中国科学院上海应用物理研究所

年报

2017-2018

(第 28 卷)

《中国科学院上海应用物理研究所年报》
编辑委员会

前　言

2017-2018 年，是应物所谋划“十三五”改革发展的关键之年，是深入实施科学院“率先行动”计划的攻坚之年，更是应物所极其不平凡、经历重大重组的变革之年。在过去两年中，应物所紧跟中科院改革创新的步伐，积极融入上海科创中心建设、支持张江实验室建设，实现了上海光源划转。与此同时，应物所持续深化体制机制改革，着力抓好重大创新成果产出，大力推进钍基熔盐堆核能系统（TMSR）研发，积极谋划研究所未来发展。

一、系统谋划改革创新发展

为了更好地发挥重大科技基础设施集群作用，支持上海科创中心和张江实验室建设，2018 年，应物所经历了重大重组的变革。按照院党组的决策部署，将上海光源等国家重大科技基础设施及其相关人员、设施、资产等划转至上海高等研究院。应物所 499 人、407 个事业编制划转至高研院/张江实验室，张江园区移交高研院/张江实验室管理。

面对新形势新变化，应物所向中科院提交了国家重大科技基础设施“十四五”项目--“钍基熔盐堆研究设施”的建设需求建议，依托应物所嘉定、武威两个园区，主要建设国际领先的小型模块化钍基熔盐堆冷态（非核）研究设施（全系统仿真实验平台）、世界首座小型模块化钍基熔盐研究堆（20MWe）和世界首座钍基乏燃料盐干法批处理研究装置等。为更加有力地推动和保障该项目的立项与实施，应物所积极建议建立 TMSR 研发的“东西联动”体制机制，将 TMSR 落实为张江综合性国家科学中心建设内容，这一建议得到了中科院、甘肃省、上海市、国家发改委等的肯定。

二、科研工作取得重要突破

2017-2018 年，应物所在 TMSR 研发、上海光源大科学装置集群建设和科学研究、基础科学与前沿交叉研究等方面取得重要突破。

钍基熔盐堆核能系统（TMSR）先导专项取得重大进展，完成 TMSR-LF1 方案设计并启动初步工程设计，实验堆选址落实在甘肃武威民勤县红砂岗镇，TMSR-LF1 建造许可证申请正式提交国家核安全局，召开 TMSR-LF1 设计方案国际专家咨询会及工程设计专家评审会；全面启动 TMSR-LF1 施工图设计和关键材料、设备加工制造工作，镍基合金材料、堆内构件（含金属、石墨）、控制棒系统、熔盐泵、主容器、换热器、核测系统、控制与保护系统等已陆续与厂家签订加工制造合同；缩比仿真堆（TMSR-SF0）全面进入工程建设阶段；优化 TMSR 技术路线，推进钍铀循环与材料研究，多渠道多领域争取科研项目；积极推进熔盐储能技术产业化，促进 TMSR

溢出技术的转移转化。并将学科领域拓展到基于 TMSR、多能互补的低碳高效复合能源系统，夯实了研究所持续发展的学科基础。结合研究所重组谋划新时期学科发展，应物所积极争取 TMSR 相关重大项目，实验堆基建落实为中科院“十三五”科教基础设施项目。TMSR 技术应用已纳入中科院“洁净能源”、“OURS”等先导专项部署。

上海光源继续保持稳定高效运行，达到国际先进水平。上海光源用户需求强劲，实验机时供不应求。用户涉及 506 家单位，实验人员达 41404 人次，共计 23254 人。目前，上海光源用户的科学研究成果已发表论文 4500 余篇，其中 SCI 1 区的文章约 1400 篇，包括 Science、Nature、Cell 等国际顶级刊物论文 83 篇。还支撑制药、化工、冶金、材料等多个领域产业用户开展高新技术研发，取得了良好的经济效益与社会效益。上海光源持续发挥支撑科技创新发展的平台作用，在 2018 年度中国科学院重大科技基础设施年会中，上海光源运行获一等奖。上海光源后续工程建设稳步推进并取得实质性进展：上海光源线站工程建安及公用设施工程完成规划验收，首批 7 条光束线站进入加工制造阶段；X 射线自由电子激光试验装置正进行自由电子激光 HGHG 模式及 EEHG 模式调试，实现 EEHG-11（24nm）FEL 饱和放大，获得 EEHG-30（8.8nm）FEL 信号；上海软 X 射线自由电子激光用户装置建安及公用设施工程基本完成，并完成规划验收；硬 X 射线自由电子激光装置项目于 2018 年 4 月正式开工，启动加速器和波荡器研制；上海大科学中心进入正式运行阶段。

基础交叉科研工作集中在纳米生物传感与生物成像、中高能核物理实验与理论、水合离子的作用等研究领域，取得了重要研究进展。核物理方面，马余刚院士、陈金辉研究院等撰写了《重离子碰撞中的反物质原子核》综述文章。文章着重阐述了马余刚团队主导的在布鲁克海文国家实验室的相对论重离子对撞机和欧洲核子中心的大型强子对撞机上的最新研究成果，包括反超氚核的发现、反氦 4 的发现以及反物质间相互作用的测量等。这篇报告也是实验核物理领域以中国学者为主发表的首篇 Physics Reports 论文。物理生物学方面提出框架核酸诱导二氧化硅沉积的团簇预水解策略（OMPC），将经典 Stöber 硅化学引入 DNA 结构体系，通过二氧化硅仿生矿化方法，成功实现了精确可控的 DNA-二氧化硅复杂纳米结构制备。相关论文被 Nature Podcast 选为当期研究亮点，以“Tougher DNA nanostructure”为题报道。

2017-2018 年，全所到位经费均超 10 亿元/年。新增基金类竞争性科研项目 107 项，共发表论文 1800 余篇（不包括会议论文），其中 SCI 收录论文 1300 余篇，影响因子大于 5 的论文共 140 余篇。专利受理专利 170 余件，授权专利 86 件。

在 2018 年度开展评选的 “中国科学院改革开放四十年 40 项标志性科技成果”中，我所 4 项科技成果入选：合成合成新核素铂-202、发现反氦核、建成上海光源和钍基熔盐堆核能系统

研发；2018 年， 我所申报的“全相干自由电子激光的前沿实验研究与新原理探索”（赵振堂、王东、邓海啸、刘波、冯超）获上海市自然科学一等奖。

三、实施人才强所战略，建设精锐科技团队

加强高层次人才队伍建设和人才国际化培养，促进队伍协调发展。开展“千人计划”、“百人计划”等高端海外人才的引进工作。按院“百人计划”引才要求引进 1 位百人（B 类）——技术英才，引进 2 位中科院百人（C 类）——青年俊才候选人。积极向国家、中科院和上海市有关部门推荐本所杰出科技工作者参评相关人才奖项评选，提升本所科技领军人才的知名度。1 人入选国家“万人计划——中青年科技创新领军人才”公示、1 人获得中科院“百人计划”终期评估优秀、3 人入选“中科院特聘研究员”、1 人入选“上海市领军人才”、1 人入选“张江人才”（卓越人才）、1 个团队入选国家“万人计划--重点领域创新团队”、1 人获得“上海市领军人才”中期评估优秀、1 人入选上海市“青年拔尖人才”，另有多人分获“上海市浦江人才”、“中科院上海分院系统杰出青年科技创新人才”和“嘉定区青年英才”等称号。

科教结合协同育人，提升研究生培养质量。共完成招收硕士研究生 193 名，招收博士研究生 157 名。申请到“联合培养本科生计划”项目等。继续做好与中科大合作的“赵忠尧应用物理科技英才班”工作，继续加强与兰大、川大、复旦等高校的合作。为支撑 TMSR 低碳新能源系统产业形成与发展，创造性地与武威职业学院共建中科低碳新能源技术学院（二级学院），培养全产业链技术人才（大专层次）；启联合学院首期确定设立核与辐射检测防护技术、应用化工（新能源方向）两个专业，“实验班”开班。

四、构建国际合作网络

2017-2018 年，共计派出 750 余人次执行因公出访任务，接待外宾来访 520 余人次。加强同欧洲各国的科技伙伴合作，推进中科院-亥姆霍兹自由电子激光联合实验室建设，由应物所与德国同步辐射光源以及上海科技大学、欧洲自由电子激光装置一起建设中科院-亥姆霍兹自由电子激光联合实验室。这是我国在发达国家设立的第一个联合研究单元，具有重大的里程碑意义；继续推动核能方面的科技合作，先进核能创新研究院与美国麻省理工学院（MIT）签订了二期合作协议，将在熔盐堆操作模拟、高温 FLiBe 熔盐中石墨的辐照后检测、氚控和熔盐储热方面开展合作；与俄罗斯门捷列夫化工大学、英国曼彻斯特大学、加拿大核科学实验室签订了框架合作协议，将在熔盐化学、材料以及燃料等领域开展合作。主办或协办了一系列的国际会议，有效地加强了相关领域的学术交流，如第一届中德自由电子激光科学与技术研讨会，第 12 届亚洲同步辐射医学成像会议等；顺利完成国际科技合作专项项目“ANSTO-SINAP 联合材料

研究”、基金委国际合作重点项目“在相对论重离子碰撞中研究重味产生以及寻找奇特粒子态和反物质原子核”。

上海光源划转后，应物所以全时承担的先导专项的核能以新领域、新团队为主，面临着高端人才流失、纵向经费占比过高、人员经费不足、科研任务重等难题，面对新形势新变化，解决的办法就是“整装、再出发”，研讨编制新发展战略与学科规划，重新确定研究所的定位、重大突破和重点培育等，积极争取国家重大科技基础设施“十四五”项目--“钍基熔盐堆研究设施”，为研究所发展成为世界一流的核科学技术研究机构奠定坚实基础。

目 录

科学引文索引 Science Citation Index

工程索引 Engineering Index

附录

科学引文索引

Science Citation Index

Development and Use of an Open-Source, User-Friendly Package To Simulate Voltammetry Experiments

Wang, Shuo Wang, Jing Gao, Yanjing

Key words Upper-Division Undergraduate, Graduate Education/Research, Chemical Engineering, Computer-Based Learning, Electrochemistry, Kinetic

An open-source electrochemistry simulation package has been developed that simulates the electrode processes of four reaction mechanisms and two typical electroanalysis techniques: cyclic voltammetry and chronoamperometry. Unlike other open-source simulation software, this package balances the features with ease of learning and implementation and can run on mainstream operating systems. In an elctroanalysis lecture for graduate students, we have simulated the cyclic voltammetry of an electron transfer reaction with varied scan rates. The dynamical concentration profiles were demonstrated in an animation to help students understand the relation between currents and evolving concentration profiles, and the relations between peak currents and scan rates were also discussed.

Journal of Chemical Education, 2017, **94(**10): 1567

Elliptic flow of electrons from heavy-flavor hadron decays in Au + Au collisions at$\sqrt{S_{NN}}$ =200, 62.4, and 39 GeV

STAR Collaboration

We present measurements of elliptic flow (v_2) of electrons from the decays of heavy-flavor hadrons (e_{HF}) by the STAR experiment. For Au+Au collisions at $\sqrt{S_{NN}}$ = 200 GeV we report v_2, for transverse momentum (pT) between 0.2 and 7 GeV/c, using three methods: the event plane method (v_2{EP}), two-particle correlations (v_2{2}), and four-particle correlations (v_2{4}). For Au+Au collisions at $\sqrt{S_{NN}}$ = 62.4 and 39 GeV we report v_2{2} for pT < 2 GeV/c. v_2{2} and v_2{4} are nonzero at low and intermediate pT at 200 GeV, and v_2{2} is consistent with zero at low pT at other energies. The v_2{2} at the two lower beam energies is systematically lower than at $\sqrt{S_{NN}}$ = 200 GeV for pT < 1 GeV/c. This difference may suggest that charm quarks interact less strongly with the surrounding nuclear matter at those two lower energies compared to $\sqrt{S_{NN}}$ = 200 GeV.

Physical Review C, 2017, **95**(3): 034907

Compact beam transport system for free-electron lasers driven by a laser plasma accelerator

Liu Tao Zhang Tong Wang Dong Huang Zhirong

Key words Extreme-Ultraviolet, Operation, Atoms

Utilizing laser-driven plasma accelerators (LPAs) as a high-quality electron beam source is a promising approach to significantly downsize the x-ray free-electron laser (XFEL) facility. Amulti-GeVLPA beam can be generated in several-centimeter acceleration distance, with a high peak current and a low transverse emittance, which will considerably benefit a compact FEL design. However, the large initial angular divergence and energy spread make it challenging to transport the beam and realize FEL radiation. In this paper, a novel design of beam transport system is proposed to maintain the superior features of the LPA beam and a transverse gradient undulator (TGU) is also adopted as an effective energy spread compensator to generate high-brilliance FEL radiation. Theoretical analysis and numerical simulations are presented based on a demonstration experiment with an electron energy of 380 MeV and a radiation wavelength of 30 nm.

Physical Review Accelerators and Beams, 2017, **20** (2): 020701

Parameter optimization and start-to-end simulation for the phase-merging enhanced harmonic generation free electron laser

Qi Zheng Feng Chao Deng Haixiao
Liu Bo Zhao Zhentang

Key words Seeded FEL, Harmonic generation, Transverse gradient, PEHG

Recently, a novel scheme called the phase-merging enhanced harmonic generation (PEHG) free-electron laser (FEL) has been developed to achieve higher harmonic bunching in a single stage set up. However, previous studies of the PEHG mechanism ignored the practical lattice configuration, leaving out the impact of the intrinsic beam divergence on the phase-merging effect. In this paper, a new method based on the beam transport matrix is proposed to comprehensively study the optimization conditions of the harmonic generation FELs. On the basis of this method, the new optimization conditions of the PEHG are obtained by taking into account both the intrinsic horizontal beam size and the intrinsic horizontal beam divergence. The parameter optimization and three dimensional start-to-end simulations are carried out using the typical beam parameters of the

Shanghai Soft X-ray Free Electron Laser user facility. The simulation results are in agreement with the theoretical analysis and demonstrate the validity of the PEHG-FEL.

Nuclear Instruments and Methods in Physics Research Section A: Accelerators, Spectrometers, Detectors and Associated Equipment, 2017, **875**: 119

Precise magnetic field control of the scanning magnets for the APTRON beam delivery system

Miao Chun-Hui Liu Ming Yin ChongXian Zhao ZhenTang

Key words Proton therapy, Scanning magnet, Hysteresis, Feedforward control

A design for precise scanning magnetic field control for the beam delivery system of the Shanghai Advanced Proton Therapy Facility (APTRON) is presented in this paper. With a novel feedforward algorithm to compensate for magnet hysteresis, the scanning magnetic field can be controlled to within a precision of +/- 2.5 G. The main advantage of the proposed feedforward algorithm is that the average settling time is shorter compared with that of a conventional feedback algorithm with acceptable tolerance.

Nuclear Science and Techniques, 2017, **28**(12): 172

Gain cascading scheme of a free-electron-laser oscillator

Li Kai Deng Haixiao

Key words X-Ray Pulses, Stimulated-Emission, Extreme-Ultraviolet, Magnetic-Field, Storage-Ring, Fel, Generation, Radiation, Coherent, Operation

The low-gain free-electron laser (FEL) oscillators are cuttingedge tools to produce fully coherent radiation in the spectral region from terahertz to vacuum ultraviolet, and potentially in hard x ray. In this paper, it is proposed to utilize an FEL oscillator with multistage undulators to enable gain cascading in a single pass, making it possible to achieve shorter single pulse lengths, higher peak power, and even higher pulse energy than the normal FEL oscillator. Theoretical analysis and numerical simulations in the infrared and hard x-ray regions show that our proposal is effective.

Physical Review Accelerators and Beams, 2017, **20**(11): 110703

Design of a nondestructive two-in-one instrument for measuring the polarization and energy spectrum at an X-ray FEL facility

Zhang Qingmin Deng Bangjie Chen Yuanmiaoliang Liu Bochao Chen Shaofei
Fan Jinquan Feng Lie Deng Haixiao Liu Bo Wang Dong

Key words Gaseous detectors, Inspection with x-rays, Instrumentation for FEL, Polarimeters

The free electron laser (FEL), as a next-generation light source, is an attractive tool in scientific frontier research because of its advantages of full coherence, ultra-short pulse duration, and controllable polarization. Owing to the demand of real-time bunch diagnosis during FEL experiments, precise nondestructive measurements of the polarization and X-ray energy spectrum using one instrument are preferred. In this paper, such an instrument based on the electron time-of-flight technique is proposed. By considering the complexity and nonlinearity, a numerical model in the framework of Geant4 has been developed for optimization. Taking the Shanghai Soft X-ray FEL user facility as an example, its measurement performances' dependence on the critical parameters was studied systematically, and, finally, an optimal design was obtained, achieving resolutions of 0.5% for the polarization degree and 0.3 eV for the X-ray energy spectrum.

Journal of Instrumentation, 2017, **12** : T1003

A new consecutive energy calibration method for X/γ detectors based on energy continuously tunable laser Compton scattering light source

Xu HangHua Wu HaiLong Fan GongTao
Chen Jian-Hui Wang Dong

Key words Laser Compton scattering (LCS), Energy calibration method, Gamma-ray application, Monte Carlo simulation

In this paper, we present an energy calibration method based on steep Compton edges of the laser Compton scattered (LCS) photon energy spectra. It performs consecutive energy calibration in the neighborhood of certain energy, hence improves calibration precision in the energy region. It can also achieve direct calibration at high energy region (several MeV) where detectors can only be calibrated by extrapolation in conventional methods. These make it suitable for detectors that need

wide-range energy calibration with high precision. The effects of systematic uncertainties on accuracy of this calibration method are studied by simulation, using the design parameters of a LCS device-SINAP III. The results show that the SINAP III device is able to perform energy calibration work over the energy region of 25-740 keV. The precision of calibration is better than 1.6% from 25 to 300 keV and is better than 0.5% from 300 to 740 keV.

Nuclear Science and Techniques, 2017, **28**(9): 121

RF design of a C-band compact spherical RF pulse compressor for SXFEL

Li Zongbin Fang Wencheng Gu Qian Zhao Zhentang

Key words RF pulse compressor; C-band; Spherical; Compact

A new C-band (5712 MHz) compact spherical radio frequency (RF) pulse compressor was designed for the Soft X-ray Free Electron Laser facility (SXFEL) at the Shanghai Institute of Applied Physics (SINAP), Chinese Academy of Sciences (CAS). Using only one high Q_0 spherical RF resonant cavity which works on two TE_{113} modes and a dual-mode polarized coupler, this pulse compressor could achieve an average power gain of 3.8. Associated with the C-band accelerator, an energy gain of 1.85 with the coupling coefficient of 4.9 could be achieved. Particularly it could make the output power stable. This paper presents the scheme of the C-band spherical pulse compressor, as well as the RF design and details of the frequency sensitivities and machining considerations.

Nuclear Instruments & Methods in Physics Research Section A-Accelerators Spectrometers Detectors and Associated Equipment, 2017, **863**: 7

Improving Touschek lifetime and synchrotron frequency spread by passive harmonic cavity in the storage ring of SSRF

Phimsen Thanapong Jiang BoCheng Hou HongTao
Tian ShunQiang Zhang ManZhou Zhang QingLei
Zhao ZhenTang

Key words Landau damping, Passive harmonic cavity, SSRF

Beam lifetime of a synchrotron is dominated by Touschek scattering. In the beamline Phase II project of Shanghai synchrotron radiation facility, a passive third harmonic cavity is to be installed

for bunch lengthening and instability suppressing. In this paper, the beam dynamics of the cavity is investigated. The parameters of passive operation are optimized to cancel the slope of RF voltage and lengthen the bunches. The Touschek lifetime increases are estimated for optimum and non-optimum voltage flattening. A tolerance of the operation is studied in case that there is a shift on detuning angle. The effect caused by reduction in harmonic voltage generated by lengthened bunch distribution is also estimated using iteration method. An increase in synchrotron frequency spread due to nonlinearity of the voltage giving to the bunch is found by using tracking simulation. This spread can help in damping coupled bunch instability through Landau damping.

Nuclear Science and Techniques, 2017, **28**(8): 108

Two-stage EEHG for coherent hard X-ray generation based on a superconducting linac

Zhao ZhenTang　Feng Chao　Zhang KaiQing

Key words　EEHG, Fresh beam, X-ray monochromator, Superconducting accelerator

A two-stage echo-enabled harmonic generation （ EEHG ） scheme is proposed for a superconducting linacdriven FEL to produce coherent hard X-rays. Electron beams of quite different bunch lengths are separately used in each stage of EEHG, and a monochromator is designed to purify the radiation from the first stage for seeding the second stage. Theoretical analysis and 3D simulations indicate that the proposed scheme can generate high-repetition-rate coherent hard X-ray pulses directly from a conventional UV seed laser.

Nuclear Science and Techniques, 2017, **28**(8): 117

Using a Bessel light beam as an ultrashort period helical undulator

Jiang, BC　Zhang, QL　Chen, JH　Zhao, ZT

Key words　Orbital Angular-Momentum, Radiation, Acceleration, Electrons

An undulator is a critical component to produce synchrotron radiation and a free electron laser. When a Bessel light beam carrying the orbit angular momentum copropagates with an electron beam bunch, a net transverse deflection force will be subjected to the latter one. As a result of dephasing effect, the deflection force will oscillate and act as an undulator. For such a laser based

undulator, the period length can reach submillimeter level, which will greatly reduce the electron energy for the required x-ray production.

Physical Review Accelerators and Beams, 2017, **20**(7): 070701

A Storage Ring Based Free-Electron Laser for Generating Ultrashort Coherent EUV and X-ray Radiation

Feng Chao Zhao Zhentang

Key words Synchrotron-Radiation, Harmonic-Generation, Operation, Pulses

Generation of ultrashort coherent radiation pulses in the extreme ultraviolet (EUV) and x-ray regime is of remarkable interest in the synchrotron radiation user community. In this work, a novel technique is proposed for directly imprinting strong coherent microbunching on the electron beam with very small laser-induced energy spread. Theoretical analysis and numerical simulations demonstrated that this technique can be used for the generation of megawatt-scale level, fully temporal coherent femtosecond EUV and soft x-ray radiation pulses at a storage ring light source.

Scientific Reports, 2017, **7**: 4724

Wakefields studies for the SXFEL user facility

Song MingHao Feng Chao Huang DaZhang Deng HaiXiao
Liu Bo Wang Dong

Key words SXFEL, Wakefields, Pulse energy, Radiation power, Spectrum, Taper

Besides the original seeded undulator line, in the soft X-ray free-electron laser (SXFEL) user facility in Shanghai, a second undulator line based on self-amplified spontaneous emission is proposed to achieve 2-nm laser pulse with extremely high brightness. In this paper, the beam energy deviation induced by the undulator wakefields is numerically calculated, and 3D and 2D results agree well with each other. The beam energy loss along the undulator degrades the expected FEL output performances, i.e., the pulse energy, radiation power and spectrum, which can be compensated with a proper taper in the undulator. Using the planned time-resolved diagnostic, a novel experiment is proposed to measure the SXFEL longitudinal wakefields.

Nuclear Science and Techniques, 2017, **28**(7): 90

Status of the SXFEL Facility

Zhao Zhentang Wang Dong Gu Qiang Yin Lixin Gu Ming
Leng Yongbin Liu Bo

Key words X-ray FEL, SXFEL, cascaded HGHG, cascaded EEHG-HGHG, water window

The Shanghai soft X-ray Free-Electron Laser facility (SXFEL) is being developed in two steps; the SXFEL test facility (SXFEL-TF), and the SXFEL user facility (SXFEL-UF). The SXFEL-TF is a critical development step towards the construction a soft X-ray FEL user facility in China, and is under commissioning at the Shanghai Synchrotron Radiation Facility (SSRF) campus. The test facility is going to generate 8.8 nm FEL radiation using an 840 MeV electron linac passing through the two-stage cascaded HGHG-HGHG or EEHG-HGHG (high-gain harmonic generation, echo-enabled harmonic generation) scheme. The construction of the SXFEL-TF started at the end of 2014. Its accelerator tunnel and klystron gallery were ready for equipment installation in April 2016, and the installation of the SXFEL-TF linac and radiator undulators were completed by the end of 2016. In the meantime, the SXFEL-UF, with a designated wavelength in the water window region, began construction in November 2016. This was based on upgrading the linac energy to 1.5 GeV, and the building of a second undulator line and five experimental end-stations. Construction status and the future plans of the SXFEL are reported in this paper.

Applied Sciences-Basel, 2017, **7**(6): 607

The front-end electronics design of dose monitors for beam delivery system of Shanghai Advanced Proton Therapy Facility

Zhao BinQin Zhao MingHua Liu Ming
Yin ChongXian Shu Hang

Key words Front-end electronics, Dose monitor, Proton therapy

A front-end electronics of dose monitor has been developed for measuring irradiation dose to the patient in Shanghai Advanced Proton Therapy Facility. The parallel plate ionization chamber is used for the dose monitoring. Unlike the traditional method of recycling capacitor integration and voltage-to-frequency conversion, this dose monitor electronics uses the trans-impedance amplifier and analog-to-digital conversion method. It performs satisfactorily, with the integral nonlinearity of less than ±0.04 nA in the range of −400 to 50 nA and the resolution of about ±0.6 nA.

Nuclear Science and Techniques, 2017, **28**(6): 83

Extending the photon energy coverage of an x-ray self-seeding FEL via the reverse taper enhanced harmonic generation technique

Zhang Kaiqing Qi Zheng Feng Chao Deng Haixiao
Wang Dong Zhao Zhentang

Key words Self-seeding, Reverse taper, Harmonic generation

In this paper, a simple method is proposed to extend the photon energy range of a soft x-ray self-seeding free-electron laser (FEL). A normal monochromator is first applied to purify the FEL spectrum and provide a coherent seeding signal. This coherent signal then interacts with the electron beam in the following reverse tapered undulator section to generate strong coherent microbunchings while maintain the good quality of the electron beam. After that, the pre-bunched electron beam is sent into the third undulator section which resonates at a target high harmonic of the seed to amplify the coherent radiation at shorter wavelength. Three dimensional simulations have been performed and the results demonstrate that the photon energy gap between 1.5 keV and 4.5 keV of the self-seeding scheme can be fully covered and 100 GW-level peak power can be achieved by using the proposed technique.

Nuclear Instruments & Methods In Physics Research Section A-Accelerators Spectrometers Detectors and Associated Equipment, 2017, **854**: 3

Design of an X-band accelerating structure using a newly developed structural optimization procedure

Huang Xiaoxia Fang Wencheng Gu Qiang Zhao Zhentang

Key words X-band, Novel structural optimization, Multipole field components, Dual-feed coupler, Racetrack

An X-band high gradient accelerating structure is a challenging technology for implementation in advanced electron linear accelerator facilities. The present work discusses the design of an X-band accelerating structure for dedicated application to a compact hard X-ray free electron laser facility at the Shanghai Institute of Applied Physics, and numerous design optimizations are conducted with consideration for radio frequency (RF) breakdown, RF efficiency, short-range wakefields, and dipole/quadrupole field modes, to ensure good beam quality and a high accelerating gradient. The designed X-band accelerating structure is a constant gradient structure

with a 4π /5 operating mode and input and output dual-feed couplers in a racetrack shape. The design process employs a newly developed effective optimization procedure-for optimization of the X-band accelerating structure. In addition, the specific design of couplers providing high beam quality by eliminating dipole field components and reducing quadrupole field components is discussed in detail.

Nuclear Instruments and Methods in Physics Research Section A: Accelerators, Spectrometers, Detectors and Associated Equipment, 2017, **854**: 45

Simplified model for fast optimization of a free-electron laser oscillator

Li Kai Song Minghao Deng Haixiao

Key words Nonmonoenergetic Beam, Radiation

A simplified one-dimensional theoretical model for free-electron laser oscillator (FELO) calculation which reserves the main physics is proposed. Instead of using traditional macroparticles sampling method, the theoretical model takes advantage of low gain theory to calculate the optical power single-pass gain in the undulator analytically, and some reasonable approximations are made to simplify the calculation of power growth in the cavity. The theoretical analysis of single-pass gain, power growth, time-dependent laser profile evolution and cavity desynchronism are accomplished more efficiently. We present the results of infrared wavelength FELO and X-ray FELO with the new model. The results are validated by simulation with GENESIS and OPC.

Physical Review Accelerators and Beams, 2017, **20**(3): 030702

Generation of double pulses at the Shanghai soft X-ray free electron laser facility

Wang Zhen Feng Chao Gu Qiang Yu LiHua Zhao ZhenTang

Key words Free electron laser, Double pulses, SXFEL

In this article, we present the promise of a new method generating double electron pulses in picosecond-scale pulse length and tunable interpulse spacing at several picoseconds. This has witnessed an impressive potential of application in pump–probe techniques, two-color X-ray free

electron laser, high-gradient witness bunch acceleration in a plasma, etc. Three-dimensional simulations are carried out to analyze the dynamic of the electron beam in a linear accelerator. Comparisons are made between the new method and existing ways.

Nuclear Science and Techniques, 2017, **28**(3): 28

Generating high-brightness and coherent soft x-ray pulses in the water window with a seeded free-electron laser

Zhou Kaishang Feng Chao Deng Haixiao Wang Dong

Key words Extreme-Ultraviolet, Harmonic-Generation, Fel, Radiation, Operation

We propose a new scheme to generate high-brightness and temporal coherent soft x-ray radiation in a seeded free-electron laser. The proposed scheme is based on the coherent harmonic generation (CHG) and superradiant principles. A CHG scheme is first used to generate a coherent signal at ultrahigh harmonics of the seed. This coherent signal is then amplified by a series of chicane-undulator modules *via* the fresh bunch and superradiant processes in the following radiator. Using a representative of a realistic set of parameters, three-dimensional simulations have been carried out and the simulations results demonstrated that 10 GW-level ultrashort (~20 fs) coherent radiation pulses in the water window can be achieved by using a 1.6 GeV electron beam based on the proposed technique.

Physical Review Accelerators and Beams, 2017, **20**(1): 010702

Chromatic effect in a novel THz generation scheme

Li Bin Zhang Wenya Liu Xiaoqin Deng Haixiao Lan Taihe
Liu Bo Liu Jia Wang Xingtao Zeng Zhinan Zhang Lijian

Key words terahertz radiation, optical rectification, nonlinear optics and parametric processes, optical chirp pulse, pulse-front tilt

Deriving single or few cycle terahertz (THz) pulse by an intense femtosecond laser through cascaded optical rectification is a crucial technique in cutting-edge time-resolved spectroscopy to characterize micro-scale structures and ultrafast dynamics. Due to the broadband nature of the ultrafast driving laser, the chromatic effect limits the THz conversion efficiency in optical rectification crystals, especially for those implementing the pulse-front tilt scheme, e.g. lithium niobate (LN) crystal, has been prevalently used in the past decade. In this research we developed a brand new type of LN crystal utilizing Brewster coupling, and conducted systematically

experimental and simulative investigation for the chromatic effect and multi-dimensionally entangled parameters in THz generation, predicting that an extreme conversion efficiency of~10% would be potentially achievable at the THz absorption coefficient of~0.5 cm^{-1} . Moreover, we first discovered that the chirp of the driving laser plays a decisive role in the pulse-front tilt scheme, and the THz generation efficiency could be enhanced tremendously by applying an appropriate chirp.

New Journal of Physics, 2017, **19**: 113025

Vacancy-assisted oxygen reduction reaction on cobalt-based catalysts in direct borohydride fuel cell revealed by in-situ XAFS and XRD

Wang Juan Lin Longxia He Yan Qin Haiying Yan Shuai
Yang Ke Li Aiguo Liu Jiabin

Key words Direct borohydride fuel cell, Oxygen reduction reaction, Cathode, Oxygen vacancy, X-ray absorption fine structure

The oxygen reduction reaction mechanism is the key issue for designing novel non-Pt electrocatalysts of H_2-O_2 fuel cells. Although the $Me^{n+}/Me^{(n+1)+}$ redox model has been widely accepted, the valence state of the Me^{n+} was found to keep unchanged in this work. Polypyrrole-modified carbon-supported cobalt oxyhydroxide catalyst (CoOOH-PPy-BP) was prepared by impregnation-chemical method and used as cathode catalyst in direct borohydride fuel cells. The CoOOH-PPy-BP exhibited compatible electrochemical properties with $Co(OH)_2$-PPy-BP and a near 4e transfer oxygen reduction reaction. The variation of the local structure around Co ions during discharging was analyzed by in-situ X-ray absorption fine structure (XAFS) and X-ray diffraction (XRD) measurements. No new phase was detected by in-situ XRD while oxygen vacancies were detected by in-situ XAFS. Oxygen vacancies at the surface of CoOOH provided favorable sites for the O_2 absorption, accelerating the activation of the O_2. The electron holes generated due to the oxygen vacancies in the CoOOH can capture electrons from the anode to form excited cationic states [Co^{3+} + e]. Then the absorption oxygen molecule is reduced by capturing electrons from [Co^{3+} + e]. A new oxygen reduction reaction mechanism based on the oxygen vacancy instead of the previous $Co^{n+}/Co^{(n+1)+}$ model is proposed. This work provides lights for the design of novel catalysts with excellent performance by introducing defects of oxygen vacancies artificially.

Electrochimica Acta, 2017, **254**: 72

Speckle-tracking X-ray phase-contrast imaging for samples with obvious edge-enhancement effect

Wang Feixiang Wang Yudan Wei Gongxiang Du Guohao Xue Yanling Hu Tao Li Ke Deng Biao Xie Honglan Xiao Tiqiao

Compared to the grating or crystal-based X-ray phase contrast imaging, the speckle-tracking method has the advantages of a simple setup and two-dimensional imaging. However, the edge-enhancement effect prevents the application of the speckle-tracking imaging to a large variety of samples. In this letter, an image reconstruction method is proposed to solve this problem. The experimental results from phantom, a biomedical sample, and a sample with a speckle-resembling structure demonstrated that the proposed method is efficacious in eliminating the effect of edge enhancement. The proposed method may greatly expand the application of the speckle-tracking method to most biomedical and material samples.

Applied Physics Letters, 2017, **111**(17): 174101

Characterization of heat treatment-induced pore structure changes in cold-sprayed titanium

Ren YQ King PC Yang YS Xiao TQ Chu C Gulizia S Murphy AB

Key words Cold spray, Ti, Additive manufacturing, Data-constrained modelling, X-ray micro-tomography

Two X-ray computed tomography (CT) datasets have been acquired for a cold-sprayed titanium sample before and after heat treatment. The datasets were collected with a beam energy of 30 keV at the Australian Synchrotron. Three-dimensional (3D) distributions of porosity in the Ti sample were reconstructed using a data-constrained modelling (DCM) technique. Quantitative analysis indicated that the heat treatment caused morphological changes to the pores and a small decrease in the overall porosity. After heat treatment, some fine porosity disappeared while the large porosity regions were essentially unaffected except for a change towards a more rounded pore shape. Interconnectivity between pores was reduced, which has implications for sealing and trapping of contaminant gases in cold-sprayed parts. The characterization technique and the workflow presented in the paper are applicable to non-destructive 3D characterization of other materials.

Materials Characterization, 2017, **132**: 69

Temperature-dependent thermal properties of Ru/C multilayers

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Zheng Yi Dong Zhaohui Tian Naxi

Key words multilayer, X-ray, interface, thermal conductivity

Multilayers made of Ru/C are the most promising candidates when working in the energy region 8–20 keV. The stability of its thermal properties, including thermal expansion and thermal conduction, needs to be considered for monochromator or focusing components. Ru/C multilayers with periodic thicknesses of 3, 4 and 5 nm were investigated in situ by grazing-incidence X-ray reflectometry and diffuse scattering in order to study their thermal expansion characteristics as a function of annealing temperature up to 400℃. The thermal conductivity of multilayers with the same structure was also measured by the transient hot-wire method and compared with bulk values.

Journal of Synchrotron Radiation, 2017, **24**(5): 975

Single bounce ellipsoidal glass monocapillary condenser for X-ray nano-imaging

Jiang Bowen Liu Zhiguo Sun Xuepeng Sun Tianxi Deng Biao
Li Fangzuo Yi Longtao Yuan Mingnian Zhu Yu
Zhang Fengshou Xiao Tiqiao Wang Jie Tai Renzhong

Key words Single bounce ellipsoidal monocapillary; Monocapillary quality; Slope error; X-ray test

A single bounce ellipsoidal glass monocapillary was designed and fabricated and its performance was measured by both an optical measurement and an X-ray test. This monocapillary had a slope error of 17 μrad. The images of the focal spot and the far-field pattern recorded by a CCD detector showed that this fabricated monocapillary had high quality and satisfied the requirement of the designed data for X-ray nano-imaging.

Optics Communications, 2017, **398**: 91

Comparative study of the low-lying valence electronic states of carbon dioxide by high-resolution inelastic x-ray and electron scattering

Ni DongDong Xu LongQuan Liu YaWei Yang Ke Hiraoka Nozomu Tsuei KuDing Zhu LinFan

Key words Generalized Oscillator-Strengths, Differential Cross-Sections, Excitation, Molecule, Helium, Impact, Co2, Spectroscopy, Transition, Vibrations

We e report a comparative study of low-lying valence electronic states of carbon dioxide by high-resolution inelastic x-ray and electron scattering. Momentum-transfer-dependent inelastic squared form factors for the two states ${}^1\sum_u^+$ and ${}^1\prod_u$ and generalized oscillator strength for the 9 eV feature from the ground state $X{}^1\sum_g^+$ have been derived from the inelastic x-ray scattering method at an impact photon energy around 10 keV, and the electron energy-loss spectra measured at an incident electron energy of 1500 eV. It is found from the comparison between the present results and the previous outcomes that the recent calculations taking the vibronic effects into consideration satisfactorily reproduce the inelastic squared form-factor profile for the ${}^1\sum_u^+$ transition and the generalized oscillator strength profile for the 9eV feature. However, the vibronic effects seem to play no role in the ${}^1\prod_u$ transition. The difference existing between the inelastic x-ray scattering and electron energy-loss spectroscopy results in the larger momentum-transfer squared region may be attributed to the increasing role of the higher-order Born terms. Furthermore, the controversy concerning the designations of electronic states around 11 eV is solved by assigning the two peaks centered at 10.98 and 11.05 eV to the vibrational progression ${}^1\sum_u^+{}'$ and ${}^1\sum_u^+$, and the peak centered at 11.16 eV to the forbidden transition $2{}^1\Delta_u$ based on the present results.

Physical Review A, 2017, **96**(1): 012518

Identification of ginseng root using quantitative X-ray microtomography

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Qi Juncheng Xiao Tiqiao

Key words Panax ginseng, Panax quinquefolius, quantitative microtomography, synchrotron radiation, X-ray phase contrast imaging

Background: The use of X-ray phase-contrast microtomography for the investigation of Chinese medicinal materials is advantageous for its nondestructive, in situ, and three-dimensional quantitative imaging properties.

Methods: The X-ray phase-contrast microtomography quantitative imaging method was used to investigate the microstructure of ginseng, and the phase-retrieval method is also employed to process the experimental data. Four different ginseng samples were collected and investigated; these were classified according to their species, production area, and sample growth pattern.

Results: The quantitative internal characteristic microstructures of ginseng were extracted successfully. The size and position distributions of the calcium oxalate cluster crystals (COCCs), important secondary metabolites that accumulate in ginseng, are revealed by the three-dimensional quantitative imaging method. The volume and amount of the COCCs in different species of the ginseng are obtained by a quantitative analysis of the three-dimensional microstructures, which shows obvious difference among the four species of ginseng.

Conclusion: This study is the first to provide evidence of the distribution characteristics of COCCs to identify four types of ginseng, with regard to species authentication and age identification, by X-ray phase-contrast microtomography quantitative imaging. This method is also expected to reveal important relationships between COCCs and the occurrence of the effective medicinal components of ginseng.

Journal of Ginseng Research, 2017, **41**(3): 290

3D investigation on polystyrene colloidal crystals by floatage self-assembly with mixed solvent via synchrotron radiation x-ray phase-contrast computed tomography

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Du Guohao Xiao Tiqiao

Key words Colloidal crystal; Floatage self-assembly; Mixed solvent; Synchrotron radiation; Computed tomography; Phase-contrast

The floatage self-assembly method was introduced with mixed solvent as the medium of polystyrene sphere suspension to fabricate the colloidal crystal. The three dimensional (3D) void system of the colloidal crystal was noninvasively characterized by synchrotron radiation phase-contrast computed tomography, and the quantitative image analysis was implemented aiming to the polystyrene sphere colloidal crystal. Comparing with gravity sedimentation method, the three samples fabricated from floatage self-assembly with mixed solvents have the lowest porosity, and when ethylene glycol and water were mixed with ratio of 1: 1, the lowest porosity of 27.49% could be achieved, that has been very close to the minimum porosity of ordered 3D monodisperse sphere array (26%). In single slices, the porosities and fractal dimension for the voids were calculated. The results showed that two factors would significantly influence the porosity of the whole colloidal crystal: the first deposited sphere layer's orderliness and the sedimentation speed of the spheres. The floatage self-assembly could induce a stable close-packing process, resulted from the powerful nucleation force-lateral capillary force coupled with the mixed solvent to regulate the floating upward speed for purpose of matching the assembly rate.

Radiation Physics and Chemistry, 2017, **135**: 49

Scan system for arbitrary-shaped samples at the synchrotron radiation facility

Lan XuYing Liang DongXu Mao ChengWen

Key words Synchrotron radiation, X-ray fluorescence mapping, EPICS, XPS controller

X-ray fluorescence (XRF) scan methodology is important for elemental mapping of samples at a synchrotron radiation facility. To save the experiment time and improve the experiment efficiency, one should develop an efficient XRF scan method. In this paper, a new scan mode is presented. It can map arbitrary-shaped areas without stopping the motors. The control and data acquisition system integrates motor controlling, detector triggering, and data acquisition and storage. The system realizes the arbitrary-shaped 2D-mapping and fluorescence data acquisition synchronously. SR-XRF mapping has been performed with a standard gold mask to verify the validity of this method at beamline $BL_{15}U_1$ of the Shanghai Synchrotron Radiation Facility. The results show that this method reduces the total scan time and improves the experiment efficiency.

Nuclear Science and Techniques, 2017, **28**(5): 60

Compensation for gravitational sag of bent mirror

Lan XuYing Liang DongXu Mao ChengWen

Key words Synchrotron radiation, X-ray fluorescence mapping, EPICS, XPS controller

The gravitational sag of aspheric bent mirrors with face-up or face-down geometry produces a nonnegligible optical error. As an effective compensation, width optimization is used to match the combined effects of the gravitational and bending moments. This method is described by analytical expressions and two calculation algorithms. The results of theoretical simulations and finite element analysis have proved that this method can reduce the slope error resulting from gravitational sag to the level of nano radians.

Nuclear Instruments and Methods in Physics Research Section A: Accelerators, Spectrometers, Detectors and Associated Equipment, 2017, **85**3: 20

Non-destructive identification of unknown minor phases in polycrystalline bulk alloys using three-dimensional X-ray diffraction

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Du Guohao Yang Sam Xiao Tiqiao

Key words Unknown minor phase, Non-destructive identification, 3DXRD

Minor phases make considerable contributions to the mechanical and physical properties of metals and alloys. Unfortunately, it is difficult to identify unknown minor phases in a bulk polycrystalline material using conventional metallographic methods. Here, a non-destructive method based on three-dimensional X-ray diffraction (3DXRD) is developed to solve this problem. Simulation results demonstrate that this method is simultaneously able to identify minor phase grains and reveal their positions, orientations and sizes within bulk alloys. According to systematic simulations, the 3DXRD method is practicable for an extensive sample set, including polycrystalline alloys with hexagonal, orthorhombic and cubic minor phases. Experiments were also conducted to confirm the simulation results. The results for a bulk sample of aluminum alloy AA6061 show that the crystal grains of an unexpected γ-Fe (austenite) phase can be identified, three-dimensionally and nondestructively. Therefore, we conclude that the 3DXRD method is a powerful tool for the identification of unknown minor phases in bulk alloys belonging to a variety of crystal systems. This method also has the potential to be used for in situ observations of the effects of minor phases on the crystallographic behaviors of alloys.

Materials Characterization, 2017, **124**: 206

Development of high-performance cathode catalyst of polypyrrole modified carbon supported CoOOH for direct borohydride fuel cell

He Yan Zhu Cai Chen Kaijian Wang Juan Qin Haiying Liu Jiabin Yan Shuai Yang Ke Li Aiguo

Key words Polypyrrole modified carbon supported cobalt catalyst, X-ray photoelectron spectroscopy, X-ray absorption fine structure, Oxygen reduction reaction, Direct borohydride fuel cell

Polypyrrole modified carbon supported CoOOH electrocatalyst (CoOOH-PPy-C) is prepared by impregnation-chemical method, and the catalytic properties for the oxygen reduction reaction (ORR) in alkaline media are investigated. The X-ray diffraction and transmission electron microscopy results confirm the presence of the expected CoOOH. The electrochemical tests show that the CoOOH-PPy-C catalyst exhibits good electrocatalytic activity towards ORR. The direct borohydride fuel cell using CoOOH-PPy-C as the cathode catalyst demonstrates a good stability performance. There is only 4% decrease of the cell voltage after 80-h operation. The ORR occurs an average 4-electron transfer pathway on the CoOOH-PPy-C catalyst. The good catalytic activity towards ORR benefits from the CoeN bond, which is identified by X-ray photoelectron spectroscopy test. X-ray absorption fine structure experiments further show that two nearest O atoms are substituted by two N atoms bonding to Co ion at a distance of 1.64 Å. The CoOOH-PPy-C exhibits better electrochemical properties than the $Co(OH)_2$ counterpart even though the valence state of Co ion is +3 in CoOOH-PPy-C. Those results indicate that the bonding of Co ion with N atoms should be a key issue regardless the valence of Co ion.

Journal of Power Sources, 2017, **339**: 13

Current Status of the Hard X-ray Nanoprobe Beamline at the SSRF

Li Aiguo Jiang Hui Wang Hua Zhang Zhaohong He Yan Zhao Gaofeng Shu Deming

The hard X-ray nanoprobe beamline (HXN) designed at the Shanghai Synchrotron Radiation facility (SSRF) will be of capability to realize a focal spot size of 10 nm for hard X-rays to satisfy requirements in biology, environmental, material sciences etc. The beamline includes two modes of operation, high energy resolution mode and high flux mode respectively. High flux mode utilizes

the multilayer KB system to obtain high-flux diffraction-limited focusing of ~10nm. An ultra-high-precision figure fabrication for diffraction-limited focusing is required to meet the Rayleigh Criterion. An idea to overcome this problem is to introduce a phase compensator upstream of the KB system to compensate the wavefront errors in the beamline. At wavelength speckle-based method will be used to measure the wavefront error in the beamline and feedback to the phase compensator. Vibration measurements have been carried out at the secondary source and endstation hutch. The flexure hinge mechanisms and high-precision actuators ensure the KB system and sample manipulator working with high stability. The building of HXN has been designed and is under construction at present.

X-Ray Nanoimaging: Instruments and Methods Ⅲ, 2017, **10389**: UNSP 103890J

X-ray multilayer mid-frequency characterizations using speckle scanning techniques

Jiang Hui Yan Shuai Liang Dongxu
Tian Naxi Wang Hua Li Aiguo

Determination of multilayer structure was developed so much, but most of studies focused on the relationship between structural imperfections and reflectivity. These imperfections, whether interfacial roughness and interdiffusion or surface feature, measured by grazing X-ray scattering, atomic force microscopy or electric microscopy, reflect relatively high-frequency characteristics. The mid-frequency figure errors were regarded as the main factor to produce large satellite peaks near the focusing spot in the multilayer K-B mirror and were found to produce stripes in the far-field imaging. We report novel method to study mid-frequency interface and layer growth characterizations of multilayer structure using at-wavelength speckle scanning technique. This work is beneficial for matching multilayer manufacture technology to the optimization of beam performances.

Advances in Metrology for X-Ray and EUV Optics VII, 2017, **10385**: UNSP 103850Q

A low dose and in-vivo imaging system based on equally sloped tomography

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Wang Dadong Xiao Tiqiao

Key words in-vivo micro-CT, equally sloped tomography, synchrotron radiation, biomedical imaging

High radiation dose impedes the development of in-vivo micro-CT. In this paper, we presents a low dose and fast in-vivo micro computed tomography (micro-CT) system based on equally sloped tomography (EST) technique and the monochromatic synchrotron X-ray source. Comparing with regular CT, the projection number required for our imaging system can be reduced by about 75%. In addition, combining with an X-ray shutter, total exposure time of 4 seconds and about 0.67Gy absorption dose for a set of CT data have been achieved. These results demonstrate that micro-CT with monochromatic synchrotron X-rays has great potential in the investigation into the microstructure evolution inside a small animal for biomedical research.

2017 IEEE 14th International Symposium on Biomedical Imaging, 2017, **63**

Monochromatic-beam-based dynamic X-ray microtomography based on OSEM-TV algorithm

Xu Liang Chen Rongchang Yang Yiming Deng Biao
Du Guohao Xie Honglan Xiao Tiqiao

Key words Image reconstruction techniques, dynamic microtomography, quantitative analysis, limited projections, X-ray imaging

Monochromatic-beam-based dynamic X-ray computed microtomography (CT) was developed to observe evolution of microstructure inside samples. However, the low flux density results in low efficiency in data collection. To increase efficiency, reducing the number of projections should be a practical solution. However, it has disadvantages of low image reconstruction quality using the traditional filtered back projection (FBP) algorithm. In this study, an iterative reconstruction method using an ordered subset expectation maximization-total variation (OSEM-TV) algorithm was employed to address and solve this problem. The simulated results demonstrated that normalized mean square error of the image slices reconstructed by the OSEM-TV algorithm was about 1/4 of that by FBP. Experimental results also demonstrated that the density resolution of OSEM-TV was high enough to resolve different materials with the number of projections less than 100. As a result, with the introduction of OSEM-TV, the monochromatic-beam-based dynamic X-ray microtomography is potentially practicable for the quantitative and non-destructive analysis to the evolution of microstructure with acceptable efficiency in data collection and reconstructed image quality.

Journal of X-Ray Science and Technology, 2017, **25**(6): 1007

Surface States in Ternary CdSSe Quantum Dot Solar Cells

Chen Zhenhu Li Hui Zhang Xiangzhi Zhang Lijuan Yu Huaina
Li Wenqin Xu Zijian Wang Yong Tai Renzhong

Key words Surface States, Ternary, Quantum Dot, Solar Cell, Synchrotron

Ternary CdSSe quantum dot-sensitized solar cells (QDSCs) have demonstrated advantages such as wide absorption ranges and tunable band structures. However, the oxygen additives absorbed on such multicomponent quantum dot (QD) surfaces induce band bending at the TiO_2/CdSSe interface and prevent charge transport in QDSCs, as determined via X-ray photoelectron spectroscopy (XPS) and synchrotron-based X-ray Absorption Near-Edge Structure (XANES) analysis. Annealing of TiO_2/CdSSe QDs photoanodes was conducted at different temperatures under Ar atmospheres to eliminate oxygen additives and interfacial band bending. The short-circuit current (J_{sc})of the annealed ternary CdSSe QDSCs is obviously improved, whereas the TiCl4 treatment and MgO coating of the TiO2 nanocrystals are assisted by the annealing to compensate for the loss of opencircuit voltage (V_{oc}) and fill factor (FF). Ternary CdSSe QDSCs with efficiencies of 4.72% have been achieved using the optimized annealing conditions.

Journal of Nanoscience and Nanotechnology, 2017, **17**(2): 1373

Fabrication of large-area high-aspect-ratio periodic nanostructures on various substrates by soft X-ray interference lithography

Xue Chaofan Zhao Jun Wu Yanqing Yu Huaina Yang Shumin
Wang Liansheng Zhao Wencong Wu Qiang Zhu Zhichao
Liu Bo Zhang Xia Zhou Wenchao Tai Renzhong

Key words Synchrotron radiation, Soft X-ray interference lithography, Large-area high-aspect-ratio nano periodic arrays, Photonic crystals

Periodic nanostructures have attracted considerable interest and been applied in many fields. However, nanostructures of sufficiently large areas and depths are necessary for the development of practical devices. In this study, large-area high-aspect-ratio periodic nanostructures were fabricated by using a hybrid technology based on X-ray interference lithography, and then the patterns were transferred onto various substrates successfully. The final periodic nanostructures on the substrate attained measurements up to square centimetres with depths greater than 200 nm.

Applied Surface Science, 2017, **425**: 553

Interfacial nanobubbles produced by long-time preserved cold water

Zhou LiMin Wang Shuo Qiu Jie Wang Lei Wang XingYa
Li Bin Zhang LiJuan Hu Jun

Key words nanobubbles, atomic force microscopy, gas saturation, solubility

Interfacial gaseous nanobubbles which have remarkable properties such as unexpectedly long lifetime and significant potential applications, are drawing more and more attention. However, the recent dispute about the contamination or gas inside the nanobubbles causes a large confusion due to the lack of simple and clean method to produce gas nanobubbles. Here we report a convenient and clean method to effectively produce interfacial nanobubbles based on a pure water system. By adding the cold water cooled at 4 ℃ for more than 48 h onto highly oriented pyrolytic graphite (HOPG) surface, we find that the average density and total volume of nanobubbles are increased to a high level and mainly dominated by the concentrations of the dissolved gases in cold water. Our findings and methods are crucial and helpful for settling the newly arisen debates on gas nanobubbles.

Chinese Physics B, 2017, **26**(10): 106803

Robust phase-retrieval-based X-ray tomography for morphological assessment of early hepatic echinococcosis infection in rats

Liu Huiqiang Zhang Chuanshan Fan Xiaoxi Duan Yingni
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Key words alveolar echinococcosis, contrast tomography, attenuation duality, fresnel region, microtomography, holotomography, optimization, ultrasound, liver, image

Propagation-based phase-contrast computed micro-tomography (PPCT) dominates the non-destructive, three-dimensional inner-structure measurement in synchrotron-based biomedical research due to its simple experimental setup. To quantitatively visualize tiny density variations in soft tissues and organs closely related to early pathological morphology, an experimental study of synchrotron-based X-ray PPCT combined with generalized phase and attenuation duality (PAD) phase retrieval was implemented with the hepatic echinococcosis (HE) infection rat model at different stages. We quantitatively analyzed and evaluated the different pathological characterizations of hepatic echinococcosis during the development of this disease via our

PAD-based PPCT and especially provided evidence that hepatic alveolar echinococcosis invades the liver tissue and spreads through blood flow systems with abundant blood supply in the early stage. Additionally, the infiltration of tiny vesicles in HE lesions can be clearly observed by our PAD-PPCT technique due to the striking contrast-to-noise ratio (CNR) and mass density resolution, which cannot be found by the medical imaging techniques, such as magnetic resonance imaging (MRI), computed tomography (CT), and ultrasound, in hospitals. The results demonstrated that our PAD-PPCT technique has a great potential for indicating the subtle structural information of pathological changes in soft biomedical specimens, especially helpful for the research of early micro-morphology of diseases.

Plos One, 2017, **12**(9): e0183396

Mutual optical intensity propagation through non-ideal mirrors

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Key words partially coherent radiation; mutual optical intensity; non-ideal mirrors; beamline design; mirror figure errors

We continue to develop MOI method to analyze the mutual optical intensity (MOI) propagation through non-ideal optics. Local stationary phase approximation is implemented to calculate the MOI propagating through a non-ideal mirror. The phase generated by the path length from the incident to exit plane is the key to solve the MOI propagation through the mirror. The effect of figure error can be expressed as phase shift. There are two methods to deal with the figure error, the analytical method and numerical one. The two methods are compared at different spatial frequency range of the figure error. An APS beamline is analyzed with the developed MOI model, in which a partially coherent beam with 10keV energy is focused to ~20nm by a non-ideal elliptical mirror. The MOI at the focal plane is acquired after propagation through the non-ideal mirror. The intensity profile, the wavefront and the global coherence degree can be get from the MOI. The results indicate that the figure error with low spatial frequency generates oscillations, redistributes coherence property and damages the wavefront on the image plane. However, the figure error does not change the global coherence degree. Comparison with other codes such as Hybrid and SRW was performed. The results show that MOI model and SRW have similar intensity profiles. The apparent oscillations from MOI model and SRW indicate high coherence. Limitation on the beam size by the BDA and mirror will increase the coherence, which can be quantitatively analyzed by global coherence degree from MOI.

Journal of Synchrotron Radiation, 2017, **24**: 954

Monte Carlo simulation on a new artificial spin ice lattice consisting of hexagons and three-moment vertices

Yu Liju Wang Yong Li Junqin Zhu Fangyuan Meng Xiangyu
Cao Jiefeng Jing Chao Wu Yanqing Tai Renzhong

Key words colloquium

A new artificial spin ice lattice called vortex lattice is proposed based on the Kagome lattice. Monte Carlo simulations were performed to investigate the magnetization reversal process of the new artificial spin ice lattice at external magnetic field and different lattice parameters. The results demonstrate some interesting phenomena which are different from Kagome lattice. There are four typical sub-structures emerged in the vortex lattice, which are clockwise and counter-clockwise hexagons, and frustrated +3q and -3q vertices. The occurrence frequency of the four sub-structures change dramatically at different lattice parameter. The new lattice can be partially frustrated at different lattice parameter

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AIP Advances, 2017, **7**(8): 085211

Independent control of the vortex chirality and polarity in a pair of magnetic nanodots

Li Junqin Wang Yon Cao Jiefeng Meng Xiangyu
Zhu Fangyuan Wu Yanqing Tai Renzhong

Key words Magnetic nanodots, Magnetic vortex, Chirality, Polarity

Independent control of the vortex chirality and polarity is realized by changing the in-plane magnetic field direction in nanodot pair through Object Oriented Micromagnetic Framework (OOMMF) simulation. The two magnetic circles are close to each other and have magnetic interaction. The two circles always have the same polarity and opposite chirality at every remanent state. There are totally four predictable magnetic states in the nanodot pair which can be obtained in the remanent state relaxed from the saturation state along all possible directions. An explanation on the formation of vortex states is given by vortex dynamics. The vortex states are stable in large out-of-plane magnetic field which is in a direction opposite to the vortex polarity. The geometry of the nanodot pair gives a way to easily realize a vortex state with specific polarity and chirality.

Journal of Magnetism and Magnetic Materials, 2017, **435**: 167

Electronic structure of $SrSn_2As_2$ near the topological critical point

Rong LY Ma JZ Nie SM Lin ZP Li ZL Fu BB Kong LY
Zhang XZ Huang YB Weng HM Qian T Ding H Tai RZ.

Key words total-energy calculations, single dirac cone, wave basis-set, phase-transition, insulator, surface, discovery, semimetal

Topological materials with exotic quantum properties are promising candidates for quantum spin electronics. Different classes of topological materials, including Weyl semimetal, topological superconductor, topological insulator and Axion insulator, etc., can be connected to each other via quantum phase transition. For example, it is believed that a trivial band insulator can be twisted into topological phase by increasing spin-orbital coupling or changing the parameters of crystal lattice. With the results of LDA calculation and measurement by angle-resolved photoemission spectroscopy (ARPES), we demonstrate in this work that the electronic structure of $SrSn_2As_2$ single crystal has the texture of band inversion near the critical point. The results indicate the possibility of realizing topological quantum phase transition in $SrSn_2As_2$ single crystal and obtaining different exotic quantum states.

Scientific Reports, 2017, **7**: 6133

Effects of temperature, mechanical motion and source positional jitter on the resolving power of beamline 02B at the SSRF

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Key words variable-line-spacing grating, mechanical vibration, source positional jitter, energy-resolving power

A detailed analysis of the effects of temperature excursions, instrumental mechanical motion and source position jitter on the energy-resolving power of beamline 02B at the Shanghai Synchrotron Radiation Facility (SSRF) is presented in this study. This beamline uses a bending-magnet-based source and includes a variable-line-spacing grating monochromator with additional optics. Expressions are derived for the monochromator output photon energy shifts for

each of the performance challenges considered. The calculated results indicate that measured temperature excursions of ±1 K produce an energy shift of less than 11% of the system's energy resolution. Mechanical displacements and vibrations measured at amplitudes of less than 0.5 mm produce changes of less than 5%, while measured source location jitter results in a change of less than 10%. Spectroscopic test experiments at 250 and 400 eV provide energy resolutions of over 10^4. This analysis, combined with the measured results, confirms the operational stability of the beamline, indicating that it meets the performance requirements for experimental use.

Journal of Synchrotron Radiation, 2017, **24**(4): 877

Soft X-ray ptychography method at SSRF

Wang ChunPeng Xu ZiJian Liu HaiGang Tao Xulei Tai RenZhong

Key words Ptychography, Coherent diffraction imaging, X-ray microscopy, Phase retrieval

Ptychography is a diffraction-based X-ray microscopy technique in which an extended sample is scanned by a coherent beam with overlapped illuminated areas and complex transmission function of the sample is obtained by applying iterative phase retrieval algorithms to the diffraction patterns recorded at each scanned position. It permits quantitatively imaging of non-crystalline specimens at a resolution limited only by the X-ray wavelength and the maximal scattering angle detected. In this paper, the development of soft X-ray ptychography method at the BL08U1A beamline of Shanghai Synchrotron Radiation Facility is presented. The experimental setup, experimental parameters selection criteria, and post-experimental data analyzing procedures are presented in detail with a prospect of high-resolution image reconstruction in real time. The performance of this newly implemented method is demonstrated through the measurements of a resolution test pattern and two real samples: Pt–Co alloy nanoparticles and a breast cancer cell. The results indicate that strong scattering specimens can be reconstructed to sub-20 nm resolution, while a sub-25 nm resolution for biological specimens can be achieved.

Nuclear Science and Techniques, 2017, **28**(6): 74

Background noise removal in x-ray ptychography

Wang Chunpeng Xu Zijian Liu Haigang
Wang Yong Wang Jian Tai Renzhong

Key words diffraction microscopy, phase retrieval, resolution, illumination

Ptychography is a diffraction-based x-ray microscopy method that removes the resolution limit imposed by image-forming optical elements. However, background noise in the recorded diffraction patterns will degrade the reconstructed images and may cause reconstruction failure. Removal of the background noise from a ptychography dataset is an important but rather ambiguous prereconstruction data processing step because high-spatial-frequency diffraction signals are inevitably partly wiped out along with the noise. In this paper, several newly designed techniques for removing background noise from experimental ptychographic datasets are provided. Meanwhile, effects of residual background noise and high-frequency signal loss on reconstructed image quality are discussed in detail. The image quality is assessed quantitatively by the power spectral density analysis method and spatial resolution calculation. Both the simulated and experimental results indicate that the positive effect of noise removal by these methods clearly exceeds the negative effect of the accompanied high-spatial-frequency signal loss because part of the lost signals can be recovered by the improved consistencies between neighboring diffraction patterns by the noise removal.

Applied Optics, 2017, **56**(8): 2099

Influence of symmetry and duty cycles on the pattern generation in achromatic Talbot lithography

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Xue Chaofan Liu Haigang Sang Huazhen
Wu Yanqing Tai Renzhong

Key words Euv Interference Lithography, Interferometric Lithography, Light, Arrays

Achromatic Talbot lithography has been proved as a robust and high throughput technique for large area nanopatterning with controllable feature sizes and duty cycles. In this work, the influence of symmetry and duty cycles on the pattern generation has been investigated in detail. Compared with square lattice case, no lattice rotation and spatial frequency multiplication can be observed in hexagonal nanopattern generation. Uniform pattern distribution with a 20 nm feature size has been obtained in square and hexagonal lattices by the masks with 144 nm period and ~50% duty cycle. For the exposure of mask with a smaller duty cycle, nonuniform dot size distribution has been

obtained in the square lattice. While, by using a smaller duty cycle hexagonal lattice mask, a highly uniform periodic hexagonal nanopattern with a 10% duty cycle has been obtained. All the experimental results were consistent with the simulation work.

Journal of Vacuum Science & Technology B, 2017, **35**(2): 021601

Fabrication of high aspect ratio nanoscale periodic structures by the soft X-ray interference lithography

Zhao Jun Wu Yanqing Xue Chaofan Yang Shumin
Wang Liansheng Zhu Fangyuan Zhu Zhichao
Liu Bo Wang Yong Tai Renzhong

Key words Periodic structures, Scintillator, Soft X-ray interference lithography, High aspect ratio

Nanoscale periodic structures have been utilized in the scintillator field to obtain enhanced light extraction efficiency. Sufficient structure depth is necessary to achieve better extraction efficiency. Recently, a soft X-ray interference lithography (SXIL) has been developed in the Shanghai Synchrotron Radiation Facility (SSRF). SXIL can be used to fabricate a high aspect ratio pattern due to the uniform distribution of the beam dose at the photoresist depth. A grating mask with a new photon stop layer was attempted, mainly consisting of Perm alloy, and it was optimized for the SXIL to increase the entire service life. Preliminary results suggest that PMMA structure with an aspect ratio of up to 3 has been successfully manufactured using SXIL techniques. Therefore, this technique has been studied to fabricate the artificial nanostructure on the scintillator in the high efficiency radiation detector area.

Microelectronic Engineering, 2017, **170**: 49

High sensitivity and homogeneity of surface enhanced Raman scattering on three-dimensional array-film hybrid platform

Liu Xing Yu Liju Yang Shumin Yu Huain Zhao Jun Wang Liansheng Wu Yanqing Tai Renzhong

Key words au nanoparticles, sers substrate, spectroscopy, performance, gaps, nanostructures, nanowires, uniform, size

We design and fabricate a substrate based on a three-dimensional array–film hybrid structure used for surface enhanced Raman scattering (SERS). This substrate exhibits improvements both in sensitivity and homogeneity for the Raman signals. As a result, the substrate increases the Raman signal of Rhodamine 6G by 12.3 times under the same measurement conditions, compared with conventional gold array sitting directly on a silica wafer. The sensitivity of SERS can be easily tuned by changing the thickness of SiO_2 separation. Meanwhile, the relative standard deviations are achieved to be less than 10%. This array–film hybrid structure provides a promising approach for future SERS applications.

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Applied Physics Letters, 2017, **110**(8): 081605

Formation of surface nanobubbles on nanostructured substrates

Wang Le Wang Xingya Wang Liansheng Hu Jun Wang Chun Lei Zhao Binyu Zhang Xuehua Tai Renzhong He Mengdong Chen Liqun Zhang Lijuan

Key words Atomic-Force Microscopy, Oriented Pyrolytic-Graphite, Solid-Water Interface, Hydrophobic Surfaces, Aqueous-Solutions, Contact Angles, Nano Bubbles, Flotation, Stability, Particle

The nucleation and stability of nanoscale gas bubbles located at a solid/liquid interface are attracting significant research interest. It is known that the physical and chemical properties of the solid surface are crucial for the formation and properties of the surface nanobubbles. Herein, we experimentally and numerically investigated the formation of nanobubbles on nanostructured substrates. Two kinds of nanopatterned surfaces, namely, nanotrenches and nanopores, were fabricated using an electron beam lithography technique and used as substrates for the formation of nanobubbles. Atomic force microscopy images showed that all nanobubbles were selectively located on the hydrophobic domains but not on the hydrophilic domains. The sizes and contact angles of the nanobubbles became smaller with a decrease in the size of the hydrophobic domains. The results indicated that the formation and stability of the nanobubbles could be controlled by

regulating the sizes and periods of confinement of the hydrophobic nanopatterns. The experimental results were also supported by molecular dynamics simulations. The present study will be very helpful for understanding the effects of surface features on the nucleation and stability of nanobubbles/nanodroplets at a solid/liquid interface.

Nanoscale, 2017, **9**(3): 1078

Interfacial gas nanobubbles or oil nanodroplets?

Wang Xingya Zhao Binyu Hu Jun Wang Shuo Tai Renzhong
Gao Xingyu Zhang Lijuan

Key words Atomic-Force Microscopy, Thin Polymer-Films, Solid-Water Interface, Surface Nanobubbles, Mica/Water Interface, Pattern-Formation, Contact Angles, Nano-Bubbles, Afm Tips, X-Ray

The existence of nanobubbles at a solid–liquid interface with high stability has been confirmed by myriad experimental studies, and their gaseous nature has also been extensively verified. However, nanodroplets of polydimethylsiloxane (PDMS) recently observed in the atomic force microscopy (AFM) measurement of nanobubbles plague the nanobubble community. It may easily lead to wrong interpretations of the AFM results and thus hinders further application of the already widely used AFM in nanobubble studies. Therefore, finding a direct experimental solution to distinguish nanobubbles from nanodroplets in AFM measurements is a matter of great urgency. Herein, we first developed an effective and reproducible method to produce PDMS nanodroplets at the highly ordered pyrolytic graphite (HOPG)/water interface. From their size, contact angle, and stiffness, the formed PDMS nanodroplets are not distinguishable from nanobubbles. However, the force curves on these two objects are strikingly different from each other, i.e., a peculiar plateau in both the approach and retraction curves was found on nanobubbles whereas they changed linearly between the jump-in and jump-off point on PDMS nanodroplets. Thus, the present study not only provided a simple and effective procedure to generate PDMS nanodroplets but also paved a simple practical and in situ way to discriminate nanobubbles from the PDMS nanodroplets by direct AFM force measurements.

Physical Chemistry Chemical Physics, 2017, **19**(2): 1108

Low-dose, high-resolution and high-efficiency ptychography at STXM beamline of SSRF

Xu Zijian Wang Chunpeng Liu Haigang
Tao Xulei Tai Renzhong

Ptychography is a diffraction-based X-ray microscopy method that can image extended samples quantitatively while remove the resolution limit imposed by image-forming optical elements. As a natural extension of scanning transmission X-ray microscopy (STXM) imaging method, we developed soft X-ray ptychographic coherent diffraction imaging (PCDI) method at the STXM endstation of BL08U beamline of Shanghai Synchrotron Radiation Facility. Compared to the traditional STXM imaging, the new PCDI method has resulted in significantly lower dose, higher resolution and higher efficiency imaging in our platform. In the demonstration experiments shown here, a spatial resolution of sub-10 nm was obtained for a gold nanowires sample, which is much better than the limit resolution 30 nm of the STXM method, while the radiation dose is only 1/12 of STXM.

Journal of Physics Conference Series, 2017, **849**: 012033

Real-Time Imaging of Single-Molecule Enzyme Cascade Using a DNA Origami Raft

Sun Lele Gao Yanjing Xu Ya Chao Jie Liu Huajie Wang Lianhui Li Di Fan Chunhai

The dynamics of enzymes are directly associated with their functions in various biological processes. Nevertheless, the ability to image motions of single enzymes in a highly parallel fashion remains a challenge. Here, we develop a DNA origami raft-based platform for in-situ real-time imaging of enzyme cascade at the single-molecule level. The motions of enzymes are rationally controlled via different tethering modes on a two-dimensional (2D) supported lipid bilayer (SLB). We construct an enzyme cascade by anchoring catalase on cholesterol-labeled double-stranded (ds) DNA and glucose oxidase on cholesterol-labeled origami rafts. DNA functionalized with cholesterol can be readily incorporated in SLB via the cholesterol–lipid interaction. By using a total internal reflection fluorescence microscope (TIRFM), we record the moving trajectory of fluorophore-labeled single enzymes on the 2D surface: the downstream catalase diffuses freely in SLB, whereas the upstream glucose oxidase is relatively immobile. By analyzing the trajectories of individual enzymes, we find that the lateral motion of enzymes increases in a substrate concentration-dependent manner and that the enhanced diffusion of enzymes can be transmitted via

the cascade reaction. We expect that this platform sheds new light on studying dynamic interactions of proteins and even cellular interactions.

Journal of the American Chemical Society , 2017, **139**(48): 17525

PCR-Free Colorimetric DNA Hybridization Detection Using a 3D DNA Nanostructured Reporter Probe

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Xu Li Li Lanying Shi Jiye Lal Ratnes Ren Shuzhen
Li Jiang Jia Nengqin Liu Gang

Key words DNA biomarker, signal amplification, magnetic microparticles, DNA tetrahedron, BRCAI

A “sandwich-like” biosensor was developed on the basis of the magnetic bead platform for sensitive detection of breast cancer 1 (BRCA1) DNA. In the present study, a tetrahedron-structured reporter probe (TSRP) was designed, in which 3 vertices of the tetrahedron were labeled with digoxin (Dig), and the other one was labeled with a detection probe. TSRP here provided accurate enzyme loading and well-organized spatial arrangement for optimized signal amplification. The detection limit of this biosensor was as low as 10 fM, which is at least 4 orders of magnitude lower than that of the single DNA probe (100 pM), and the signal gain was 2 times higher than the analysis using three one-dimensional (1D) reporter probes. We could distinguish DNA sequences with only 1 base mismatch, and the performance of our TSRP biosensor was proven to be equally good in both PCR products and real fetal calf serum (FCS) sample as in buffer. We believe this work provided a novel avenue for the development of signal amplification strategies.

ACS Applied Materials & Interfaces, 2017, **9**(44): 38281

Organelle-Specific Triggered Release of Immunostimulatory Oligonucleotides from Intrinsically Coordinated DNA–Metal–Organic Frameworks with Soluble Exoskeleton

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Chen Nan Wang Qi Tu Yaoquan Wang Lihua
Song Shiping Ling Daishun Song Haiyun
Kong Xueqian Fan Chunhai

DNA has proven of high utility to modulate the surface functionality of metal–organic frameworks (MOFs) for various biomedical applications. Nevertheless, current methods for

preparing DNA–MOF nanoparticles rely on either inefficient covalent conjugation or specific modification of oligonucleotides. In this work, we report that unmodified oligonucleotides can be loaded on MOFs with high density (~2500 strands/particle) via intrinsic, multivalent coordination between DNA backbone phosphate and unsaturated zirconium sites on MOFs. More significantly, surface-bound DNA can be efficiently released in either bulk solution or specific organelles in live cells when free phosphate ions are present. As a proof-of-concept for using this novel type of DNA–MOFs in immunotherapy, we prepared a construct of immunostimulatory DNA–MOFs (isMOFs) by intrinsically coordinating cytosine–phosphate–guanosine (CpG) oligonucleotides on biocompatible zirconium MOF nanoparticles, which was further armed by a protection shell of calcium phosphate (CaP) exoskeleton. We demonstrated that isMOFs exhibited high cellular uptake, organelle specificity, and spatiotemporal control of Toll-like receptors (TLR)-triggered immune responses. When isMOF reached endolysosomes *via* microtubule-mediated trafficking, the CaP exoskeleton dissolved in the acidic environment and in situ generated free phosphate ions. As a result, CpG was released from isMOFs and stimulated potent immunostimulation in living macrophage cells. Compared with naked CpG–MOF, isMOFs exhibited 83-fold up-regulation in stimulated secretion of cytokines. We thus expect this isMOF design with soluble CaP exoskeleton and an embedded sequential “protect–release” program provides a highly generic approach for intracellular delivery of therapeutic nucleic acids.

Journal of the American Chemical Society, 2017, **139**(44): 15784

Enzyme-Triggered Fluorescence Turn-on: A Probe for Specifically Imaging Ovarian-Cancer-Related γ-Glutamyltranspeptidase

Tian Jie Yan Qinglong Zhu Ying Zhang Jichao Li Jiao Shi Ben Xu Ge Fan Chunhai Zhao Chunchang

Key words fluorescence turn-on, GGT, the aromatic hydrocarbon transfer, living cells, specifically targeting

A fluorescent turn-on probe for specifically targeting γ-glutamyltranspeptidase (GGT) was designed and synthesized by integrating boron-dipyrromethene (BODIPY) as a chromophore and glutathione (GSH) as the GGT substrate. GGT-catalyzed the cleavage of the γ-glutamyl bond and generated the aromatic hydrocarbon transfer between the sulfur and the nitrogen atom in BODIPY, leading to distinct optical changes. Such specific responsiveness provides an easily distinguishable

fluorescence signal to visualize the GGT activity in living cells and differentiate GGT-positive cancer cells from GGT-negative cells.

Chinese Journal of Chemistry, 2017, **35**(11): 1711

Computation in Chemistry: A Summary of the Development and Models of DNA Computing

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Key words DNA computing, NP hard problem, parallel overlap assemble model, sticker model, splicing model, DNA Tile self-assembly, biochemical signal logic gate

The development in computer science has brought a great impetus to the advance of human society. However, as the manufacturing process goes to the limit, there is an urgent need to find a new computing system to meet the growing demand for computing. DNA computing has attracted great attention due to its advantages in huge information storage, large scale parallelism and very low energy consumption. Many different models have been established ever since the experimental implementation of solving a 6 vertices Hamilton pathway problem by Adleman in 1994. In this paper, a brief introduction to the basic principles and experimental operations in DNA computing is first given, and the theories in this field are illustrated, including the DNA sequence design, complexity of different models and the proof of universal computing power. Moreover, the models regarded as breakthroughs in the field are summarized. All the models are classified based on the specific means in conducting the experiment, and reviewed according to different classes. More detailed descriptions are further set forth for a classical model in each class. At last, a prospect is made based on our work in this area.

Progress in Chemistry, 2017, **29**(11): 1297

Evolution of grain boundary carbides in thermal exposed Ti-modified alloy N

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Song Changjiang Li Zhijun Zhou Xingtai

Key words MC carbides, Hastelloy N, Thermal exposure, Orientation relationship

The evolution of grain boundary MC carbides during the thermal exposure has been investigated in the Ti-modified Hastelloy N alloy. MC carbides precipitate at the grain boundaries

after exposed at 650 °C and 750 °C for 500 hours (h). The morphology of MC carbides at the grain boundaries was characterized as separated particles with a cube-on-cube orientation relationship with the matrix. The MC/Matrix interface exhibits a semi-coherent character, on which misfit dislocations are repeated in every sixth layer of $(111)_{MC}$. With the further thermal exposure, the size of MC carbides remain stable at 650 °C. By contrast, M_2C carbides undergo the initial coarsening and subsequent re-dissolution at 750 °C. At the same time, the deviation angles from the cube-cube orientation relationship (OR) between MC carbides and the matrix become larger at both 650 °C and 750 °C, which indicate the semi-coherent interfaces are transforming to the incoherent ones.

Materials Characterization, 2017, **133**: 54

Engineering nucleic acid structures for programmable molecular circuitry and intracellular biocomputation

Li Jiang Green Alexander A Yan Hao Fan Chunhai

Key words Tetrahedral DNA Nanostructure, Origami

Nucleic acids have attracted widespread attention due to the simplicity with which they can be designed to form discrete structures and programmed to perform specific functions at the nanoscale. The advantages of DNA/RNA nanotechnology offer numerous opportunities for in-cell and in-vivo applications, and the technology holds great promise to advance the growing field of synthetic biology. Many elegant examples have revealed the potential in integrating nucleic acid nanostructures in cells and in vivo where they can perform important physiological functions. In this Review, we summarize the current abilities of DNA/RNA nanotechnology to realize applications in live cells and then discuss the key problems that must be solved to fully exploit the useful properties of nanostructures. Finally, we provide viewpoints on how to integrate the tools provided by DNA/RNA nanotechnology and related new technologies to construct nucleic acid nanostructure-based molecular circuitry for synthetic biology.

Nature Chemistry, 2017, **9**(11): 1056

Recognizing single phospholipid vesicle collisions on carbon fiber nanoelectrode

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Shi Jiye Wang Lihua Fan Chunhai Zuo Xiaolei

Key words single vesicle, carbon fiber nanoelectrode, high resolution, electrochemical detection 3

We recognize the stochastic collisions of dopamine contained phospholipid vesicle on carbon fiber nanoelectrode, extending the observation of discrete collision events on nanoelectrode to biologically relevant analytes. To decrease noise interference to the technique, the dimensions of nanoelectrode was systematically investigated and optimized. Scanning electron microscopy (SEM) further supported the comparable sizes of nanoelectrode and vesicles (~100 nm in diameter). Vesicles collision and rupture on the surface of nanoelectrode led to the dopamine release from vesicles, which could be electrochemically oxidized to dopamine-o-quinone and detected via voltammetry. The comparable size of the nanoelectrode with vesicles and fast voltammetry allowed differentiation of single collision events from the current magnitudes and peak widths in the electrochemical collision experiments, which shows the efficacy of the method to characterize vesicle samples. This work provides a foundation upon which quantitative sensor technology might be built for the detection of dopamine contained vesicles with high spatial and temporal resolution.

Science China Chemistry, 2017, **60**(11): 1474

Special topic for "single-molecule, single-particle and single-cell bioimaging"

Fan Chunhai Fang Xiaohong

Science China Chemistry, 2017, **60**(10): 1265

Sub-diffraction-limit cell imaging using a super-resolution microscope with simplified pulse synchronization

Gao Zhaoshuai Deng Suhui Li Jiang Wang Kun Li Jiajun
Wang Lihua Fan Chunhai

Key words fluorescence microscope, far field super-resolution, stimulated emission depletion (STED) microscope, pulse synchronization

Stimulated emission depletion (STED) microscope is one of the most prominent super-resolution bio-imaging instruments, which holds great promise for ultrahigh-resolution imaging of cells. To construct a STED microscope, it is challenging to realize temporal synchronization between the excitation pulses and the depletion pulses. In this study, we present a simple and low-cost method to achieve pulse synchronization by using a condensed fluorescent dye

as a depletion indicator. By using this method, almost all the confocal microscopes can be upgraded to a STED system without losing its original functions. After the pulse synchronization, our STED system achieved sub-100-nm resolution for fluorescent nanospheres and single-cell imaging.

Science China Chemistry, 2017, **60**(10): 1305

Assembling and Powering Up Nanostructures!

Nam JwaMin Fan Chunhai Gianneschi Nathan

This special issue, guest edited by Jwa-Min Nam, Chunhai Fan and Nathan Gianneschi, highlights emerging concepts and important advances in the directed assembly of nanostructures, their emergent properties, and applications.

ChemNanoMat, 2017, **3**(10): 668

A Gold-Nanoparticle-Based SERS Reporter that Rolls on DNA Origami Templates

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Wang Jun Zhu Dan Su Shao Peng Hongzhen
Wang Lihua Wang Lianhui Chao Jie

Key words AuNPs, DNA origami, gold, plasmonic nanostructures, surface-enhanced Raman scattering (SERS)

Plasmonic nanostructures with distinct spatial configuration and geometry are of considerable significance because of their desired optical response. These optical responses have close relationship with the inter-particle parameters in plasmonic nanostructures. However, the precise control of the consecutive variation of these parameters remains a formidable challenge. Here, we demonstrate a gold nanoparticle (AuNP) -based plasmonic nano-reporter, in which a AuNP performs as a walker to stepwise roll directionally and progressively on DNA origami. Using another AuNP as a stator, the rolling of the AuNP reporter could generate the inter-particle distance variation, which would be monitored by surface-enhanced Raman scattering (SERS). Our method opens up a door to develop an optical reporter that monitors inter-particle variations in plasmonic nanostructures.

ChemNanoMat, 2017, **3**(10): 760

Humidity-Responsive Single-Nanoparticle-Layer Plasmonic Films

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Zuo Xiaolei Liu Gang Shi Jiye Wang Lihua
Zhou Ruhong Cheng Wenlong Fan Chunhai

Key words chromogenic films; DNA; gold nanoparticles; plasmon coupling; single nanoparticle layers

2D materials possess many interesting properties, and have shown great application potentials. In this work, the development of humidity-responsive, 2D plasmonic nanostructures with switchable chromogenic properties upon wetting–dewetting transitions is reported. By exploiting DNA hybridization-directed anchoring of gold nanoparticles (AuNPs) on substrates, a series of single-nanoparticle-layer (SNL) plasmonic films is fabricated. Due to the collective plasmonic responses in SNL, these ultrathin 2D films display rapid and reversible red-blue color change upon the wetting–dewetting transition, suggesting that hydration-induced microscopic plasmonic coupling between AuNPs is replicated in the macroscopic, centimeter-scale films. It is also found that hydration finely tunes the electric field distribution between AuNPs in the SNL film, based on which responsive surface-enhanced Raman scattering substrates with spatially homogeneous hot spots are developed. Thus it is expected that DNA-mediated 2D SNL structures open new avenues for designing miniaturized plasmonic nanodevices with various applications.

Advanced Materials, 2017, **29**(35): 1606796

Multifunctional Yolk–Shell Nanostructure as a Superquencher for Fluorescent Analysis of Potassium Ion Using Guanine-Rich Oligonucleotides

Lu Na Wen Yanli Liu Gang Ding Lei Zeng Caixia
Aldalbahi Ali Khan Muhammad Naziruddin
Periyasami Govindasami Rahaman Mostafizur Alrohaili Abdulaziz
Shi Jiye Song Shipin Wang Lihua Zhang Min

Key words multifunctional yolk-shell nanoparticles, superquencher, fluorescent sensing, potassium ion, G-rich oligonucleotides

The excellent performance of a biosensor generally depends on the high signal-to-noise ratio, and the superquencher plays a dominant role in fluorescent sensors. Novel nanoquenchers exhibited

high quenching efficiency in various fluorescent assays of biological/chemical molecules. Here, we developed a novel nano-biosensor using Fe_3O_4@C yolk–shell nanoparticles (YSNPs) and studied their quenching effect. We found Fe3O4@C YSNP was a superquencher and exhibited an ultrastrong quenching ability, up to almost 100% quenching efficiency, toward fluorophores. Also, Fe_3O_4@C YSNPs possessed the most superior fluorescence restoration efficiency, due to biomolecular recognition event, compared to the other nanoquenchers, including bare Fe3O4 NPs, graphene oxide (GO), and single-wall carbon nanotubes (SWCNTs). On the basis of that, a fluorescent sensing platform for potassium-ion (K^+) analysis with guanine (G)-rich oligonucleotides was designed. As a result, Fe_3O_4@C YSNP-based fluorescent sensors demonstrated excellent performance, with an ultrahigh sensitivity of a detection limit as low as 1.3 μM, as well as a wide dynamic range from 50 μM to 10 mM. The proposed method is fast, simple, and cost-effective, suggesting the great potential for practical applications in biomedical detection and clinical diagnosis.

ACS Applied Materials & Interfaces, 2017, **9**(6): 30406

DNA Hydrogel with Aptamer-Toehold-Based Recognition, Cloaking, and Decloaking of Circulating Tumor Cells for Live Cell Analysis

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Liu Huajie Hwang Michael T. Chao Jie Su Shao Wang Lihua
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Key words Circulating tumor cell, DNA hydrogel, CTC capture, CTC release, live cell analysis

Circulating tumor cells (CTCs) contain molecular information on the primary tumor and can be used for predictive cancer diagnostics. Capturing rare live CTCs and their quantification in whole blood remain technically challenging. Here we report an aptamer-trigger clamped hybridization chain reaction (atcHCR) method for in situ identification and subsequent cloaking/decloaking of CTCs by porous DNA hydrogels. These decloaked CTCs were then used for live cell analysis. In our design, a DNA staple strand with aptamer-toehold biblocks specifically recognizes epithelial cell adhesion molecule (EpCAM) on the CTC surface that triggers subsequent atcHCR via toehold-initiated branch migration. Porous DNA hydrogel based-cloaking of single/cluster of CTCs allows capturing of living CTCs directly with minimal cell damage. The

ability to identify a low number of CTCs in whole blood by DNA hydrogel cloaking would allow high sensitivity and specificity for diagnosis in clinically relevant settings. More significantly, decloaking of CTCs using controlled and defined chemical stimuli can release living CTCs without damages for subsequent culture and live cell analysis. We expect this liquid biopsy tool to open new powerful and effective routes for cancer diagnostics and therapeutics.

Nano Letters, 2017, **17**(9): 5193

Sequence-dependent interactions between model peptides and lipid bilayers

Lei HaoZhi Tian Tian Du Qiqige Hu Jun Zhang Yi

Key words Peptides, Lipid membrane, Atomic force microscopy, Fluorescence methods

Studying interaction between peptides and lipid membranes is helpful for understanding the working mechanism of amyloidogenic peptides and antimicrobial peptides, which are toxic to cells through disruption of the cell membrane. Although many efforts have been made to find out common mechanisms of the peptide-induced membrane disruption, detailed information on how the peptide's amino acid sequence affects its interaction with lipid bilayers is still lacking. In this study, three peptides termed as Pep_{11}, $P_{11\text{-}2}$, and QQ_{11}, which share a similar backbone, were employed to explore how modifications on the peptide sequence as well as terminal groups influenced its interaction with the lipid membrane. Atomic force microscopy data revealed that the peptides could deposit on the membranes and induce defects with varied morphologies and stiffness. Fluorescence resonance energy transfer (FRET) experiments indicated that the introduction of the three peptides resulted in different FRET effects on either liquid or gel lipid membranes. DPH fluorescence anisotropy and Laurdan's generalized polarization analysis showed that $P_{11\text{-}2}$ could insert into the lipid membrane and impact the lipid hydrophobic region while QQ_{11} influenced the order of the hydrophilic head of the lipid membrane. With these results, we have illustrated how these peptides interacted differently with the lipid membrane because of the modification of their sequences. Although these peptides did not relate to disease and antibiosis, we hope these results still could provide some clues for partly understanding the working mechanism of amyloidogenic peptides and antimicrobial peptides.

Nuclear Science and Techniques, 2017, **28**(9): 124

Dual-mode electrochemical analysis of microRNA-21 using gold nanoparticle-decorated MoS_2 nanosheet

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Fan Chunhai Wang Lianhui

Key words Dual-mode, Molybdenum disulfide, Gold nanoparticles, MicroRNA, Biosensor

The detection of microRNA plays an important role in early cancer diagnosis. Herein, a dual-mode electronic biosensor was developed for microRNA-21 (miRNA-21) detection based on gold nanoparticle-decorated MoS_2 nanosheet (AuNPs@MoS_2). A classical DNA "sandwich" structure was employed to construct MoS_2-based electrochemical sensor, including capture DNA, target miRNA-21 and DNA-modified nanoprobe. $[Fe(CN)_6]^{3-/4-}$ and $[Ru(NH3)_6]^{3+}$ were selected as electrochemical indicators to monitor the preparation process and evaluate the performance of MoS_2-based electrochemical biosensor by electrochemical impedance spectroscopy (EIS) and differential pulse voltammetry (DPV), respectively. Such MoS_2-based biosensor exhibited excellent performance for miRNA-21 detection in the range from 10 fM to 1 nM with detection limit of 0.78 fM and 0.45 fM for DPV and EIS technique, respectively. Furthermore, the proposed MoS_2-based biosensor displayed high selectivity and stability, which could be used to determine miRNA-21 in human serum samples with satisfactory results. All data suggested that such MoS_2-based nanocomposite may be a potential candidate for biosensing ranging from nucleic acid to protein detection.

Biosensors and Bioelectronics, 2017, **94**: 552

Nuclease-free target recycling signal amplification for ultrasensitive multiplexing DNA biosensing

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Key words DNA detection, Nuclease-free, Target recycling, Multiplexing biosensing

Ultrasensitive biosensing technologies without gene amplification held great promise for direct detection of DNA. Herein we report a novel biosensing method, combining target recycling signal-amplification strategy and a homemade electrochemical device. Especially, the target recycling was achieved by a strand displacement process, no needing the help of any nucleases. In the presence of target DNA, the recycling system could be activated to generate a cascade of assembly steps with three hairpin DNA segments. Each recycling process were accompanied by a disassembly step that the last hairpin DNA segment displaces target DNA from the complex at the

end of each circulation, freeing targets to activate the self-assembly of more trefoil DNA structures. This biosensing method could detect target DNA at aM level and can distinguish target DNA from interfering DNAs, demonstrating its high sensitivity and high selectivity. Importantly, the biosensing method could work well with serum samples.

Biosensors and Bioelectronics, 2017, **94**: 605

Enzymatic O-GlcNAcylation of α-synuclein reduces aggregation and increases SDS-resistant soluble oligomers

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Key words α-Synuclein, O-GIcNAcylation, Aggregation, SDS-resistant oligomers

Neurodegenerative diseases including dementia with Lewy bodies, Lewy body variant of Alzheimer's disease, and Parkinson's disease are associated with the aberrant aggregation of α-synuclein, which is influenced by several post-translational modifications (PTMs). O-GlcNAcylation is one PTM that has an important role in many fundamental processes. The O-GlcNAcylation of endogenous α-synuclein at residues 53, 64, 72 and 87 has been reported in an unbiased mass spectrum analysis. The consequences of O-GlcNAcylation at residues 72 or 87 have been studied by using a synthetic α-synuclein bearing O-GlcNAcylation at threonine residue 72 or serine 87, respectively. O-GlcNAcylation at Thr72 or Ser87 suppresses the aggregation of α-synuclein. However, the effect of enzymatic O-GlcNAcylation of α-synuclein at multiple residues is not clear. Here, we successfully generated O-GlcNAcylated α-synuclein by co-expressing a shorter form of OGT (sOGT) with α-synuclein. The O-GlcNAcylation inhibited α-synuclein aggregation and promoted the formation of soluble SDS-resistant and Thioflavine T negative oligomers. Our data warrant further studies on the role of O-GlcNAcylation in the progression/treatment of Parkinson's disease in animal models.

Neuroscience Letters, 2017, **655**: 90

Programming Cell Adhesion for On-Chip Sequential Boolean Logic Functions

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Key Words Strand Displacement Cascades, Dna Nanostructures, Computation, Microenvironments, Amplification, Monolayers, Delivery, Robots, Array, Ecm

Programmable remodelling of cell surfaces enables high-precision regulation of cell behavior. In this work, we developed in vitro constructed DNA-based chemical reaction networks (CRNs) to program on-chip cell adhesion. We found that the RGD-functionalized DNA CRNs are entirely noninvasive when interfaced with the fluidic mosaic membrane of living cells. DNA toehold with different lengths could tunably alter the release kinetics of cells, which shows rapid release in minutes with the use of a 6-base toehold. We further demonstrated the realization of Boolean logic functions by using DNA strand displacement reactions, which include multi-input and sequential cell logic gates (AND, OR, XOR, and AND-OR). This study provides a highly generic tool for self-organization of biological systems.

Journal of The American Chemical, 2017, **139**(30): 10176

Synchrotron-based X-ray microscopy for sub-100 nm resolution cell imaging

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Key Words Fluorescence Microscopy, Diffraction Microscopy, Tio2 Nanoparticles, Quantum Dots, Metal-Ions, Nanoscale, Cytotoxicity, Tomography, Breaking, Whole

Microscopic imaging provides a straightforward approach to deepen our understanding of cellular events. While the resolution of optical microscopes is generally limited to 200–300 nm due to the diffraction limit, there has been ever growing interest in studying cells at the sub-100 nm regime. By exploiting the short wavelength, long penetration depth and elemental specificity of X-rays, synchrotron-based X-ray microscopy (XRM) has demonstrated its power in exploring the structure and function of cells at the nanometer resolution. Here we summarize recent advances in using XRM for imaging ultrastructure of organelles and specific biomolecular locations in cells, and provide a perspective on potentials and applications of XRM.

Current Opinion in Chemical Biology, 2017, **39**: 11

In situ TEM studies of the shape evolution of Pd nanocrystals under oxygen and hydrogen environments at atmospheric pressure

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Zhang Ze Gao Yi Wang Yong

Key Words Co Oxidation, Electron-Microscopy, Copper Nanocrystals, Nanoparticles, Palladium, Catalysts, Size, Visualization, Combustion, Particles

We demonstrate an atomic scale TEM observation of shape evolutions of Pd nanocrystals under oxygen and hydrogen environments at atmospheric pressure. Combined with multi-scale structure reconstruction model calculations, the reshaping mechanism is fully understood.

Chemical Communications, 2017, **53**(99): 13213

Effect of pH on the Stability of DNA Origami

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Key words DNA origami, Self-assembly, Stability, pH

The response of DNA origami nanostructures to pH is systematically investigated from two aspects in this work. At first, self-assembly of DNA origami triangle in different pH buffer was tested by putting M13 scaffold and staple strands into a series of sodium citrate buffer (10 mmol/L with 12.5 mmol/L Mg^{2+}), the as-prepared sample was characterized by AFM. The formation of the origami structure was affected by pH and the structure was observed only in the pH range of 6-9. Tolerance of DNA origami to pH in the external environment was investigated by immersing them (pH = 8) into acidic and basic solutions for 2 h at room temperature, followed by characterization of the samples by AFM and 0.5% agarose gel respectively. The AFM results showed that the DNA origami triangle maintained the original structure at pH range of 5-10, and the structure was broken at higher or lower pH. The agarose gel suggested that the most stable state of DNA origami triangle was in pH range of 7-8, where the intensity and mobility of the sample band remained the same. Compared with the origami self-assembled in different pH buffers, the pre-prepared origami showed better resistance to acidic and alkali environments. In order to test the long time-stability of DNA origami, pH value of the prepared triangle origami was adjusted in the range of 5-10 and the reaction time was extended to 12 h. AFM test results indicated that the DNA origami could maintain its original structure for at least 12 h. Another common origami nanostructure was also tested; like origami triangle, rectangle structure showed a similar pH tolerance which could keep

the stability at pH range of 5-10 for at least 12 h. The long time pH stability experiment of the triangle and the rectangle structures indicated that the origami structure based on M13 owned a relatively high pH tolerance. Based on the above results, possible mechanism of pH effect on DNA origami stability was also proposed. In the process of the origami preparation, excess H^+ or OH-will affect the formation of the hydrogen bond thus affecting the hybridization of DNA double helixes. In the pH tolerance experiment, excessive H^+ or OH-will attack the formed hydrogen bonds and make the origami structure floppy. In both aspects, more H+ or OH-will undermine the primary structure of DNA, and eventually affect the formation and stability of DNA origami structures.

Acta Polymerica Sinica, 2017, (12): 1993

Application Progress of DNA Nanostructures in Drug Delivery and Smart Drug Carriers

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Key words DNA nanostructures, Drug delivery carriers, Smart drug delivery, Review

The nanocarrier systems have been widely used for improving solubility, stability and therapeutic activity of drugs due to their high drug-loading efficiency, good target specificity and long circulation time. To achieve precisely controlled loading and tumor-selective release of drugs, extensive researches have been focused on developing nanocarriers with low toxicity, excellent biocomapatibility and biodegradability. As a type of nano-biomaterials with various functions and applications, self-assembled DNA nanostructures explored new ways to develop drug carriers in smart drug delivery based on their well-defined structures, good biocompatibility and stability, high cell membrane permeability and controlled drug releasing property. In this review, we summarized the developing course and the recent advances of DNA nanostructures for drug delivery, including the application of both static and dynamic DNA nanostructures. The application of dynamic DNA nanostructures for controllable drug release showed great potential in smart drug delivery.

Chinese Journal of Analytical, 2017, **45**(7): 1078

Real-Time Imaging of Endocytosis and Intracellular Trafficking of Semiconducting Polymer Dots

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Shi Jiye Wang Lihua Zhao Yun
Wu Changfeng Chen Nan

Key words fluorescent polymer dots, endocytosis, intracellular trafficking, theranostic nanoparticles, live cell imaging

Semiconducting polymer dots (Pdots) have shown great promise in biomedical applications, including biosensing, drug delivery, and live imaging of cells and biomolecules. Insight into the mechanism and regulation of cellular uptake and intracellular metabolism of Pdots is important for the development of superior Pdots-based theranostic nanoconjugates. Herein, we performed real-time imaging of endocytosis and intracellular trafficking of a type of fluorescent Pdots that showed excellent biocompatibility in various types of cells. The endocytic routes and kinetics of Pdots were differently regulated in distinct cell types. Following endocytosis, Pdots were transported in vesicles along microtubule and destined for lysosomes. Furthermore, our results revealed exosome-mediated extracellular release of Pdots and have tracked the dynamic process at the single particle level. These results provide new insight into the design of more effective and selective imaging probes as well as drug carriers.

ACS Applied Materials & Interfaces, 2017, **9**(25): 21200

Preservation of DNA Nanostructure Carriers: Effects of Freeze - Thawing and Ionic Strength during Lyophilization and Storage

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Shen Ju wen Shi Jiye Li Jiang Wang Lihua

Key words lyophilization, DNA nanostructures, structure friendly, ionic strength, storage

DNA rianostiuctures have: attracted wide interest-in biomedical applications, especially as nanocarriers for drug delivery. Therefore, it is.important to ensure: the structural integrity of DNA nanostructures under ambient temperature storage. In this study, we examined lyophilization-based preservation of DNA nanostructures by investigating the structural integrity of different DNA

nanostructures reconstituted from lyophilization. We demonstrated that lyophilization Under appropriate ionic strength is amenable to the storage of DNA. nanostructures Compared with that stored in liquid solutiOn, DNA nanostructure carriers reconstituted from lyophilization showed significantly better structural integrity after an accelerated aging test equivalent to 100-day room-temperature storage.

ACS Applied Materials & Interfaces, 2017, **9**(22): 18434

Nanodiamonds Mediate Oral Delivery of Proteins for Stem Cell Activation and Intestinal Remodeling in Drosophila

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Key words nanodiamonds, protein delivery, oral delivery, stem cells microenvironment, intestinal remodeling

Introduction of exogenous biomacromolecules into living systems is of great interest in genome editing, cancer immunotherapy, and stem cell reprogramming. Whereas current strategies generally depend on nucleic acids transfection, direct delivery of functional proteins that provides enhanced specificity, increased safety, and fast and temporal regulation is highly desirable. Nevertheless, intracellular delivery of intact and bioactive proteins, especially in vivo, remains poorly explored. In this study, we developed a nanodiamonds (NDs)-based protein delivery system in cultured cells and in Drosophila that showed high adsorption, high efficiency, and effective cytosolic release of fully functional proteins. Through live-cell imaging, we observed a novel phenomenon wherein a substantial amount of internalized NDs–protein complex rejected fusion with the early endosome, thereby evading protein degradation in the lysosome. More significantly, we demonstrated that dietary NDs–RNase induced apoptosis in enterocytes, stimulating regenerative divisions in intestinal stem cells and increasing the number of stem cells and precursor cells in Drosophila intestine. As stem cells are poorly accessible by exogenous agents in vivo, NDs-mediated oral delivery of proteins provides a new approach to modulate the stem cell microenvironment for intestinal remodeling, which has important implications for colorectal cancer therapy and regenerative medicine.

ACS Applied Materials & Interfaces, 2017, **9**(22): 18575

Size-Dependent Regulation of Intracellular Trafficking of Polystyrene Nanoparticle-Based Drug-Delivery Systems

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Key words nanopartides, imaging, exocytosis, endocytosis, intracellular trafficking

Nanoparticles (NPs) have shown great promise as intracellular imaging probes or nanocarriers and are increasingly being used in biomedical applications. A detailed understanding of how NPs get “in and out” of cells is important for developing new nanomaterials with improved selectivity and less cytotoxicity. Both physical and chemical characteristics have been proven to regulate the cellular uptake of NPs. However, the exocytosis process and its regulation are less explored. Herein, we investigated the size-regulated endocytosis and exocytosis of carboxylated polystyrene (PS) NPs. PS NPs with a smaller size were endocytosed mainly through the clathrin-dependent pathway, whereas PS NPs with a larger size preferred caveolae-mediated endocytosis. Furthermore, our results revealed exocytosis of larger PS NPs and tracked the dynamic process at the single-particle level. These results indicate that particle size is a key factor for the regulation of intracellular trafficking of NPs and provide new insight into the development of more effective cellular nanocarriers.

ACS Applied Materials & Interfaces, 2017, **9**(22): 18619

Study on physisorption between G-actin and amphiphilic polymer-coated gold nanoparticles

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Key words amphiphilic polymer, binding constant, G-actin, gold nanoparticle, photoluminescence quenching

Physisorptions occurs everywhere and constantly in living organisms and between nanomaterials and biomolecules. In this study, one of the most important proteins, G-actin, was selected to investigate its bio-nano physisorption with a model nanoparticle coated with a amphiphilic polymer. Using a photoluminescence quenching method, both the binding constant and the Hill constant were determined as 1.79×10^7 M^{-1} and 0.84, respectively. Thermodynamic

calculations proved that such a physisorption was a spontaneous procedure. The physisorption-mediated protein–nanoparticle conjugates were robust enough to resist gel electrophoresis, and protein conformation was kept intact, as revealed using circular dichroism. This conjugate might be a promising candidate for nanofabrication or could play a significant role in actin–related bioactivities.

Luminescence, 2017, **32**(4): 618

Real-time visualization of clustering and intracellular transport of gold nanoparticles by correlative imaging

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Li Jiajun Lv Min Chen Nan Song Haiyun Lee Joon
Shi Jiye Wang Lihua Lal Ratnesh Fan Chunhai

Key words Clathrin-Mediated Endocytosis, Cell, Mechanisms, Microscopy, Endosomes, Dynamics, Platform, Motors, Cancer, Virus

Mechanistic understanding of the endocytosis and intracellular trafficking of nanoparticles is essential for designing smart theranostic carriers. Physico-chemical properties, including size, clustering and surface chemistry of nanoparticles regulate their cellular uptake and transport. Significantly, even single nanoparticles could cluster intracellularly, yet their clustering state and subsequent trafficking are not well understood. Here, we used DNA-decorated gold (fPlas-gold) nanoparticles as a dually emissive fluorescent and plasmonic probe to examine their clustering states and intracellular transport. Evidence from correlative fluorescence and plasmonic imaging shows that endocytosis of fPlas-gold follows multiple pathways. In the early stages of endocytosis, fPlas-gold nanoparticles appear mostly as single particles and they cluster during the vesicular transport and maturation. The speed of encapsulated fPlas-gold transport was critically dependent on the size of clusters but not on the types of organelle such as endosomes and lysosomes. Our results provide key strategies for engineering theranostic nanocarriers for efficient health management.

Nature Communications, 2017, **8**: 15646

Graphene Nanoprobes for Real-Time Monitoring of Isothermal Nucleic Acid Amplification

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Key words interaction of graphene oxide and DNA, length and position dependent, various DNA structures, real-time detection,
isothermal amplification

Isothermal amplification is an efficient way to amplify DNA with high accuracy; however, the real-time monitoring for quantification analysis mostly relied on expensive and precisely designed probes. In the present study, a graphene oxide (GO)-based nanoprobe was used to real-time monitor the isothermal amplification process. The interaction between GO and different DNA structures was systematically investigated, including single-stranded DNA (ssDNA), double-stranded DNA (dsDNA), DNA 3-helix, and long rolling circle amplification (RCA) and hybridization chain reaction (HCR) products, which existed in one-, two-, and three-dimensional structures. It was found that the high rigid structures exhibited much lower affinity with GO than soft ssDNA, and generally the rigidity was dependent on the length of targets and the hybridization position with probe DNA. On the basis of these results, we successfully monitored HCR amplification process, RCA process, and the enzyme restriction of RCA products with GO nanoprobe; other applications including the detection of the assembly/disassembly of DNA 3-helix structures were also performed. Compared to the widely used end-point detection methods, the GO-based sensing platform is simple, sensitive, cost-effective, and especially in a real-time monitoring mode. We believe such studies can provide comprehensive understandings and evocation on design of GO-based biosensors for broad application in various fields.

ACS Applied Materials & Interfaces, 2017, **9**(18): 15245

Carbides Evolution in a Ni-16Mo-7Cr Base Superalloy during Long-Term Thermal Exposure

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Zhou Xingtai

Key words nickel base superalloy, carbide, thermal exposure, in situ transformation

The effect of long-term thermal exposure on the carbide evolution in a Ni-16Mo-7Cr base superalloy was investigated. The results show that $M_{12}C$ carbides are mainly precipitated on the

grain boundaries during thermal exposure, and the primary massive M_6C carbides can be completely transformed to $M_{12}C$ carbides in situ at temperatures above 750 °C for long-term thermal exposure. The transformation from M_6C carbides to $M_{12}C$ carbides is attributed to the release of C atoms from M_6C, which results in the morphology changes of massive carbides, and stabilization of the sizes of $M_{12}C$ carbides precipitated on the grain boundaries.

Materials, 2017, **10**(5): 521

Synthesis and Applications of Triangular Gold Nanoplates

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Key words triangular gold nanoplates, crystal growth, plasmonics, surface-enhanced Raman, superlattices

Colloidal metal nanoparticles are emerging as key materials because of their localized surface plasmon resonance (LSPR) property and the enormous applications in catalysis, plasmonics, sensing, and photonics. Anisotropic nanoparticles have attracted increasing attention due to the novel and unusual chemical and physical behavior along with the decreased symmetry. In the case of the anisotropic nanoparticles, triangular gold nanoplates stand out owing to their unique shape and excellent LSPR properties, which is of great significance to develop a new generation of photonic and electronic devices. However, compared with the spherical nanoparticles, the controllable synthesis of triangular. gold nanoplates is much more difficult. Therefore, numerous efforts have been put into their controlled synthesis and a variety of methods have been developed successfully, providing opportunities for the better use of this new material. In this review, we highlight the synthetic achievements, the shape-directing mechanism and separation methods of triangular gold nanoplates. We also address the recent breakthroughs of Au triangular structures in constructing anisotropic superlattices and taking advantage of their enhanced electromagnetic field for single-molecular fluorescence detection and surface-enhanced Raman scattering. Finally, with the development of the self-assembly technology, we believe that Au triangular nanoplates are powerful building blocks for the bottom-up materials engineering and it will play a more important role in chemistry, materials and other fields.

Progress in Chemistry, 2017, **29**(5): 459

Precisely Tailored DNA Nanostructures and their Theranostic Applications

Zhu Bing Wang Lihua Li Jiang Fan Chunhai

Key words DNA nanostructure, DNA nanotechnology, imaging, theranostic, biomedicine

A critical challenge in nanotechnology is the limited precision and controllability of the structural parameters, which brings about concerns in uniformity, reproducibility and performance. Self-assembled DNA nanostructures, as a newly emerged type of nano-biomaterials, possess low-nanometer precision, excellent programmability and addressability. They can precisely arrange various molecules and materials to formspatially ordered complex, resulting in unambiguous physical or chemical properties.Because of these, DNA nanostructures have shown great promise in numerous biomedical theranostic applications. In this account, we briefly review the history and advances on construction of DNA nanoarchitectures and superstructures with accurate structural parameters. We focus on recent progress in exploiting these DNA nanostructures as platforms for quantitative biosensing, intracellular diagnosis, imaging, and smart drug delivery. We also discuss key challenges in practical applications.

Chemical Record, 2017, **17**(12): 1213

The Inhibition Effect of Graphene Oxide Nanosheets on the Development of Streptococcus mutans Biofilms

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Fan Chunhai Lv Min Tang Zisheng

Key words biofilm formation, extracellular polymeric substances (EPS), graphene oxide, Streptococcus mutans biofilms

Bacterial biofilms play a critical role in dental pathogenic mechanisms due to their ability to tolerate many traditional antibacterial agents. Thus, it is crucial to find effective methods to inhibit the occurrence and development of biofilms. Recently, graphene oxide (GO) nanosheets have become a promising antibacterial nanomaterial for use in various applications. This study focuses on the effect of GO nanosheets on the development of Streptococcus mutans biofilms. It is found that GO nanosheets are highly effective at inhibiting the formation of bacterial biofilms at concentrations ranging from low to high in early development stages. After GO treatment, the ratio

of living cells in the biofilm decreases significantly, and the biofilm structure is destroyed. In contrast, GO has a minimal effect on mature biofilms.

Particle & Particle Systems Characterization, 2017, **34**(5): 1700001

EDXRF and XAFS Analysis on the White Porcelains of Ding Kiln of Successive Dynasties

Zhang Maolin Wang Lihua Li Qijiang Wu Junming

Key words Ding Kiln, EDXRF, XAFS, Firing technique

Among the five famous kilns of the Song Dynasty, Ding kiln is the only one famous for white porcelain production, whose superb technique processes such as engraved designs and original upside down firing, had a profound influence on many kilns home and abroad. Nondestructive Energy Dispersive X-Ray Fluorescence (EDXRF) analysis method was applied to analyze the chemical composition and the recipe of the Ding white porcelain from the Tang Dynasty (618-907A.D.) to the Jin Dynasty (1115-1234A.D.). The valence state of Fe in the glaze of Ding white porcelains was analyzed with X-Ray Absorption Fine Structure (XAFS) for the first time while discussing the firing technique. It was found that the bodies of Ding white porcelains were characterized as “high alumina and low silicon” of typical northern porcelains, and raw mineral materials rich in CaO was intentionally added to the bodies' recipe in order to promote the sintering of the body. TiO_2 in the bodies was generally introduced by impurity of kaoline. The glazes of Ding white porcelains were characterized as “high calcium and high magnesium”, which generally belonged to Calcium magnesium glaze or Calcium magnesium alkaline glaze. Its recipe should contained a certain content of dolomite or talc. The increasing content of K2O in the glazes reflected the transition from Calcium magnesium glaze to Calcium magnesium alkaline glaze. In addition, wood ash and kaoline should be added to the recipe of glazes according to the chemical composition characteristics of Al_2O_3, MnO and P_2O_5. The XAFS results showed that the Fe^{3+} proportion in the Ding white glaze of the Late Tang Dynasty and the Five Dynasties was the highest, while that of the Jin Dynasty taked the second place, followed by that of the Song Dynasty. So it implied that Ding white porcelains of successive dynasties were fired in a reducing atmosphere. The yellowish colour of Ding white porcelain in the Song and Jin Dynasties was probably caused by Fe-S compound produced in the firing process by the interaction of glaze and sulfur enriched in the fuel coal.

Spectroscopy and Spectral Analysis, 2017, **37**(5): 1542

Yolk-shell nanostructured Fe_3O_4@C magnetic nanoparticles with enhanced peroxidase-like activity for label-free colorimetric detection of H_2O_2 and glucose

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Song Shiping Zuo Xiaolei Wang Lihua

Key Words Catalytic-Activity, Enzyme, Design, Copper(Ⅱ), Sensor, Adenosine, Chemistry, Growth

Herein, we have developed a simple and facile method to synthesize yolk–shell nanostructured Fe_3O_4@C nanoparticles (NPs) as a multifunctional biosensing platform for the label-free colorimetric detection of H_2O_2 and glucose. It was demonstrated that Fe_3O_4@C yolk–shell nanostructures (YSNs) retained the magnetic properties that can be used for separation and concentration. Also importantly, the Fe_3O_4@C YSNs exhibited an intrinsic peroxidase-like activity that could quickly catalyze the enzyme substrate in the presence of H_2O_2 and produce a blue color. Compared to other similar ferric oxide-based NPs with different structures, Fe_3O_4@C YSNs exhibited greatly enhanced catalytic activities due to their unique structural features. Moreover, steady-state kinetics indicated the catalytic behaviors in agreement with the classic Michaelis–Menten models. Taking advantage of the high catalytic activity, Fe_3O_4@C YSNs were employed as novel peroxidase mimetics for label-free, rapid, sensitive, and specific colorimetric sensing of H_2O_2 and glucose, suggesting that Fe_3O_4@C YSNs have the potential for construction of portable sensors in the application of point-of-care (POC) diagnosis and on-site tests.

Nanoscale, 2017, **9**(13): 4508

Discrimination of foodborne pathogenic bacteria using synchrotron FTIR microspectroscopy

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Hu Jun Lu JunHong

Key words Synchrotron FTIR microspectroscopy, Foodborne pathogens, Bacterial discrimination, Subdivided spectral regions, Multivariate statistical analysis

Traditional Fourier transform infrared (FTIR) spectroscopy has been recognized as a valuable method to characterize and classify kinds of microorganisms. In this study, combined with multivariate statistical analysis, synchrotron radiation-based FTIR (SR-FTIR) microspectroscopy

was applied to identify and discriminate ten foodborne bacterial strains. Our results show that the whole spectra (3000–900 cm^{-1}) and three subdivided spectral regions (3000–2800, 1800–1500 and 1200–900 cm^{-1}, representing lipids, proteins and polysaccharides, respectively) can be used to type bacteria. Either the whole spectra or the three subdivided spectra are good for discriminating the bacteria at levels of species and subspecies, but the whole spectra should be given preference at the genus level. The findings demonstrate that SR-FTIR microspectroscopy is a powerful tool to identify and classify foodborne pathogenic bacteria at the genus, species and subspecies level.

Nuclear Science and Techniques, 2017, **28**(4): 49

The effect of aluminum ion on the aggregation of human islet amyloid polypeptide (11-28)

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Zhang Gongjun Zhou Xingfei Li Bin

Key words metal ion, hIAPP peptides, atomic force microscopy, Thioflavin T fluorescence, X-ray photoelectron spectroscopy

Metal ions play a critical role in human islet amyloid polypeptide (hIAPP) aggregation, which is believed to be closely associated with β-cell death in type II diabetes. In this work, the effect of Al3+ on the aggregation of hIAPP (11-28) was studied by several different experimental approaches. Atomic force microscopy measurements showed that Al^{3+} could remarkably inhibit hIAPP(11-28) fibrillogenesis, while Zn^{2+} had a slight promotion effect on peptide aggregation, which was also confirmed by Thioflavin T fluorescence observation. Furthermore, X-ray photoelectron spectroscopy measurement indicated that Al ions might form chemical bonds with neighboring atoms and destroy the secondary structures of the protein. Our studies could deepen the understanding of the role of metal ions in the aggregation of amyloid peptides.

Acta Biochimica et Biophysica Sinica, 2017, **49**(4): 355

Construction of DNA-based logic gates on nanostructured microelectrodes

Wei Tao Li Min Zhang YueYue Aldalbahi Ali Wang
LiHua Zuo XiaoLei Zhao Yun

Key words Logic gates, Microelectrode, Bio-computing, Electrochemical, Nanostructured electrode

Electrochemical logical operations utilizing biological molecules (protein or DNA), which can be used in disease diagnostics and bio-computing, have attracted great research interest. However, the existing logic operations, being realized on macroscopic electrode, are not suitable for implantable logic devices. Here, we demonstrate DNA-based logic gates with electrochemical signal as output combined with gold flower microelectrodes. The designed logic gates are of fast response, enzyme-free, and micrometer scale. They perform well in either pure solution or complex matrices, such as fetal bovine serum, suggesting great potential for in vivo applications.

Nuclear Science and Techniques, 2017, **28**(3): 35

Multicolor Gold–Silver Nano-Mushrooms as Ready-to-Use SERS Probes for Ultrasensitive and Multiplex DNA/miRNA Detection

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Zhao Zhihan Dou Yanzhi Peng Tianhuan Shi Jiye
Mathur Sanjay Fan Chunhai Song Shiping

Key words Enhanced Raman-Scattering, Plasmonic Nanoparticles, Signal Amplification, Optical-Properties, Interior Nanogap, Nanostructures, Dna, Sensor, Tags, Nanomaterials

Uniform silver-containing metal nanostructures with strong and stable surface-enhanced Raman scattering (SERS) signals hold great promise for developing ultrasensitive probes for biodetection. Nevertheless, the direct synthesis of such ready-to-use nanoprobes remains extremely challenging. Herein we report a DNA-mediated gold–silver nanomushroom with interior nanogaps directly synthesized and used for multiplex and simultaneous SERS detection of various DNA and RNA targets. The DNA involved in the nanostructures can act as not only gap DNA (mediated DNA) but also probe DNA (hybridized DNA), and DNA's involvement enables the nanostructures to have the inherent ability to recognize DNA and RNA targets. Importantly, we were the first to establish a new method for the generation of multicolor SERS probes using two different strategies. First Raman-labeled alkanethiol probe DNA was assembled on gold nanoparticles, and second, thiol-containing Raman reporters were coassembled with the probe DNA. The ready-to-use probes also give great potential to develop ultrasensitive detection methods for various biological molecules.

Analytical Chemistry, 2017, **89**(4): 2531

Clamped Hybridization Chain Reactions for the Self-Assembly of Patterned DNA Hydrogels

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Wang Lianhui Huang Wei Willner Itamar Fan Chunhai

Key words DNA hydrogels, DNA nanotechnology, nucleic acid hybridization, self-assembly, sol-gel process

DNA hydrogels hold great potential for biological and biomedical applications owing to their programmable nature and macroscopic sizes. However, most previous studies involve spontaneous and homogenous gelation procedures in solution, which often lack precise control. A clamped hybridization chain reaction (C-HCR)-based strategy has been developed to guide DNA self-assembly to form macroscopic hydrogels. Analogous to catalysts in chemical synthesis or seeds in crystal growth, we introduced DNA initiators to induce the gelation process, including crosslinked self-assembly and clamped hybridization in three dimensions with spatial and temporal control. The formed hydrogels show superior mechanical properties. The use of printed, surface-confined DNA initiators was also demonstrated for fabricating 2D hydrogel patterns without relying on external confinements. This simple method can be used to construct DNA hydrogels with defined geometry, composition, and order for various bioapplications.

Angewandte Chemie-International, 2017, **56**(8): 2171

An Exonuclease III-Powered, On-Particle Stochastic DNA Walker

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Chao Jie Liu Huajie Zuo Xiaolei Wang Lihua Shi Jiye
Wang Lianhui Huang Wei Pei Hao Fan Chunhai

Key words Brownian motions, DNA nanotechnology, enzymes, molecular machines, nanoparticles

DNA-based machines have attracted rapidly growing interest owing to their potential in drug delivery, biocomputing, and diagnostic applications. Herein, we report a type of exonuclease III (Exo III)-powered stochastic DNA walker that can autonomously move on a spherical nucleic acid (SNA)-based 3D track. The motion is propelled by unidirectional Exo III digestion of hybridized DNA tracks in a burnt-bridge mechanism. The operation of this Exo III-propelled DNA walker was monitored in real time and at the single-particle resolution using total internal reflection

fluorescence microscopy (TIRF). We further interrogated the morphological effect of the 3D track on the nuclease activity, which suggested that the performance of the DNA walker was critically dependent upon the DNA density and the track conformation. Finally, we demonstrated potential bioanalytical applications of this SNA-based stochastic DNA walker by exploiting movement-triggered cascade signal amplification.

Angewandte Chemie-International, 2017, **56**(7): 1588

Catalysis-Driven Self-Thermophoresis of Janus Plasmonic Nanomotors

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Hu Xiaocai Wang Kun Shi Jiye
Li Di Ren Jicun Fan Chunhai

Key words Janus nanoparticles, nanomotors, plasmons, thermophoresis

It is highly demanding to design active nanomotors that can move in response to specific signals with controllable rate and direction. A catalysis-driven nanomotor was constructed by designing catalytically and plasmonically active Janus gold nanoparticles (Au NPs), which generate an asymmetric temperature gradient of local solvent surrounding NPs in catalytic reactions. The self-thermophoresis behavior of the Janus nanomotor is monitored from its inherent plasmonic response. The diffusion coefficient of the self-thermophoresis motion is linearly dependent on chemical reaction rate, as described by a stochastic model.

Angewandte Chemie-International, 2017, **56**(2): 515

Nanoplasmonic Biological Sensing and Imaging

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Li Di Fan Chunhai

Key words nanophotonics, noble metal nanomaterial, localized surface plasmon resonance (LSPR), sensing, bioimaging

The localized surface plasmon resonance of metal nanoparticles is the collective oscillation of electrons on particle surface. The localized electromagnetic interaction brings a series of novel functions and applications. Plasmonic nanomaterials have been the significant part of nanophotonics, since its' localized surface plasmon resonance (LSPR) can focus incident phonons on the nanoscale surface. The unique plasmonic property is highly sensitive to their size, shape,

coupling between particles as well as local dielectric environment. These properties can be utilized for the development of new biosensing and bioimaging applications. To date, many LSPR sensing strategies have been developed with outstanding measurement capabilities, enabling detection down to the single-molecule level, including LSPR-based sensing, surface-enhanced Raman scattering, metal-enhanced fluorescence, dark-field light-scattering, metal-mediated fluorescence resonance energy transfer. Moreover, the unique optical stability of plasmonic nanoparticles enables them as ideal probes in cellular imaging. Here, recent examples on application of plasmonic nanostructures in sensing and bioimaging are summarized, and perspectives are provided as well.

Acta Chimica Sinica, 2017, **75**(11): 1036

Self-Assembly of Amyloid-Like Peptides at Interfaces Investigated by Atomic Force Microscopy

Lei Haozhi Zhang Xueqiang Hu Jun Zhang Yi

Key words Peptide, Self-Assembly, AFM, Interface

In the past few years, numerous researches have focused on the self-assembly of amyloid peptides and proteins. Especially, the self-assembly of peptides and proteins at interfaces has attracted much attention, on account of the potential applications as well as understanding mechanism of some neurodegenerative diseases. In this review, we centered topic on recent progress of the self-assembly of amyloid-like peptides at interfaces, which was mainly carried out in our group by employing atomic force microscopy (AFM). In the first part of the review, we introduced how the amyloid peptides assembled at the solid substrate/water interface. And nanoscale control of the assembly of the peptides by AFM has also been introduced. In the second part of this review, we focused on how the amyloid-like peptides assembled at air/solid interface, in which diffusion and self-assembly of peptides occurred with the help of a water nanofilm confined from ambient environment onto the solid surface. These results indicate that interfaces play an important role in peptide assembly, and also prove that AFM is one of the powerful instruments in studying peptide self-assembly.

Science of Advanced Materials, 2017, **9**(1): 65

DNA Nanostructure-Based Engineering of the Biosensing Interface for Biomolecular Detection

Ye Dekai Zuo Xiaolei Fan Chunhai

Key words biosensing, interfacial engineering, DNA nanostructure, electrochemical, cell imaging

The biosensing technology plays an important role in environmental monitoring, safety control and medical diagnosis. Precise control of the interaction between bio-recognition probe and the interface is critical to improve the sensitivity, specificity and selectivity of biosensors. In a typical bioprobe immobilization, the heterogeneity of self-assembled monolayers on the surface increases the binding energy barrier and decreases the recognition efficiency and rate. We found that DNA nanostructures, such as tetrahedral DNA nanostructures (TDNs), could increase the homogeneity of self-assembled monolayers via enthalpy-entropy compensation, which enables precise regulation of interfacial property at the nanoscale. By regulating the intermolecular distance of bioprobes, the hybridization efficiency and hybridization rate of DNA probes can be improved significantly. The detection limit of DNA and microRNA can be pushed down to 10 aM limit. The detection limit of antigen detection can be improved to 100 pM and the detection limit of small molecule (cocaine) can be pushed to 33 nM. By using TDNs, we developed a universal detection platform for nucleic acids, proteins, small molecules and cells with superior detection sensitivity. To further use TDN probes in cells and in vivo, we explored the transport pathways of TDNs into the cell and directed their targeting location to specific organelles. We aim to develop DNA nanostructure-based bioprobes for intracellular and in-vivo imaging.

Progress in Chemistry, 2017, **29**(1): 36

BIOSENSING CRISPR-powered diagnostics

Zuo Xiaolei Fan Chunhai Chen HongYuan

A CRISPR-associated nuclease that can promiscuously cleave RNAs enables a rapid and cheap test for the single-molecule detection and single-base discrimination of nucleic acids.

Nature Biomedical Engineering, 2017, **1**(6): 0091

Nanodiamonds Interfere with Wnt-Regulated Cell Migration and Adipocyte Differentiation in Cells and Embryonic Development In Vivo

Yi Hongyang Li Xiaojiao Wang Zhuyao Yin Min Wang Lihua Aldalbahi Ali El-Sayed Nahed Nasse Wang Hui Chen Nan Chen Luonan Fan Chunhai Song Haiyun

Key words cancer cell migration, embryonic development, nanodiamonds, obesity, signal transduction

Biocompatible nanoparticles hold a great promise for biomedical applications, whereas their biosafety has raised extensive concerns. Nanodiamonds (NDs) are generally regarded as “inert” nanocarriers and widely employed in biomedical studies; however, it is yet to explore their biological effects in more general contexts. In this study, the authors observe that intracellular NDs block signal transduction of the Wnt signaling pathway, an effect that is not caused by general cytotoxicity. The authors find that NDs attenuate activities of Wnt signaling in several types of cell lines and in Zebrafish, and interfere with Wnt signaling-controlled biological processes, including cancer cell migration, adipocyte differentiation, and embryonic development. Significantly, the authors show that intracellular NDs trigger degradation of the disheveled protein, a key component of Wnt signaling cascade, while they do not affect protein stability of other Wnt signal transducers or other signaling molecules. This work thus illustrates a novel crosstalk between nanoparticles and the Wnt signaling pathway, and expands the understanding of biological effects induced by nanoparticles. In addition, given the clinical implications of Wnt signaling in tumorigenesis and cancer metastasis, this study also provides the rationale for potential applications of NDs in cancer therapies.

Particle & Particle Systems Characterization, 2017, **34**(1): 1600208

Programming Cell Adhesion for On-Chip Sequential Boolean Logic Functions

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Key Words Strand Displacement Cascades, Dna Nanostructures, Computation, Microenvironments, Amplification, Monolayers, Delivery, Robots, Array, Ecm

Programmable remodelling of cell surfaces enables high-precision regulation of cell behavior. In this work, we developed in vitro constructed DNA-based chemical reaction networks (CRNs) to program on-chip cell adhesion. We found that the RGD-functionalized DNA CRNs are entirely noninvasive when interfaced with the fluidic mosaic membrane of living cells. DNA toehold with different lengths could tunably alter the release kinetics of cells, which shows rapid release in minutes with the use of a 6-base toehold. We further demonstrated the realization of Boolean logic functions by using DNA strand displacement reactions, which include multi-input and sequential cell logic gates (AND, OR, XOR, and AND-OR). This study provides a highly generic tool for self-organization of biological systems.

Journal of The American Chemical, 2017, **139**(30): 10176

Expression and radiolabeling of Cas9 protein

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Key words Cas9, Radiolabeling , ^{125}I labeling yield, Stability

As a robust platform for genome editing, CRISPR/Cas9 is currently being explored for engineering biology or therapeutics, yet means for quantitative detection of Cas9 proteins remain to be fully realized. Here, we expressed Cas9 proteins and developed a novel detection method that traced Cas9 based on radiolabeled iodine. Through optimizing the reaction conditions of reaction time, temperature and cycles, we obtained ^{125}I-Cas9 of high labeling yield. The prepared ^{125}I-Cas9 was stable in various media and preserved excellent genome editing efficiency. Thus, our strategy provides a convenient and efficient tool for further tracing biological behaviors of Cas9 proteins in living systems.

Nuclear Science and Techniques, 2017, **28**(1): 11

Silicone oil promotes amyloid-like aggregation of αB-crystallin

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Key words Retinal-Detachment Surgery, Proliferative Vitreoretinopathy, Protein Aggregation, Cataract Formation, Nuclear Cataract, Liquid Silicone, Lens, Complications, Injection, Eyes

Silicone oil is a chemically inert and biocompatible material. However, the use of silicone oil as an adjunct for internal tamponade in the treatment of retinal detachment is accompanied by the sequelae of cataract, the molecular mechanism of which has been a mystery for scientists. In this study, we focused on the influence of silicone oil on the aggregating behaviors of one of the important proteins in the eyes, αB-crystallin (CRYAB). We found that silicone oil could promote the amyloid-like aggregation of CRYAB, verified using atomic force microscopy (AFM), transmission electron microscopy (TEM), laser granularity and number analysis (Nanosight), and turbidity measurements. Furthermore, fluorescent experiments using Thioflavin T (ThT), Congo red, and 1-anilinonaphthalene-8-sulfonic acid (ANS) suggested formation of a β-sheet structure in CRYAB in the presence of silicone oil, which was also confirmed by far-UV circular dichroism (CD) spectroscopy. These findings provide a direct evidence of the changes in the secondary structures of CRYAB protein and amyloid aggregation behavior upon adding silicone oil in the solution, and could be helpful for understanding the molecular mechanisms of the cataract formed in silicone oil-filled eyes.

RSC Advances, 2017, **7**(10): 6000

Autophagy and lysosomal dysfunction: A new insight into mechanism of synergistic pulmonary toxicity of carbon black-metal ions co-exposure

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Key Words Particulate Matter, Air-Pollution, Oxidative Stress, Ultrafine Particles, Cellular Toxicity, Fine, Nanoparticles, Cytotoxicity, Exposure, Coarse

Fine particulate matter (PM 2.5) is the principal instigators of adverse health events, yet gaps still remain in understanding the mechanism mediating its toxic response. Similar to nanoparticles, PM 2.5, with large surface area to volume ratio, can absorb multipollutants in air, displaying toxicity profiles that are very different from those of coarse particles of the same composition. One particularly relevant interaction is that of PM 2.5 and the anthropogenic metals. In this study, we used carbon black nanoparticle (CBs) and metal ions as model materials to investigate the synergistic pulmonary toxicity and its mechanism. We demonstrated that excessive metal contaminants adsorbed on CBs contributed to the observed toxic effects both in vitro and in

C57BL6 mice intratracheal instillation model. Significantly, we found that autophagy and lysosomal dysfunction accounted for the synergistic pulmonary toxic effect of co-exposure to CBs and metals. Our findings provide a new insight into understanding the toxicological and healthy effects of fine particles, which have potential to aid in mitigating their adverse health effect.

Carbon, 2017, **111**: 322

pH and thermal-dependent ultrafiltration membranes prepared from poly (methacrylic acid) grafted onto polyethersulfone synthesized by simultaneous irradiation in homogenous phase

Fan Kai Huang Jianxi Yang Haijun Lu Runsan
Sun Xueqing Hu Jun Hou Zhengchi

Key words Membrane, Polyethersulfone, Graft polymerization, gamma-ray irradiation, PH- and thermal-dependent

Polyethersulfone (PES) and monomer methacrylic acid (MAA) were chosen to synthesize the grafted polymer PES-g-PMAA by simultaneous γ-ray irradiation in homogenous phase. Membranes prepared from pristine PES and PES-g-PMAA with different degrees of grafting (DGs), have been obtained. The kinetics of grafting reaction and the DG values were studied through sulphur elemental analysis. The morphology study of the membranes showed formation of sponge-like structure in the sub-layer of membrane, along with grafting PMAA onto the PES chains. By ultrafiltration experiments, a regular pH-dependent permeability and thermal-dependent permeability of PES-g-PMAA membranes was demonstrated through introduction of PMAA onto the PES which reduced the water flux of the membranes. The pH-dependent permeability could be attributed to pH-sensitive reconfiguration of PMAA molecule chains on the surface of membrane pore, while thermal-dependent permeability might be caused by better thermal-sensibility of PMAA chains inside the membrane.

Journal of Membrane Science, 2017, **543**: 335

An infrared spectroscopy study of PES PVP blend and PES-g-PVP copolymer

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Hou Zhengchi Wu Minghong

Key words FTIR, Graft copolymerization, Poly(ether sulfone), N-vinyl pyrrolidone, Blue-shift

Systematic study of FTIR spectra was carried out on the PES/PVP blends and PES-g-PVP copolymers. In the blends, no shift of carbonyl group absorbance was observed. In the copolymers, there was an occurrence of blue-shift that increases with the grafting degree, which can be used as a compelling evidence of PVP being grafted onto PES. This phenomenon was interpreted from the stereo-hindrance effect. Besides, as the intensity of carbonyl group absorbance increased proportionally with the degree of grafting obtained by elementary analysis, FTIR, a simple and easy tool, became feasible for the quantitative determination of PVP content in the graft copolymers. Calibration curves with high correlation coefficient were established from which the quantitative relationship between the intensity of carbonyl group absorbance normalized by a chosen internal reference and the grafting degree can be obtained.

Polymer Testing, 2017, **59**: 212

Magic compositions in Pd-Au nanoalloys

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Legrand Bernard Mottet Christine

Key words Monte Carlo simulations, Metallic alloy nanoparticles, Surface segregation, Chemical ordering

We identified new magic compositions of Pd-Au nanolloys of simple symmetries according to the icosahedral and the cubic truncated octahedral structures. Chemically ordered structures as well as segregated ones are characterized using Monte Carlo simulations in semi-grand canonical ensemble and tight-binding semi-empirical potential fitted to ab initio calculations for the Pd-Au system. Ordering and surface (or core) segregation phenomena can be distinguished by their behavior as a function of the temperature: chemical ordering at surface or in the core disappears above a critical temperature (which is lower or equal to the bulk alloy order-disorder temperature), whereas surface/core segregation (core-shell structures) remains at high temperature, although the interfacial profile is less abrupt.

Computational and Theoretical Chemistry, 2017, **1107**(S1): 49

S-shaped velocity deformation induced by ionic hydration in aqueous salt solution flow

Fan Wen Chen Jige Lei Xiaoling Fang Haiping

Key Words Molecular-Dynamics Simulation, Frequency Raman-Scattering, Initio Qm/Mm Dynamics, Liquid Water, Electrolyte-Solutions, Dielectric-Relaxation, Nacl Solutions, Solvation, Mobility, Chloride

Ionic hydration shells are the most noticeable microscopic feature in an aqueous salt solution, and have attracted attention due to their possible contribution to its flow behavior. In this paper, we find by molecular dynamic simulations that an S-shaped velocity profile is induced by the ionic hydration shells in the nano channel flow. Our theoretical analysis implies a linear relationship between the energy density inside the first hydration shell of the ions and the deformation strength of the velocity profiles of aqueous salt solutions, where the deformation strength is quantified by the curvature length defined by the linear deviation extended from the velocity profile. Our simulation results confirm that such a linear relationship holds for chloride salt solutions with monatomic cations, e.g., K, Na, Ca, Mg, Al and the Na/Ca models by varying the valence number of Na and Ca in the salt solutions. Furthermore, the influence of the flow velocity and the channel width upon the velocity deformation strength are also investigated. Our results indicate that the calculated curvature length provides a numerical evaluation for nano flow behavior and would be helpful in nanofluidic device design.

Physical Chemistry Chemical Physics, 2017, **19**(44): 30055

Reply to 'On the bonding in ligand-protected gold clusters'

Xu Wen Wu Zeng Xiao Cheng Gao Yi

Key Words Molecules, Motifs, Block

Nature Communications, 2017, **8**: 1351

Graphene Oxide Facilitates Solvent-Free Synthesis of Well-Dispersed, Faceted Zeolite Crystals

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Key words faceted crystals, graphene oxide, oriented growth, solvent-free synthesis, zeolites

Zeolites with molecular dimension pores are widely used in petrochemical and fine-chemical industries. While traditional solvothermal syntheses suffer from environmental, safety, and efficiency issues, the newly developed solvent-free synthesis is limited by zeolite crystal aggregation. Herein, we report well-dispersed and faceted silicalite ZSM-5 zeolite crystals obtained using a solvent-free synthesis facilitated by graphene oxide (GO). The selective interactions between the GO sheets and different facets, which are confirmed by molecular dynamics simulations, result in oriented growth of the ZSM-5 crystals along the c-axis. More importantly, the incorporation of GO sheets into the ZSM-5 crystals leads to the formation of mesopores. Consequently, the faceted ZSM-5 crystals exhibit hierarchical pore structures. This synthetic method is superior to conventional approaches because of the features of the ZSM-5 zeolite.

Angewandte Chemie-International, 2017, **56**(45): 14090

Ultra-Broadband THz Antireflective Coating with Polymer Composites

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Zhao Hongwei　Sugihara Okihiro

Key words COP-TiO_2 composite; epoxy-TiO_2 composite; antireflection; THz; ultra-broadband; graded refractive index

Achieving an ultra-broadband range is an essential development direction in terahertz techniques; however, a method to cover the full terahertz band by using a highly efficient antireflection (AR) coating that could greatly increase the efficiency of terahertz radiation is still lacking. It is known that structures possessing a graded-index profile can offer a broadband AR effect, and such structures have been widely used, especially in the visible range. In this paper, first, we tuned the refractive index of a cyclo-olefin polymer (COP) by using a TiO_2 dopant, and a polymer–TiO_2 composite with a refractive index of 3.1 was achieved. We then fabricated a surface-relief structure with a graded-index profile by using a hot-embossing method. The structure on the silicon substrate can provide an excellent AR effect, but the working band is still limited by its scale of sag and swell. To obtain an ultra-broadband AR effect, we then proposed a flat six-layer structure; a graded-index profile was obtained by casting epoxy–TiO_2 composites in the order of a high index to lower indices. With a very well controlled refractive index and thickness of each layer, we achieved an AR effect of <2% in the ultra-broadband of 0.2–20 THz.

Polymers, 2017, **9**(11): 574

Ion sieving in graphene oxide membranes via cationic control of interlayer spacing

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Li Deyuan Qian Zhe Xu Gang Liu Gongping
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Key Words Carbon Nanotubes, Layered Graphene, Porous Graphene, Transport, Separation, Mechanism, Ultrathin, Future

Graphene oxide membranes-partially oxidized, stacked sheets of graphene-can provide ultrathin, high-flux and energy-efficient membranes for precise ionic and molecular sieving in aqueous solution. These materials have shown potential in a variety of applications, including water desalination and purification, gas and ion separation, biosensors, proton conductors, lithium-based batteries and super-capacitors. Unlike the pores of carbon nanotube membranes, which have fixed sizes, the pores of graphene oxide membranes-that is, the interlayer spacing between graphene oxide sheets (a sheet is a single flake inside the membrane)-are of variable size. Furthermore, it is difficult to reduce the interlayer spacing sufficiently to exclude small ions and to maintain this spacing against the tendency of graphene oxide membranes to swell when immersed in aqueous solution. These challenges hinder the potential ion filtration applications of graphene oxide membranes. Here we demonstrate cationic control of the interlayer spacing of graphene oxide membranes with ångström precision using K^+, Na^+, Ca^{2+}, Li^+ or Mg^{2+} ions. Moreover, membrane spacings controlled by one type of cation can efficiently and selectively exclude other cations that have larger hydrated volumes. First-principles calculations and ultraviolet absorption spectroscopy reveal that the location of the most stable cation adsorption is where oxide groups and aromatic rings coexist. Previous density functional theory computations show that other cations (Fe^{2+}, Co^{2+}, Cu^{2+}, Cd^{2+}, Cr^{2+} and Pb^{2+}) should have a much stronger cation-pi interaction with the graphene sheet than Na+ has, suggesting that other ions could be used to produce a wider range of interlayer spacings.

Nature, 2017, **550**(7676): 415

Preparation of graphene oxides with different sheet sizes by temperature control

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Shi, Guo-Sheng Xu, Gang Fang, Hai-Ping Wu, Ming-Hong

Key words graphene oxide, sheet size, temperature control, degree of oxidation

The sheet size of a graphene oxide (GO) can greatly influence its electrical, optical, mechanical, electrochemical and catalytic property. It is a key challenge to how to control the sheet size during its preparation in different application fields. According to our previous theoretical calculations of the effect of temperature on the oxidation process of graphene, we use Hummers method to prepare GOs with different sheet sizes by simply controlling the temperature condition in the process of the oxidation reaction of potassium permanganate ($KMnO_4$) with graphene and the dilution process with deionized water. The results detected by transmission electron microscopy (TEM) and atomic force microscopy (AFM) show that the average sizes of GO sheets prepared at different temperatures are about 1 μm and 7 μm respectively. The ultraviolet–visible spectroscopy (UV-vis) shows that lower temperature can lead to smaller oxidation degrees of GO and less oxygen functional groups on the surface. In addition, we prepare GO membranes to test their mechanical strengths by ultrasonic waves, and we find that the strengths of the GO membranes prepared under low temperatures are considerably higher than those prepared under high temperatures, showing the high mechanical strengths of larger GO sheets. Our experimental results testify our previous theoretical calculations. Compared with the traditional centrifugal separation and chemical cutting method, the preparation process of GO by temperature control is simple and low-cost and also enables large-size synthesis. These findings develop a new method to control GO sheet sizes for large-scale potential applications.

Chinese Physics B, 2017, **26**(10): 106101

Dynamic Cooperation of Hydrogen Binding and Π Stacking in ssDNA Adsorption on Graphene Oxide

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Song Bo Fang Haiping

Key words graphene oxide, hydrogen bonds, molecular simulation, ssDNA, π-π stacking interaction.

Functional nanoscale structures consisting of a DNA molecule coupled to graphene or graphene oxide (GO) have great potential for applications in biosensors, biomedicine,

nanotechnology, and materials science. Extensive studies using the most sophisticated experimental techniques and theoretical methods have still not clarified the dynamic process of single-stranded DNA (ssDNA) adsorbed on GO surfaces. Based on a molecular dynamics simulation, this work shows that an ssDNA segment could be stably adsorbed on a GO surface through hydrogen bonding and π-π stacking interactions, with preferential binding to the oxidized rather than to the unoxidized region of the GO surface. The adsorption process shows a dynamic cooperation adsorption behavior; the ssDNA segment first captures the oxidized groups of the GO surface by hydrogen bonding interaction, and then the configuration relaxes to maximize the π-π stacking interactions between the aromatic rings of the nucleobases and those of the GO surface. We attributed this behavior to the faster forming hydrogen bonding interaction compared to π-π stacking; the π-π stacking interaction needs more relaxation time to regulate the configuration of the ssDNA segment to fit the aromatic rings on the GO surface.

Chemistry-A European Journal, 2017, **23**(53): 13100

Inert Gas Deactivates Protein Activity by Aggregation

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Wang Xingya Zhang Meng Gao Yi Hu Jun
Zhang Xuehua Lu Junhong Li Guohui
Tai Renzhong Fang Haiping

Key Words Der-Waals Complexes, Xenon, Binding, Xe, Myoglobin, Pathways, Nitrogen, Cavity, Kr, Ionization

Biologically inert gases play important roles in the biological functionality of proteins. However, researchers lack a full understanding of the effects of these gases since they are very chemically stable only weakly absorbed by biological tissues. By combining X-ray fluorescence, particle sizing and molecular dynamics (MD) simulations, this work shows that the aggregation of these inert gases near the hydrophobic active cavity of pepsin should lead to protein deactivation. Micro X-ray fluorescence spectra show that a pepsin solution can contain a high concentration of Xe or Kr after gassing, and that the gas concentrations decrease quickly with degassing time. Biological activity experiments indicate a reversible deactivation of the protein during this gassing and degassing. Meanwhile, the nanoparticle size measurements reveal a higher number of “nanoparticles” in gas-containing pepsin solution, also supporting the possible interaction between inert gases and the protein. Further, MD simulations indicate that gas molecules can aggregate into a tiny bubble shape near the hydrophobic active cavity of pepsin, suggesting a mechanism for reducing their biological function.

Scientific Reports, 2017, **7**: 10176

Catalytic role of vacancy diffusion in ceria supported atomic gold catalyst

Han ZhongKang Wang YangGang Gao Yi

Key Words Gas Shift Reaction, Co Oxidation, Active Oxygen, Au/Tio2, States, Au, Activation, Stability, Hydrogen, Surface

Dynamics of intrinsic defects are considered fundamental in the chemistry of reducible oxides, and their effect on catalytic reactions have been rarely reported. Herein, we propose a new O_v diffusion assisted Langmuir-Hinshelwood mechanism for CO oxidation, which may largely account for the origin of high reactivity of supported atomic gold catalysts.

Chemical Communications, 2017, **53**(65): 9125

Defect-Induced Wetting Behavior on Solid Polar Surfaces with Small Charge Dipole Length

Qiu Yifei Liu Yang Tu Yusong
Wang Chunlei Xu Yousheng

Key Words Water Channel, Molecular-Structure, Room-Temperature, Contact-Angle, Ordered Water, Proteins, Hydrophobicity, Simulation, Interfaces, Nanotubes

Previous work showed that solid polar surfaces with a very small dipole length still might be quite hydrophobic even with large values of charge. Using molecular dynamics simulations, we have found that the presence of the point defects on a solid polar surface greatly influences the wetting behavior of water, even at a very low defect ratio of 1%. As the defect ratio increases, the coverage of the water layer over the solid surface also increases. Because of the breakdown of steric exclusion, the water molecules strongly bind to the solid surface mainly through electrostatic interactions between their hydrogen atoms and the negative charges near the positive-vacancy defects on the surface, or between their oxygen atoms and the positive charges near the negative-vacancy defects.

Journal of Physical Chemistry C, 2017, **121**(32): 17365

$Ti_{12}Xe$: A twelve-coordinated Xe-containing molecule

Miao Junjian Xu Wenwu Zhu Beien Gao Yi

Key words Xenon, Coordination number, Density functional theory, Xenon-titanium cluster complex, Chemical bonding

A twelve-coordinated Xe-containing molecule $Ti_{12}Xe$ has been predicted by DFT calculations with quasi-icosahedral symmetry. Structural and NBO analyses show the chemical bonding exists between the central Xe atom and peripheral Ti atoms, which leads to the high stability of the molecule to a considerable degree. First principle molecular dynamics simulations further reveal the particularly high thermal stability of $Ti_{12}Xe$ up to 1500 K. This unique species may disclose new physics and chemistry of xenon element and stir interest in the Xe-transition metal cluster physics and chemistry.

Physics Letters A, 2017, **381**(29): 2363

$Au_3(\mu_3\text{-}S)(0e)$ elementary block: new insights into ligated gold clusters with μ_3-sulfido motifs

Xu WenWu Zeng XiaoCheng Gao Yi

Key Words Crystal-Structure, Theoretical-Analysis, Structure Evolution, Complexes, Pseudopotentials, Transformation, Nanomolecules, Luminescence, Nanoclusters, Fullerene

An understanding of the structural stability and formation mechanism of ligated gold nanoclusters with triply coordinated μ_3-sulfido (μ_3-S) motifs is important not only for gold chemistry but also for the design of more effective catalysts or drug carriers for various applications. In this article, a new elementary block $Au_3(\mu_3\text{-}S)$ with zero valence electrons [referred to as $Au_3(\mu_3\text{-}S)(0e)$] has been identified, which describes all crystallized ligated gold clusters with μ_3-S motifs, in conjunction with the previously reported $Au_3(2e)$ and $Au_4(2e)$ elementary blocks, in a grand unified model (GUM). This $Au_3(\mu_3\text{-}S)(0e)$ elementary block has a tripod structure with the S atom bonding to three Au atoms in a μ3 bridging mode, and can be considered as a μ_3-S atom balancing out the 2e valence electrons of the $Au_3(2e)$ block. Using $Au_3(\mu_3\text{-}S)$ as a building block, a special group of quasi-fullerene hollow-cage $[Au_{3n}(\mu_3\text{-}S)_{2n}]^{n-}$ gold(I) μ_3-S clusters are designed, which exhibit high stabilities. In addition, a series of theoretical structures are predicted to be increasingly stable after introducing μ_3-S atoms, based on the crystallized clusters. Overall, the

introduction of a $Au_3(\mu_3\text{-}S)(0e)$ elementary block can help with the understanding of diverse structures of ligated gold clusters with μ3-S motifs, thereby assisting the rational design of new forms of gold nanoclusters.

Nanoscale, 2017, **9**(26): 8990

Terahertz Spectra of Ninhydrin and Indane-1,2,3-Trione

Zou Tao Li Shaoping Pan Tingting Zhang Bo Yu Zheng
Li Xindi Zhang Jianbing Zhao Hongwei

Key words Indane-12,3-trione, Ninhydrin, Terahertz, Density functional theory, The vibrational mode

Distinctive terahertz (THz) absorption spectra of ninhydrin and indane-1,2,3-trione ranging from 0.5 to 4.5 THz were observed firstly in our experiment by terahertz time-domain spectroscopy (THz-TDS). The dehydration process of ninhydrin was also monitored online. The experimental results indicate that THz spectroscopy is highly sensitive to the crystal structure, weak intermolecular interactions, and the environmental change. Multitechniques including differential scanning calorimetry (DSC) and powder X-ray diffraction (PXRD) were also carried out to further investigate ninhydrin and indane-1,2,3-trione. And the results support the reliability of THz spectroscopy. Density functional theory (DFT) calculations based on the samples' crystalline structures were performed for better understanding the THz characteristic spectra. The calculations agree with the experimental observation, and the corresponding vibrational modes of ninhydrin and indane-1,2,3-trione are assigned.

Journal of Infrared, Millimeter, and Terahertz Waves, 2017, **38** (7): 896

Formation and Stability of Bulk Nanobubbles Generated by Ethanol-Water Exchange

Qiu Jie Zou Zhenglei Wang Shuo Wang Xingya
Wang Lei Dong Yaming Zhao Hongwei
Zhang Lijuan Hu Jun

Key words dynamic light scattering, exchange interactions, liquids, nanostructures, solvent effects

Bulk nanobubbles have unique properties and find potential applications in many important processes. However, their stability or long lifetime still needs to be understood and has attracted

much attention from researchers. Bulk nanobubbles are generated based on ethanol-water exchange, a method that is generally used in the study of surface nanobubbles. Their formation and stability is further studied by using a new type of dynamic light scattering known as NanoSight. The results show that the concentration of the bulk nanobubbles produced by this method is about five times greater than that in the degassed group, which indicates the existence of bulk gas nanobubbles. The effects of ethanol/water ratios and temperature on the stability of the bulk nanobubbles have also been studied and their numbers reach a maximum at a ratio of about 1: 10 (v/v).

ChemPhysChem, 2017, **18**(10): 1345

Terahertz spectra of L-phenylalanine and its monohydrate

Pan Tingting Li Shaoping Zou Tao Yu Zheng
Zhang Bo Wang Chenyang Zhang Jianbing
He Mingxia Zhao Hongwei

Key words L-Phenylalanine; Monohydrate; Terahertz absorption spectrum; Low-frequency vibration; DFT

The low-frequency vibrational property of l-phenylalanine (L-Phe) and l-phenylalanine monohydrate (L-Phe·H_2O) has been investigated by terahertz time-domain spectroscopy (THz-TDS) at room and low temperature ranging from 0.5 to 4.5 THz. Distinctive THz absorption spectra of the two compounds were observed. Density functional theory (DFT) calculations based on the crystal structures have been performed to simulate the vibrational modes of L-Phe and L-Phe·H_2O and the results agree well with the experimental observations. The study indicates that the characterized features of L-Phe mainly originate from the collective vibration of molecules. And the characterized features of L-Phe·H_2O mainly come from hydrogen bond interactions between L-Phe and water molecules. L-Phe and L-Phe·H_2O were also verified by differential scanning calorimetry and thermogravimetry (DSC-TG) and powder X-ray diffraction (PXRD) examinations.

Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy, 2017, **178**: 19

Au_{13}(8e): A secondary block for describing a special group of liganded gold clusters containing icosahedral Au_{13} motifs

Xu WenWu Zeng XiaoCheng Gao Yi

A grand unified model (GUM) has been proposed recently to understand structure anatomy and evolution of liganded gold clusters. In this work, besides the two types of elementary blocks

(triangular Au_3(2e) and tetrahedral Au_4(2e)), we introduce a secondary block, namely, the icosahedral Au_{13} with 8e valence electrons, noted as Au_{13}(8e). Using this secondary block, structural anatomy and evolution of a special group of liganded gold nanoclusters containing icosahedral Au13 motifs can be conveniently analyzed. In addition, a new ligand-protected cluster $Au_{49}(PR_3)_{10}(SR)_{15}Cl_2$ is predicted to exhibit high chemical and thermal stability, suggesting likelihood of its synthesis in the laboratory.

Chemical Physics Letters, 2017, **675**: 35

Mechanism of degradation of a nitrogenous heterocycle induced by a reductive radical: decomposition of a sym-triazine ring

Lyu Gengxin Shi Guosheng Tang Liang
Fang Haiping Wu Minghong

Cyanuric acid is a major component of many materials and chemicals, and is the most important intermediate in the degradation processes of sym-triazine compounds in the natural environment, as well as being used for water treatment. However, the degradation mechanism of cyanuric acid is still unclear in various advanced oxidation processes (AOPs), where ˙OH is usually regarded as the dominant radical. Here, using a combination of density functional theory calculations and experimental observations, we unexpectedly show that the sym-triazine ring structure is broken efficiently by reductive free radicals – hydrogen radicals (˙H), rather than traditional ˙OH. The energy barrier of cyanuric acid reacting with ˙H to form the $–NH_2$ group and break the sym-triazine ring is only 4.96 kcal mol^{-1}, which is clearly lower than that of cyanuric acid reacting with ˙OH (13.32 kcal mol^{-1}). Our theoretical predictions are further confirmed by γ photon irradiation experiments, which show that when ˙H is present in the reaction, the nitrogen in cyanuric acid (or other nitrogenous compounds including primidone and bezafibrate) rapidly degrades into NH_4^+. In contrast, when ˙H is scavenged, cyanuric acid stops degrading into NH_4^+. Our results provide new insight for understanding the decomposition of nitrogenous materials, and we are the first to shed light on the key role of ˙H in organic transformation processes.

Physical Chemistry Chemical Physics, 2017, **19**(14): 9354

Accelerated evaporation of water on graphene oxide

Wan Rongzheng Shi Guosheng

Using molecular dynamics simulations, we show that the evaporation of nanoscale volumes of water on patterned graphene oxide is faster than that on homogeneous graphene oxide. The evaporation rate of water is insensitive to variation in the oxidation degree of the oxidized regions, so long as the water film is only distributed on the oxidized regions. The evaporation rate drops when the water film spreads onto the unoxidized regions. Further analysis showed that varying the oxidation degree observably changed the interaction between the outmost water molecules and the solid surface, but the total interaction for the outmost water molecules only changed a very limited amount due to the correspondingly regulated water–water interaction when the water film is only distributed on the oxidized regions. When the oxidation degree is too low and some unoxidized regions are also covered by the water film, the thickness of the water film decreases, which extends the lifetime of the hydrogen bonds for the outmost water molecules and lowers the evaporation rate of the water. The insensitivity of water evaporation to the oxidation degree indicates that we only need to control the scale of the unoxidized and oxidized regions for graphene oxide to regulate the evaporation of nanoscale volumes of water.

Physical Chemistry Chemical Physics, 2017,**19**(13): 8843

DNA origami-based shape IDs for single-molecule nanomechanical genotyping

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Liu Ke Cui Chengjun Chen Jianhua Huang Qing Hu Jun
Wang Lianhui Huang Wei Shi Yongyong Fan Chunhai

Variations on DNA sequences profoundly affect how we develop diseases and respond to pathogens and drugs. Atomic force microscopy (AFM) provides a nanomechanical imaging approach for genetic analysis with nanometre resolution. However, unlike fluorescence imaging that has wavelength-specific fluorophores, the lack of shape-specific labels largely hampers widespread applications of AFM imaging. Here we report the development of a set of differentially shaped, highly hybridizable self-assembled DNA origami nanostructures serving as shape IDs for magnified nanomechanical imaging of single-nucleotide polymorphisms. Using these origami shape IDs, we directly genotype single molecules of human genomic DNA with an ultrahigh resolution of ~10 nm and the multiplexing ability. Further, we determine three types of

disease-associated, long-range haplotypes in samples from the Han Chinese population. Single-molecule analysis allows robust haplotyping even for samples with low labelling efficiency. We expect this generic shape ID-based nanomechanical approach to hold great potential in genetic analysis at the single-molecule level.

Nature Communications, 2017, **8**: 14738

Supersonic thermal excitation-induced shock wave in black phosphorene

Chen Jige Chen Shunda Gao Yi

Thermal transport in low-dimensional materials possesses various novel features since anomalous energy carriers may heavily contribute. Black phosphorene exhibits excellent thermal properties and thus it attracts attention about the possible existence of anomalous energy carriers. In this paper, we find that shockwave appears as a dominant energy carrier in the zigzag direction of black phosphorene when a supersonic thermal excitation above a critical strength is exerted. Comparing with the diffusive thermal transport, shockwave carries a considerable amount of excitation energy and propagates faster than the local acoustic speed. It leads to a strong anisotropic enhancement in the transport speed of thermal energy in the zigzag direction, up to a factor of twofold compared with no shockwave. The linear increase of velocity with intensity and exponential decay of intensity with time of the shockwave are observed. Unlike solitary waves, the collision of shockwaves exhibits no phase shift in the spatial-temporal trajectory. Moreover, it shows that shockwave velocity decreases with tensile strain, which is favorable for modulation. Our results reveal a possible anomalous energy transport process and may help in designing black phosphorene-based thermal devices.

Physical Review B, 2017, **95**(13): 134301

Asymmetric nanoparticle may go "active" at room temperature

Sheng Nan Tu YuSong Guo Pan Wan RongZheng
Wang ZuoWei Fang HaiPing

Key words asymmetric nanoparticle, curved trajectory, active

Using molecular dynamics simulations, we show that an asymmetrically shaped nanoparticle in dilute solution possesses a spontaneously curved trajectory within a finite time interval, instead

of the generally expected random walk. This unexpected dynamic behavior has a similarity to that of active matters, such as swimming bacteria, cells, or even fish, but is of a different physical origin. The key to the curved trajectory lies in the non-zero resultant force originated from the imbalance of the collision forces acted by surrounding solvent molecules on the asymmetrically shaped nanoparticle during its orientation regulation. Theoretical formulae based on microscopic observations have been derived to describe this non-zero force and the resulting motion of the asymmetrically shaped nanoparticle.

Science China Physics, Mechanics & Astronomy, 2017, **60**(4): 040511

Flow effect on ^{135}I and ^{135}Xe evolution behavior in a molten salt reactor

Wu Jianhui Guo Chen Cai Xiangzhou Yu Chenggang
Zou Chunyan Han Jianlong Chen Jingen

Key words Molten salt reactor, Core burnup, Flow effect

Molten Salt Reactor (MSR) employs fissile material dissolved in the fluoride salt as fuel which continuously circulates through the primary loop with the flow cycle time being a few tens of seconds. The nuclei evolution law is quite different from that in a solid fuel reactor. In this paper, we analytically deduce the nuclei evolution law of ^{135}Xe and ^{135}I which are entrained in the flowing salt, evaluate its concentration changing with the burnup time, and validate the result with the SCALE6. The circulation of fuel salt could decrease the concentration of ^{135}Xe and ^{135}I, and the reduction can achieve to around 40% and 50% for ^{135}Xe and ^{135}I respectively at a small power level (e.g., 2 MW) when the core has the same fuel salt volume as that of the outer-loop. Furthermore, it can be found that the reduction is inversely proportional to the core to outer-loop volume ratio, but uncorrelated with the mass flow rate under normal operating condition of a MSR. At low core power scale, the flow effect on ^{135}Xe concentration reduction is apparent, but it is mitigated as the core power scale increases because of the rise of ^{135}I concentration, which raises its decay to ^{135}Xe and compensates the loss of ^{135}Xe due to decay at the outer-loop. The decreased ^{135}Xe concentration results in a core reactivity increase varying from around 150 pcm to 1000 pcm depending on the core power and core to outer-loop volume ratio.

Nuclear Engineering and Design, 2017, **314**: 318

Equilibrium Shape of Metal Nanoparticles under Reactive Gas Conditions

Zhu Beien Meng Jun Gao Yi

Characterization and control of the shape of nanoparticles has a primary importance in nanoscience and nanotechnology since most of the physical and chemical properties are shape-dependent. In recent years, many in situ experimental observations have shown that metal nanoparticles can change their shapes and structures dramatically and reversibly under reactive gas conditions. However, despite the experimental achievements, the precise theoretical prediction of this kind of shape evolution is still a challenging and demanding task. In this work, using CO@Pt as a benchmark, we develop a multiscale structure reconstruction model to quantitatively illuminate the equilibrium geometries of metal nanoparticles at given temperature and gas pressure. This model perfectly reproduces the experimental results and explains some intriguing phenomena, including the CO-induced breakup of Pt surfaces. The shape evolution results of Pt, Pd, Cu, and Au nanoparticles under CO and NO gas environments are presented. Our study provides useful guidelines for improving and developing real catalysts.

Journal of Physical Chemistry C, 2017, **121**(10): 5629

A nonmonotonic dependence of the contact angles on the surface polarity for a model solid surface

Qi Chonghai Zhou Bo Wang Chunlei
Zheng Yujun Fang Haiping

Based on molecular dynamics simulations, we found a nonmonotonic relationship between the contact angle of water droplets and the surface polarity on a solid surface with specific hexagonal charge patterns at room temperature. The contact angle firstly decreases and then increases as polarity (denoted as charge q) increases from 0 e to 1.0 e with a vertex value of q = 0.5 e. We observed a different wetting behavior for a water droplet on a conventional nonwetted solid surface when $q \leq 0.5$ e, and a water droplet on an ordered water monolayer adsorbed on a highly polar solid surface when $q > 0.5$ e. The solid–water interaction, density of water, hydrogen bonds, and water structures were analyzed. Remarkably, there was up to six times difference in the solid–water interactions despite the same value of the apparent contact angle values.

Physical Chemistry Chemical Physics, 2017, **19**(9): 6665

Design of High-Performance Pd-Based Alloy Nanocatalysts for Direct Synthesis of H_2O_2

Xu Haoxiang Cheng Daojian Gao Yi

Key words direct synthesis of H_2O_2, Pd-based alloys, nanoparticle, selectivity, catalyst design, density functional theory, electronegativity

The direct synthesis of hydrogen peroxide (H_2O_2) is a promising alternative to the commercialized indirect process. However, it is still a big challenge for the development of Pd-based catalysts with outstanding activity and selectivity, because the design and optimization of the efficient catalysts cannot be effectively achieved solely on the basis of the well-known Sabatier analysis. In this paper, we proposed a strategy to design more efficient Pd-based nanocatalysts combining density functional theory (DFT) calculations and Sabatier analysis. The average valence electron of Pd-shell atoms is identified as the intrinsic factor for the activity and selectivity of the Pd-based nanocatalysts, which can be effectively tuned by the dopants. By introducing dopants with suitable electronegativity, the valence electrons of Pd-shell atoms could be adjusted to the optimal range to enhance the activity and selectivity of the nanocluster simultaneously. With this strategy, Pd-W, Pd-Pb, Au-Pd-W, Au-Pd-Pb, Au-Pd-Mo, and Au-Pd-Ru are predicted as the potential candidates with catalytic performance far exceeding the state of the art experimental systems by a scan of the periodic table. This work not only predicts potential Pd-based alloy nanocatalysts for direct synthesis of H_2O_2 for future experiments but also provides a viable way for the design of highly efficient heterogeneous catalysts in extensive applications.

ACS Catalysis , 2017, **7**(3): 2164

Water flow in carbon-based nanoporous membranes impacted by interactions between hydrated ions and aromatic rings

Liu Jian Shi Guosheng Fang Haiping

Key words nanoporous membrane; carbon-based material; carbon nanotube; desalination; cation-pi interaction

Carbon-based nanoporous membranes, such as carbon nanotubes (CNTs), graphene/graphene oxide and graphyne, have shown great potential in water desalination and purification, gas and ion separation, biosensors, and lithium-based batteries, etc. A deep understanding of the interaction

between hydrated ions in an aqueous solution and the graphitic surface in systems composed of water, ions and a graphitic surface is essential for applications with carbon-based nanoporous membrane platforms. In this review, we describe the recent progress of the interaction between hydrated ions and aromatic ring structures on the carbon-based surface and its applications in the water flow in a carbon nanotube. We expect that these works can be extended to the understanding of water flow in other nanoporous membranes, such as nanoporous graphene, graphyne and stacked sheets of graphene oxide.

Nanotechnology, 2017, **28**(8): 084004

Graphene Oxide Restricts Growth and Recrystallization of Ice Crystals

Geng Hongya Liu Xing Shi Guosheng Bai Guoying
Ma Ji Chen Jingbo Wu Zhuangyuan Song Yanlin
Fang Haiping Wang Jianjun

Key words cryopreservation, Gibbs-Thompson effect, graphene oxide, hydrogen bonds, ice formation

We show graphene oxide (GO) greatly suppresses the growth and recrystallization of ice crystals, and ice crystals display a hexagonal shape in the GO dispersion. Preferred adsorption of GO on the ice crystal surface in liquid water leads to curved ice crystal surface. Therefore, the growth of ice crystal is suppressed owing to the Gibbs–Thompson effect, that is, the curved surface lowers the freezing temperature. Molecular dynamics simulation analysis reveals that oxidized groups on the basal plane of GO form more hydrogen bonds with ice in comparison with liquid water because of the honeycomb hexagonal scaffold of graphene, giving a molecular-level mechanism for controlling ice formation. Application of GO for cryopreservation shows that addition of only 0.01 wt % of GO to a culture medium greatly increases the motility (from 24.3 % to 71.3 %) of horse sperms. This work reports the control of growth of ice with GO, and opens a new avenue for the application of 2D materials.

Angewandte Chemie International Edition, 2017, **56**(4): 997

The switch of the binding behaviours between Xe and Π system induced by the change of oxidation state of Cu ion

Miao Junjian Gao Yi

Key words Aerogen-π interaction, ab initio calculations, copper ion, xenon anaesthesia, noble gas chemistry

The interaction between a xenon atom and aromatic π electron system is generally of van der Waals force with a specifically weak strength. In this work, we suggest the introduction of Cu ion will highly affect the binding behaviour between the xenon and π systems. Once Cu^{2+} ion locates above the benzene ring, the binding is surprisingly strengthened to 11.98 kcal mol−1 at CCSD(T)/CBS level, which is significantly stronger than average strength of the H-bonds in Watson-Crick guanine-cytosine base pair. If the Cu^{2+} is reduced to Cu^{+}, the interaction of interest returns to the weak van der Waals interaction again. This phenomenon indicates the oxidation state shift of Cu ion could regulate the binding strength of Xe with π systems, which would be important for their potential biological functions. This study may provide a plausible understanding of the recent experimental observations of xenon anaesthesia.

Molecular Simulation, 2017, **43**(13-16): 1256

Effect of water molecules on nanoscale wetting behaviour of molecular ethanol on hydroxylated SiO2 substrate

Nie Xuechuan Chen Jige Sheng Nan Zeng Li
Yang Haijun Wang Chunlei

Key words Wetting behaviour, ethanol, SiO2, molecular dynamics

The wettability property of silica (SiO_2) substrate by the ethanol molecules may play important roles in nanomedicine and nanomaterials fabrication. In this paper, by molecular dynamics (MD) simulations, we show that ethanol molecules can form an ordered monolayer on hydroxylated β-cristobalite SiO_2 (1 1 1) substrate, therefore an ethanol droplet can form on this ordered monolayer. We found that water molecules could affect the formation of ethanol monolayer on SiO_2 surface when the amount of water molecules is large, thus regulates the wetting transformation of ethanol molecules. The absorbed water molecules would disrupt the ordered ethanol monolayer and the ethanol molecules could not form the droplet.

Molecular Simulation, 2017, **43**(13-16): 1377

Minor actinide incineration and Th-U breeding in a small FLiNaK Molten Salt Fast Reactor

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Ma Yuwen Wu Jianhui Han Jianlong Chen Jingen

Key words Molten Salt Fast Reactor, Minor actinide incineration, FLiNaK salt, Th-U breeding

Minor actinide (MA) accumulated in spent fuel is the primary contributor to the long-term radiological hazards of high-level nuclear waste. Due to its outstanding features such as fast neutron spectrum, no fuel assembly fabrication, on-line refueling and reprocessing, Molten Salt Fast Reactor (MSFR) is regarded as one of the candidate reactors for MA incineration. In the present work, we evaluate the MA incineration capability for a 500 MW_{th} FLiNaK MSFR by considering on-line MA feeding into the fuel salt and/or ^{233}U extraction from the fertile salt, where the initial FLiNaK fuel salt is composed of 70 mol% (LiF, NaF and KF) and 30 mol% (ThF4, and MAF3). The simulated results show that, during a 50-year operation, the MA incineration efficiency with on-line MA feeding and ^{233}U extraction scenario is significantly higher compared with the case without either MA feeding or ^{233}U extraction. Based on the scenario of on-line MA feeding and ^{233}U extraction, the initial MA loading is further adjusted to keep a small excess reactivity during the whole operation. And the MA incineration amount, the depletion ratio between MA and total heavy nuclides and the MA incineration efficiency at 50-year operating time are 7301 kg, 77.4% and 33.3 kg/TWh, respectively, with a doubling time of 39-year for ^{233}U breeding. We also analyze and discuss the evolutions of the fuel temperature feedback coefficient, the effective delayed neutron fraction and the intensity of spontaneous fission neutron during the whole operating time.

Annals of Nuclear Energy, 2017, **99**: 335

FEA-based structural optimization design of a side cooling collimating mirror at SSRF

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Bian FengGang Xu ZhongMin

Key words Finite element analysis (FEA), Synchrotron radiation, Heat load, Structural optimization

Based on finite element analysis of thermal mechanical behavior, structural optimization design was proposed for a side cooling collimating mirror subjected to high heat load for a

beamline at SSRF (Shanghai Synchrotron Radiation Facility). The temperature distribution, stress concentration effect, maximum equivalent (von-Mises) stress, and slope error of the mirror were analyzed. In particular, the cooling water channels of the traditional structural design were optimized, and the modified designs were further optimized. Although the traditional structural and the improved designs could meet requirements for the temperature and thermal stress, the deformation gradients were relatively large for several structural designs, and this led to larger slope error. The further improved structural designs could be of better performance.

Nuclear Science and Techniques, 2017, **28**(11): 159

Cleaning of carbon-contaminated optics using O_2/Ar plasma

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Chen Ming Liu JunNan

Key words RF plasma cleaning, Carbon-coated samples, Roughness, Cable's conductivity, Beamline photon flux

Cleaning of carbon-contaminated beamline optics was studied by RF plasma discharge process using O_2/Ar. Carbon-coated samples were prepared, and through their cleaning processes key parameters were determined, such as the optimal RF output power, mixing rates of O_2/Ar, and chamber vacuum. Considerations were made against possible adverse effects in cleaning the beamline optics, such as comparing the roughness of samples before and after cleaning, and possible detrimental kinetic effects on cable insulation. Under the cleaning parameters to clean the beamline optics, the thickness of removed carbon film and the change in beamline photon flux were analyzed.

Nuclear Science and Techniques, 2017, **28**(9): 127

Normal tracing deflectometry using a secondary light source

Peng Chuanqian He Yumei Wang Jie

Key words normal tracing method, secondary light source, deflectometric profiler, beam lateral motion, aberration, inhomogeneity

Scanning deflectometric profilers based on an f-θ system are typical optical tools used to measure mirror profiles at many synchrotron facilities. Unlike these profilers, which are based on a pencil beam, here a secondary light source and a pinhole are used to construct a system that automatically selects a beam that will always pass through the pinhole and propagate along the normal direction of the measured area on the surface under test. By measuring the angle variation

of the selected beam, slope variations of the surface under test can be measured. Systematic errors introduced by manufacturing defects or aberrations of an optical element, which greatly degrade the performance of traditional profilers, could be minimized by using the developed method. Simulation values of the proposed method and a conventional method are compared.

Journal of Synchrotron Radiation, 2017, **24**: 765

Measurement of the spatial coherence of hard synchrotron radiation using a pencil beam

Hua Wenqiang Zhou Guangzhao Wang Yuzhu Zhou Ping
Yang Shumin Peng Chuanqian Bian Fenggang
Li Xiuhong Wang Jie

We present a simple method to measure the spatial coherence of hard x-ray beams. Based on the convolution of Gaussian functions, we analyze the diffraction patterns of a grating irradiated by partially coherent hard x rays with a constrained beam diameter. The spatial coherence properties of an x-ray beam are obtained from the width of the diffraction peaks with high accuracy. The results of experiments conducted by combining a pinhole with a grating show a good agreement with our calculation using the Gaussian–Schell model.

Chinese Optics Letters, 2017, **15**(3): 033401

Injection transient study using a two-frequency bunch length measurement system at the SSRF

Duan LiWu Leng YongBin Yuan RenXian Chen ZhiChu

Key words Bunch length measurement, Two-frequency method, Bunch-by-bunch, Injection

The bunch length can be measured by comparison of two frequency components of a synchrotron beam signal. An online bunch length measurement system has been implemented based on this method. Working frequencies of 3 GHz and 500 MHz were selected, and the raw data was acquired by digital oscilloscope and was resampled and analyzed using the MATLAB software platform at bunch-by-bunch rate. The constructed system was employed to study the bunch length synchronous oscillation phenomenon during injection. The beam experiments demonstrated a time resolution of less than 0.5 ps.

Nuclear Science and Techniques, 2017, **28**(7): 93

Beam test results of high Q CBPM prototype for SXFEL

Chen Jian Leng YongBin Yu LuYang Lai LongWei
Yuan RenXian

Key words High Q CBPM, SXFEL, Position resolution, RF front end, DBPM

In pursuit of high-precision beam position measurements at micrometers or submicrometers for the Shanghai soft X-ray free-electron laser (SXFEL) facility which is under construction in the vicinity of the Shanghai Synchrotron Radiation Facility, a high Q cavity beam position monitor (CBPM) with a resonant frequency of 4.7 GHz is developed by the Shanghai Institute of Applied Physics, and the relevant BPM electronics with a dedicated RF front end, and a digital BPM, are completed. The cavity design, cold test, system architecture, and first beam test are performed at the Shanghai deep ultraviolet free-electron laser (Zhao et al. in Nucl Instrum Meth A 528(1–2): 591–594, 2004. doi: 10.1016/j.nima.2004.04.108) facility. Results of the beam experiment show that the performance of the CBPM is consistent with basic expectations, and the beam position resolution can fulfill the requirements for the SXFEL project if the beam conditions are optimized.

Nuclear Science and Techniques, 2017, **28**(4): 51

In vitro anticoagulant activity of polyanionic graft chains modified poly(vinyl alcohol) particles

Li Rong Wu Guozhong Cai Ximing Ye Yin

Key words γ-ray simultaneous irradiation induced graft, polymerization, Poly(vinyl alcohol), Acrylic acid, Sodium styrenesulfonate, Anticoagulant activity

Poly(acrylic acid), poly(sodium styrenesulfonate), and poly(acrylic acid-co-sodium styrenesulfonate) chains were immobilized onto poly(vinyl alcohol) (PVA) particles via a facile γ-ray simultaneous irradiation induced graft polymerization technique, which were confirmed by the attenuated total reflection Fourier transform infrared spectroscopy and the high swelling ratios of modified PVA particles. The effects of absorbed dose, dose rate, Cu^{2+} concentration and monomer concentration on the degree of grafting (DG) of PVA particles were investigated to find out a feasible process for preparing polyanionic chains graft-modified PVA particles. The clotting time results illustrated that both PVA-g-PAA and PVA-g-PSSS particles presented excellent anticoagulant activity, and the activated partial thromboplastin time (APTT), prothrombin time (PT) and thrombin time (TT) were effectively prolonged with the increase of DG_{AA} and DG_{SSS}, respectively. Furthermore, the anticoagulant activity of PVA-g-PSSS samples was more efficient

than that of PVA-g-PAA samples. However, the anticoagulant effect of PVA-g-P(AA-co-SSS) samples was different from that of PVA-g-PAA and PVA-g-PSSS samples, and was similar to that of heparin, mainly elongating the APTT and TT. This might be due to both of them containing the same negative-charged groups. Additionally, the grafted PVA particles were all nonhemolytic, showing good blood compatibility.

Radiation Physics and Chemistry, 2017, **134**: 27

Microstructure variations induced by excess PbX_2 or AX within perovskite thin films

Zheng Guanhaojie Zhu Cheng Chen Yihua Zhang Juchen
Chen Qi Gao Xingyu Zhou Huanping

We systematically investigated the impact of stoichiometric ratio variation between PbX_2 and AX on hybrid perovskite films from the perspective of microstructure, especially on the plane stacking directions, using the two-dimensional synchrotron radiation grazing incidence wide-angle X-ray scattering (GIWAXS) technique. The tuned crystal plane stacking in perovskite films can consequently enlighten further explorations about the relationship between microstructure and solar cell performance.

Chemical Communications, 2017, **53**(96): 12966

The crystal structure of Pyrococcus furiosus RecJ implicates it as an ancestor of eukaryotic Cdc45

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Chen Jia-Nan Xu Chun-Yan Wang Feng-Ping
Xiao Xiang He Jian-Hua Liu Xi-Peng

RecJ nucleases specifically degrade single-stranded (ss) DNA in the 5′ to 3′ direction. Archaeal RecJ is different from bacterial RecJ in sequence, domain organization, and substrate specificity. The RecJ from archaea Pyrococcus furiosus (PfuRecJ) also hydrolyzes RNA strands in the 3′ to 5′ direction. Like eukaryotic Cdc45 protein, archaeal RecJ forms a complex with MCM helicase and GINS. Here, we report the crystal structures of PfuRecJ and the complex of PfuRecJ and two CMPs. PfuRecJ bind one or two divalent metal ions in its crystal structure. A channel consisting of several positively charged residues is identified in the complex structure, and might be responsible for binding substrate ssDNA and/or releasing single nucleotide products. The deletion

of the complex interaction domain (CID) increases the values of k_{cat}/K_m of 5′ exonuclease activity on ssDNA and 3′ exonuclease activity on ssRNA by 5- and 4-fold, respectively, indicating that the CID functions as a regulator of enzymatic activity. The DHH domain of PfuRecJ interacts with the C-terminal beta-sheet domain of the GINS51 subunit in the tetrameric GINS complex. The relationship of archaeal and bacterial RecJs, as well as eukaryotic Cdc45, is discussed based on biochemical and structural results.

Nucleic Acids Research, 2017, **45**(21): 12551

Detailed structure of a new bioactive glass composition for the design of bone repair materials

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Key words \Structural characterization; Bioactive glass; Sol-gel; Phosphosilicate

Detailed structure of a new bioactive glass composition (PSC, 54 mol% SiO_2, 35 mol% CaO and 11 mol% P_2O_5) was studied, and conventional glasses (45S5 and S70C30) were used as comparison. The structure information were obtained by HEXRD and solid NMR techniques. It was found that all the samples have different silicon and phosphorous coordination environment, there is Si-O-P network formed for PSC samples but not for 45S5 and S70C30 samples. These results may hopefully advance the design of new bioactive glasses.

Journal of Non-Crystalline Solids, 2017, **475**: 10

Facile Construction of Novel 3-Dimensional Graphene/Amorphous Porous Carbon Hybrids with Enhanced Lithium Storage Properties

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Key words amorphous porous carbon, graphene, core shell, lithium ion batteries, $NaBiO_3$

Presently, porous materials have become essential to many technological applications. In this account, 3-dimensional skeleton composite materials consisting of a core–shell amorphous porous carbon/multilayer graphene are synthesized by chemical vapor deposition on Ni foam using a facile

one-step growth method. The data suggest that these composites have not only outstanding electrical and mechanical properties of the multilayer graphene but also the mesoporous characteristics of the amorphous carbon. Moreover, the composited carbon materials perfectly inherit the macroporous structure of Ni foam, and the amorphous carbon core in the skeleton serves as a cushion to buffer the volume variation after the removal of Ni. The carbon composites reveal ultralow density (4.45 mg cm^{-3}) and high conductivity (45 S cm^{-1}), essentially issued from the perfectly preserved structural integrity of graphene. The novel carbon composites can be used as anodes for lithium ion batteries. After these carbon composites are incorporated with $NaBiO_3$, superior electrochemical activities above 2 V can be achieved with a discharge capacity of ~300 mAh g^{-1}.

ACS Applied Materials & Interfaces, 2017, **9**(40): 35191

Discovery of a novel small inhibitor RJ19 targeting to human Hsp90

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Key words Heat shock protein 90, Drug target, Inhibitor, X-ray diffraction, Complex crystal structure

AHeat shock protein 90 (Hsp90) can promote growth and proliferation of cancer cells by helping in folding, conformational maturation, and activation of various client proteins. Therefore, Hsp90 has been paid more attention to as an anticancer drug target. Reported Hsp90 inhibitors have several limitations such as poor solubility, limited bioavailability, and hepatotoxicity. Here, a novel small inhibitor RJ19 has been designed using fragment-based drug discovery and synthesized. Additionally, a crystal structure of $Hsp90^N$–RJ19 was determined by X-ray diffraction (resolution limit, 2.0 Å, PDB code 4L90). The crystal structure of $Hsp90^N$–RJ19 was analyzed in detail and compared with that of native $Hsp90^N$, $Hsp90^N$-ATP, and $Hsp90^N$-GDM, respectively. It was indicated that RJ19 interacted with $Hsp90^N$ at the ATP-binding pocket, which suggests that RJ19 may replace nucleotides to bind with $Hsp90^N$ to result in chaperone function failure of Hsp90. RJ19, therefore, has emerged as a promising anticancer lead compound. Rearrangement and displacement of L2 Loop in $Hsp90^N$–RJ19 play a key role in the functio+n failure, which also makes the pocket wider and longer facilitating structure modification of RJ19 later. The complex crystal structure and interaction between RJ19 and $Hsp90^N$ provide a rational basis for the design and optimization of novel anticancer drugs.

Nuclear Science and Techniques, 2017, **28**(10): 148

In Situ Observation of Thermal Proton Transport through Graphene Layers

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Xu Zijian Ji Gengwu Jiang Sheng Zhao Bin Yin
Guangzhi Li Li Yang Tieying Wang Yong Yi Lin Li
Xiaolong Tai Renzhong

Key words in situ technique, graphene, thermal proton, synchrotron X-ray, transport

Protons can penetrate through single-layer graphene, but thicker graphene layers (more than 2 layers), which possess more compact electron density, are thought to be unfavorable for penetration by protons at room temperature and elevated temperatures. In this work, we developed an in situ subsecond time-resolved grazing-incidence X-ray diffraction technique, which fully realizes the real-time observation of the thermal proton interaction with the graphene layers at high temperature. By following the evolution of interlayer structure during the protonation process, we demonstrated that thermal protons can transport through multilayer graphene (more than 8 layers) on nickel foil at 900 °C. In comparison, under the same conditions, the multilayer graphenes are impermeable to argon, nitrogen, helium, and their derived ions. Complementary in situ transport measurements simultaneously verify the penetration phenomenon at high temperature. Moreover, the direct transport of protons through graphene is regarded as the dominant contribution to the penetration phenomenon. The thermal activation, weak interlayer interaction between layers, and the affinity of the nickel catalyst may all contribute to the proton transport. We believe that this method could become one of the established approaches for the characterization of the ions intercalated with 2D materials in situ and in real-time.

ACS Nano, 2017, **11**(9): 8970

Enhanced Crystalline Phase Purity of $CH_3NH_3PbI_{3-X}Cl_X$ Film for High- Efficiency Hysteresis-Free Perovskite Solar Cells

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Li Li Zhang Xingmin Ji Gengwu Zhang Xiaonan)
Wang Zhaokui Xiong Yimin Cao Liang
Sun Baoquan Gao Xingyu

Key words Solution-processed perovskite films, GIXRD, dual phases, conventional planar, inverted planar PSCs

Despite rapid successful developments toward promising perovskite solar cells (PSCs) efficiency, they often suffer significant hysteresis effects. Using synchrotron-based grazing incidence X-ray diffraction (GIXRD) with different probing depths by varying the incident angle, we found that the perovskite films consist of dual phases with a parent phase dominant in the interior and a child phase with a smaller (110) interplanar space (d(110)) after rapid thermal annealing (RTA), which is a widely used post treatment to improve the crystallization of solution-processed perovskite films for high-performance planar PSCs. In particular, the child phase composition gradually increases with decreasing depth till it becomes the majority on the surface, which might be one of the key factors related to hysteresis in fabricated PSCs. We further improve the crystalline phase purity of the solution-processed $CH_3NH_3PbI_{3-x}Cl_x$ perovskite film (referred as g-perovskite) by using a facile gradient thermal annealing (GTA), which shows a uniformly distributed phase structure in pinhole-free morphology with less undercoordinated Pb and I ions determined by synchrotron-based GIXRD, grazing incidence small-angle X-ray scattering, scanning electron microscopy, and X-ray photoelectron spectroscopy. Regardless of device structures (conventional and inverted types), the planar heterojunction PSCs employing $CH_3NH_3PbI_{3-x}Cl_x$g-perovskite films exhibit negligible hysteresis with a champion power conversion efficiency of 17.04% for TiO_2-based conventional planar PSCs and 14.83% for poly(3,4-ethylenedioxythiophene: poly(styrenesulfonate) (PEDOT: PSS)-based inverted planar PSCs. Our results indicate that the crystalline phase purity in $CH_3NH_3PbI_{3-x}Cl_x$ perovskite film, especially in the surface region, plays a crucial role in determining the hysteresis effect and device performance.

ACS Applied Materials & Interfaces, 2017, **9**(27): 23141

Mini-beam modes on standard MX beamline BL17U at SSRF

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Pan Qiangyan Zhong Changyou Liu Ke
Zhou Huan Sun Bo He Jianhua

The macromolecular crystallography beamlines at third-generation synchrotron facilities play a central role in solving macromolecular crystal structures and also in understanding the biological function at molecular levels. The MX beamline BL17U at Shanghai Synchrotron Radiation Facility is a typical standard MX beamline with a focused beam size (H × V) of FWHM around 80 μm × 45 μm. However the protein samples brought to the beamline are down to 5-10 m from the important and challenging science project now. These samples require smaller size beam. In order to achieve

the mini-size beamline, two mini-beam modes have been developed on BL17U: the pinhole-based mini-beam and the focused mini-beam by compound refractive lens (CRL). Compared to the pinhole-based mode, three times increase in flux is obtained by the CRL mode at a similar beam size. The flux gain obtained by the CRL needs to be considered for data collection strategies. It takes few minutes to switch the beamline from the normal to CRL mini-beam mode.

Review of Scientific Instruments, 2017, **88**(7): 073301

Atomic pair distribution function method development at the Shanghai Synchrotron Radiation Facility

Zhou XiaoJuan Tao JuZhou Guo Han Lin He

Key words atomic pair distribution function, x-ray scattering, local structure, high energy x-ray

The atomic pair distribution function (PDF) reveals the interatomic distance in a material directly in real-space. It is a very powerful method to characterize the local structure of materials. With the help of the third generation synchrotron facility and spallation neutron source worldwide, the PDF method has developed quickly both experimentally and theoretically in recent years. Recently this method was successfully implemented at the Shanghai Synchrotron Radiation Facility (SSRF). The data quality is very high and this ensures the applicability of the method to study the subtle structural changes in complex materials. In this article, we introduce in detail this new method and show some experimental data we collected.

Chinese Physics B, 2017, **26**(7): 076101

Novel phenomenon of magnetism and superconductivity in Fe-doped superconductor $Bi_{4-x}Fe_xO_4S_3$ ($0 \le x \le 0.1$)

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We report the effects of Fe doping on the BiS_2-based superconductor $Bi_4O_4S_3$. It has been found that the superconducting transition temperature (T_C^{onset}) is slightly enhanced by Fe doping. The magnetic susceptibility results reveal the coexistence of superconductivity and long-range ferrimagnetism in these samples. A new magnetic transition temperature T_V (Verwey transition) from the M–T curves at ~112 K is observed. The isothermal magnetization curves (M–H) indicate a

weak ferrimagnetism, which is probably due to the antiparallel ordering of Fe^{2+} and Fe^{3+} magnetic moments. The coexistence of superconductivity and ferro/ferrimagnetism makes bismuth oxysulfide superconductor a platform for understanding superconductivity from a new perspective.

Applied Physics A, 2017, **123**(6): 427

Annealing Induced Re-crystallization in $CH_3NH_3PbI_{3-x}Cl_x$ for High Performance Perovskite Solar Cells

Yang Yingguo Feng Shanglei Li Meng Xu Weidong Yin Guangzhi Wang Zhaokui Sun Baoquan Gao Xingyu

Using poly(3,4-ethylenedioxythiophene): polystyrene sulfonate (PEDOT: PSS) as hole conductor, a series of inverted planar $CH_3NH_3PbI_{3-x}Cl_x$ perovskite solar cells (PSCs) were fabricated based on perovskite annealed by an improved time-temperature dependent (TTD) procedure in a flowing nitrogen atmosphere for different time. Only after an optimum annealing time, an optimized power conversion efficiency of 14.36% could be achieved. To understand their performance dependence on annealing time, an in situ real-time synchrotron-based grazing incidence X-ray diffraction (GIXRD) was used to monitor a step-by-step gradual structure transformation from distinct mainly organic-inorganic hybrid materials into highly ordered $CH_3NH_3PbI_3$ crystal during annealing. However, a re-crystallization process of perovskite crystal was observed for the first time during such an annealing procedure, which helps to enhance the perovskite crystallization and preferential orientations. The present GIXRD findings could well explain the drops of the open circuit voltage (V_{oc}) and the fill factor (FF) during the ramping of temperature as well as the optimized power conversion efficiency achieved after an optimum annealing time. Thus, the present study not only illustrates clearly the decisive roles of post-annealing in the formation of solution-processed perovskite to better understand its formation mechanism, but also demonstrates the crucial dependences of device performance on the perovskite microstructure in PSCs.

Scientific Reports , 2017, **7**: 46724

Facile synthesis the nitrogen and sulfur co-doped carbon dots for selective fluorescence detection of heavy metal ions

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Key words Co-doped carbon dots, Carbon materials, Luminescence, Heavy metal ion-detection

In this article, we prepare the nitrogen (N) and sulphur (S) co-doped carbon dots (NS-CDs) via a one-step hydrothermal method using the methionine as the precursor. The N and S doping content reach as high as 15.2 at.% and 19.5 at.%, separately. The analysis of the photoluminescence dates exhibits that the relationship between the excitation and the corresponding emission wavelength can be summarized as a linear fitting function. In addition, the as prepared NS-CDs also exhibits sensitive detection properties for heavy metal cations. With these excellent characteristics, there are extensive potential applications for NS-CDs in industry and environmental monitoring.

Materials Letters , 2017, **193**: 236

Dehydration behaviour and structural evolution of graphene oxide membranes on silicon substrate

Wang Rui Gao Hui Zhu Daming Yang Tieying Zhang Xingmin Li Li Yin Guangzhi Zhu Lina Feng Zhenjie Li Xiaolong

The dehydration kinetics of graphene oxide (GO) were investigated by in-situ two-dimensional grazing incident X-ray diffraction. We found that the interlayer spacing of the GO membrane gradually decreased as the annealing temperature increased and as time elapsed. Surprisingly, we observed the formation of an intermediate “water-rich” GO layers at 25 °C with an interlayer spacing of approximately 15.2 Å, which was caused by the intercalation of two additional layers of water into the interlayers of the GO membrane. Moreover, three types of water trapped in GO were clearly distinguished upon isothermal annealing at various temperatures. Below 160 °C, the removal of “bulk water” and “confined water” resulted in a smaller interlayer spacing and the preservation of oxygen-containing functional groups. At 160 °C or higher, “bound water” was removed and oxygen-containing functional groups were lost, which contributed to the reduction of GO. The dehydration behaviour and structural evolution of GO investigated here is useful for understanding and controlling the properties of GO membranes for permeation, separation and electronic applications.

Carbon, 2017, **114**: 23

Microwave Hydrothermal Synthesis of Terbium Ions Complexed with Porous Graphene for Effective Absorbent for Organic Dye

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Liu Wenjing Li Xiaolong

Key words Microwave; Absorbent; Rare earth ions; Graphene

A luminescent terbium ions/reduced graphene oxide complex (Tb-RGO) was successfully and rapidly synthesized by the microwave hydrothermal reaction via the interactions between terbium ions and the active oxygen functional groups of graphene oxide. The as-prepared material was porous stacked by multilayer graphene in all directions. Thus, the resulting product owed the high specific surface area, high adsorption capacity and ultra-fast adsorption rate. Combined with the characteristic photoluminescence derived from terbium ions, the material has potential applications in biosensing and environmental protection.

Nanoscale Research Letters, 2017, **12**: 204

Origin of Magnetism in Hydrothermally Aged 2-Line Ferrihydrite Suspensions

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As an iron oxyhydroxide, nanosized ferrihydrite (Fh) is important in Earth science, biology, and industrial applications. However, its basic structure and origin of its magnetism have long been debated. We integrate synchrotron-based techniques to explore the chemical structures of 2-line ferrihydrite and to determine the origin of its magnetism during hydrothermal aging in air. Our results demonstrate that both the magnetism and X-ray magnetic circular dichroism (XMCD) signal of 2-line ferrihydrite are enhanced with aging time, and that XMCD spectral patterns resemble that of maghemite (γ-Fe_2O_3) rather than magnetite (Fe_3O_4). Fe L-edge and K-edge X-ray absorption spectroscopy (XAS) further indicate formation of both maghemite and hematite (α-Fe_2O_3) with increasing concentrations with longer hydrothermal aging time. Thus, magnetic enhancement with longer hydrothermal aging time is attributed to increasing maghemite concentration instead of a

magnetically ordered ferrihydrite as previously reported. Moreover, L-edge and K-edge XAS spectra with different probing depths yield different ratios of these Fe oxides, which suggest the formation of a core (ferrihydrite-rich)-shell (with a mixture of both allotropes; α-Fe_2O_3 and γ-Fe_2O_3) structure during hydrothermal aging. Our results provide insights into the chemical evolution of 2-line ferrihydrite that reveal unambiguously the origin of its magnetism.

Environmental Science & Technology, 2017, **51**(5): 2643

Interfacial electronic structures revealed at the rubrene/$CH_3NH_3PbI_3$ interface

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Zhang Xiaonan Shen Kongchao Yang Yingguo
Xiong Yimin Gao Xingyu Cao Liang Qi DongChen

The electronic structures of rubrene films deposited on $CH_3NH_3PbI_3$ perovskite have been investigated using in situ ultraviolet photoelectron spectroscopy (UPS) and X-ray photoelectron spectroscopy (XPS). It was found that rubrene molecules interacted weakly with the perovskite substrate. Due to charge redistribution at their interface, a downward 'band bending'-like energy shift of ~0.3 eV and an upward band bending of ~0.1 eV were identified at the upper rubrene side and the $CH_3NH_3PbI_3$ substrate side, respectively. After the energy level alignment was established at the rubrene/$CH_3NH_3PbI_3$ interface, its highest occupied molecular orbital (HOMO)–valence band maximum (VBM) offset was found to be as low as ~0.1 eV favoring the hole extraction with its lowest unoccupied molecular orbital (LUMO)–conduction band minimum (CBM) offset as large as ~1.4 eV effectively blocking the undesired electron transfer from perovskite to rubrene. As a demonstration, simple inverted planar solar cell devices incorporating rubrene and rubrene/poly(3,4-ethylenedioxythiophene): poly(styrenesulfonate) (PEDOT: PSS) hole transport layers (HTLs) were fabricated in this work and yielded a champion power conversion efficiency of 8.76% and 13.52%, respectively. Thus, the present work suggests that a rubrene thin film could serve as a promising hole transport layer for efficient perovskite-based solar cells.

Physical Chemistry Chemical Physics, 2017, **19**(9): 6546

Local structural characteristics of Sb_2Te_3 films studied by reverse Monte Carlo modeling

Zhang Ling Song SanNian Lin He Cheng Yan Xi Wei Li Le He Yan Song ZhiTang

Key words Phase-change material, Reverse Monte Carlo, Atomic configuration

Atomic configuration and connectivity of Sb2Te3 thin film are investigated using high-energy X-ray diffraction and reverse Monte Carlo simulation. Atomic model details of Sb2Te3 thin film are compared with liquid and amorphous Sb2Te3 reported in other article. Simulations show that both Sb–Sb and Te–Te homopolar bonds are present in the models. In phase transition process, atomic configuration of the sample rearranges gradually through the forming of Sb–Te bonds and the breaking of Sb–Sb and Te–Te bonds.

Nuclear Science and Techniques, 2017, **28**(3): 38

The structure of filled skutterudites and the local vibration behavior of the filling atom

Zhou Xiaojuan Zong Pengan Chen Xihong Tao Juzhou Lin He

Key words Atomic pair distribution function, Extended x-ray absorption fine structure, Local vibration

oth of atomic pair distribution function (PDF) and extended x-ray absorption fine structure (EXAFS) experiments have been carried out on unfilled and Yb-filled skutterudites $Yb_xCo_4Sb_{12}$ (x=0, 0.15, 0.2 and 0.25) samples. The structure refinements on PDF data confirm the large amplitude vibration of Yb atom and the dependence of Yb vibration amplitude on the filling content. Temperature dependent EXAFS experiment on filled skutterudites have been carried out at Yb LⅢ-edge in order to explore the local vibration behavior of filled atom. EXAFS experiments show that the Einstein temperature of the filled atom is very low (70.9 K) which agrees with the rattling behavior.

Physica B: Condensed Matter, 2017, **507**: 131

The Evidence of Giant Surface Flexoelectric Field in (111) Oriented $BiFeO_3$ Thin Film

Yang Tieying Zhang Xingmin Chen Bin Guo Haizhong Jin Kuijuan Wu Xiaoshan Gao Xingyu Li Zhong Wang Can Li Xiaolong

Key words Surface layer, ferroelectric thin films, X-ray diffraction, flexoelectrics, microstructure

In this work, the surface structure of a single-domain epitaxial $BiFeO_3$ film with (111) orientation was investigated by in situ grazing incidence X-ray diffraction and X-ray reflectivity. We found that a large strain gradient exists in the surface region (2-3 nm) of the $BiFeO_3$ film. The strain gradient is approximately 10^7 m^{-1}, which is 2 or 3 orders of magnitude larger than the value inside the film. Moreover, we found that a surface layer with a lower electron density compared with the underlying $BiFeO_3$ layer exists on the surface of $BiFeO_3$ film, and this layer exhibits an irreversible surface structure transition occurs at 500 K, which should be associated with the surface flexoelectric field. We considered that this large strain gradient is originated from the surface depolarization field of ferroelectrics. Our results suggest a coupling between the surface structure and the flexoelectricity and imply that the surface layer and properties would be controlled by the strain gradient in ferroelectric films.

ACS Applied Materials & Interfaces, 2017, **9**(6): 5600

The energy level alignment at the $CH_3NH_3PbI_3$/pentacene interface

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Key words Perovskite solar cell, Interface electronic structure, Energy level alignment

Pentacene thin film on $CH_3NH_3PbI_3$ was studied by in-situ X-ray photoelectron spectroscopy and ultraviolet photoelectron spectroscopy to determine their interfacial energy level alignment. A 0.2 eV downward band bending together with a 0.1 eV interfacial dipole was found at the pentacene side, whereas there was no band bending found at the $CH_3NH_3PbI_3$ side. The offset between $CH_3NH_3PbI_3$ Valance Band Maximum (VBM) and pentacene Highest Occupied Molecular Orbital (HOMO) and that between $CH_3NH_3PbI_3$ Conduction Band Minimum (CBM)

and pentacene Lowest Unoccupied Molecular Orbital (LUMO) was determined to be 0.7 and 1.35 eV, respectively. The band alignment at this interface is favor of efficient hole transfer, which suggests pentacene as a viable HTL candidate to be explored in perovskite solar cells.

Applied Surface Science, 2017, **393**: 417

Structural consistency analysis of recombinant and wild-type human serum albumin

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Key words rystal structure, Consistency analysis, Wild-type human serum albumin (HSA), Recombinant human serum albumin (rHSA)

Recombinant human serum albumin (rHSA) is potential alternatives for human serum albumin (HSA) which may ease severe shortage of HSA worldwide. In theory, rHSA and HSA are the same. Structure decides function. Therefore, the 3D structural consistency analysis of rHSA and HSA is outmost importance, which is the base of their function consistency. In this paper, the crystal structures of rHSA at resolution limit of 2.22 Å and HSA at 2.30 Å were determined by X-ray diffraction (XRD), which were deposited in the Protein Data Bank (PDB) with accession codes 4G03 (rHSA) and 4G04 (HSA). The differences between rHSA and HSA were systematically analyzed from the crystallization behavior, diffraction data and three-dimensional (3D) structure. The superimposed contrasted analysis indicated that rHSA and HSA achieved a structural similarity of 99% with an r.m.s. deviation of 0.397 Å for the corresponding overall Cα atoms. In addition, the number of α-helices in the rHSA or HSA molecule was verified to be 30. As a result, rHSA can potentially replace HSA. The study provides a theoretical and experimental basis for the clinical and additional applications of rHSA. Meanwhile, it is also a good example for applications of genetic engineering.

Journal of Molecular Structure, 2017, **1127**: 1

Thermal Stable Perovskite Solar Cells Improved by ZnO/Graphene Oxide as Electron Transfer Layers

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Key words GIXRD, ZnO/GO, perovskite, ETL (electron transfer layers)

ZnO/graphene oxide (GO) nano-particles (NPs) layer was prepared using a facile solution process and employed as an electron conductor to improve the thermal stability of perovskite solar

cells. Structural changes during the degradation process in high temperature environment were characterized via in situ grazing incidence X-ray diffraction. The optical properties and surface morphologies of the films were characterized. It was observed that smooth and compact structure of ZnO/GO layer works as a protection layer to prevent decomposition of perovskite film which is converted into PbI_2 during the annealing process reaction. The perovskite film grown on ZnO/GO layer exhibited enhanced crystallization, high surface coverage ratio as well as preferred in-plane orientation of the (110) plane.

Journal of Inorganic Materials, 2017, **32**(1): 96

Stress Analysis and Structural Integrity Evaluations of Pressure Vessel in Molten Salt Reactor

Wang Xiaoyan Zhu Shifeng Wang Xiao Cao Yun

To guarantee the safety of nuclear reactor, the stress analysis and structural integrity evaluations of the reactor pressure vessel (RPV) are very important for Thorium-based Molten Salt Reactor (TMSR), whose design temperature and design pressure are 700 ℃ and 0.5MPa respectively. In this paper, the structural analysis is firstly carried out by using a 3D coarse model of the RPV. Secondly, the reactor core support are recalculated by a sub-model with a fine mesh and the analysis results are evaluated according to ASME NH code, including stress evaluation, strain and deformation evaluation and creep-fatigue evaluation. It was found that the initial structural did not meet the requirements of creep-fatigue limits. Finally, structural optimization designs are proposed, such as T-shaped modified structure and fillet design, whose results can satisfy the requirements of creep-fatigue limits. These analysis methods and results provide some practical engineering guidance to the structural design and safety evaluation of the RPV in TMSR.

Proceedings Of The Asme Pressure Vessels And Piping Conference (2016), 2017, **3**: UNSP V003T03A036

The critical role of Si doping in enhancing the stability of M_6C carbides

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Key words Si doping; M_6C carbides; Stability; Si K-edge XANES; First-principles calculations

M6C carbides are one of the most common second phases in high speed steels and superalloys, and also an alternative catalytic materials for energy applications. Although the influences of Si doping on the stability of M6C carbides have been frequently observed in different alloys, the atomic-scale mechanism of which remains poorly understood. Here we obtain the Ni3Mo3C-type M6C carbides in GH3535 alloys and evaluate the dependence of their structure and composition on Si contents. Combining high-energy synchrotron X-ray diffraction and first-principle calculations, Si atoms are found to preferentially occupy Ni (16d) sites in Ni3Mo3C structure. The electronic structures and Si K-edge x-ray absorption near edge structures demonstrate the band hybridization and charge transfer between Si atoms and the nearest-neighbor Ni (32e) and Mo (48f) atoms in Si-doped Ni3Mo3C structures, which is responsible for the stability of M6C carbides.

Journal of Alloys and Compounds, 2017, **728**: 917

Grain boundary engineering for control of tellurium diffusion in GH3535 alloy

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Key words Grain-clusters, Tellurium diffusion, EPMA, EBSD, Grain boundary engineering, GH3535 alloy

The effect of grain boundary engineering (GBE) on the Te diffusion along the surface grain boundaries was investigated in GH3535 alloy. It can be found that GBE treatment increases obviously the fraction of low-Σ coincidence site lattice (CSL) boundaries, especially the Σ3 ones, and introduces the large-size grain clusters. When the as-received (AR) and GBE-treated (GBET) specimens were exposed to Te vapor, only Σ3 boundaries were found to be resistant to Te diffusion. From the cross section and the surface, the fewer Te-attacked grain boundaries and the thinner corrosion layer can be observed in the GBET sample. The improvement of resistance to Te diffusion in the GBET sample can be attributed to the large size grain-clusters associated with high proportion of the $\Sigma 3^n$ boundaries.

Journal of Nuclear Materials, 2017, **497**: 76

Effect of thermal exposure time on tellurium-induced embrittlement of Ni–16Mo–7Cr–4Fe alloy

Chu XiangWei Cheng HongWei Fu CaiTao Leng Bin
Jia YanYan Liu Fang Li ZhiJun

Key words Tellurium, Grain boundary, Embrittlement, Intergranular cracking, Nickel-based alloy, Molten salt reactor

The embrittlement of nickel-based structural alloys by fission-produced tellurium (Te) is a major challenge for molten salt reactors (MSR). In this study, the effects of thermal exposure time on tellurium diffusion in a candidate MSR structural alloy (Ni–16Mo–7Cr–4Fe) and the consequent mechanical property degradation of the alloy were investigated through surrogate diffusion experiments at 700 °C. The results show that some tellurium reacted with the alloy to form tellurides on the surface, while some tellurium diffused into the alloy along grain boundaries. Ni_3Te_2 and CrTe were the most stable reaction products at the tested temperature, and the formation of CrTe on the surface induced the Cr depletion at grain boundaries of the alloy. The diffusion depth of Te increased gradually with thermal exposure time, and the diffusion rate kept stable within the test duration of up to 3000 h. The Te diffusion in the alloy caused the embrittlement of grain boundaries, inducing crack formation and strength degradation in tensile test at room temperature.

Nuclear Science and Techniques, 2017, **28**(12): 178

Microstructure and Mechanical Properties of Fiber Laser Welded GH3535 Superalloy

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Key words Laser beam welding, GH3535 superalloy, Microstructure, M6C-gamma eutectic phases, Microhardness, Tensile properties

As a primary material of the thorium molten salt reactor (TMSR) that is a suitable candidate reactor of the Generation IV nuclear reactors, GH3535 superalloy was successfully welded. The effect of laser beam welding (LBW) on microstructure evolution of fusion zone (FZ) and heat affected zone (HAZ), such as element segregation, precipitate behavior and grain evolution, was investigated. The microhardness and tensile properties were tested and discussed. The results of microstructure evolution showed that a number of fine M_6C-γ eutectic phases precipitated at

solidification grain boundaries and interdendritic region in FZ. Compared to base metal zone (BMZ), the grain size of HAZ has no obvious change. While a few of M_6C-γ eutectic phases were observed in partially melted zone (PMZ) of HAZ. The results of microhardness indicated that the hardness of FZ was higher than that of HAZ and BMZ. The results of tensile test showed that the ultimate tensile strength of joints at room temperature, 650 and 700 °C were 98%, 97% and 99% of that of BM, respectively. All the tensile specimens of joints failed in BMZ rather than in PMZ where M_6C carbides had been transformed into M_6C-γ eutectic phases.

Journal of Materials Science & Technology, 2017, **33**(11): 1289

Control rod drop dynamic analysis in the TMSR-SF1 based on numerical simulation and experiment

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Zhang Xiaochun Cao Yun Wang Naxiu

Key words Scram, Thorium base molten salt reactor, Rod drop time, Hydraulic buffer

The scram function renders the core subcritical in response to plant upsets, which is realized by fast drop of the control rods. In the solid fuel (SF) thorium molten salt reactor system (TMSR), denoted as the TMSR – SF1 project, the drop time of the rod is obviously affected by the driving mechanical drag and the hydraulic resistance of the liquid environment. An inner-house code is developed to analyze the rod drop in the TMSR – SF1. In the code, the total transmission efficiency of the driving mechanism is deduced as a relationship with dropping velocity of the rod. With the experimental and theoretic analysis, the motion process of the rod drop is simulated in this study. And it turns out that the drop time in the molten salt is satisfied with the limiting drop time in the TMSR – SF1. In addition, a hydraulic buffer is designed to alleviate the dropping shock from the scram and the calculation results are presented in the paper as well.

Nuclear Engineering and Design, 2017, **322**: 131

Characteristics of the laminar convective heat transfer of molten salt in concentric tube

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Fu Yuan Tang ZhongFeng Zhu HaiHua Wang NaXiu

Key words Molten salt, Concentric tube, Laminar flow, Convective heat transfer, Heat transfer correlation

In this paper, laminar convective heat transfer performance of molten salt with Reynolds number of 300–2300 and Grashof number of 8.56×10^4–3.95×10^6 in a concentric tube heat exchanger is reported. The effects of temperature on the heat transfer coefficient of molten salt are experimentally studied with the temperature of 473 K–573 K. Results show that the measured Nusselt number is larger than that predicted by pure forced convective heat transfer correlations and the deviations decrease as Reynolds number increases. In addition, the experimental result displays a completely different dependence on the temperature from forced convective correlations. It is presumably that the radial density gradient gives rise to buoyancy motion resulting in the formation of natural convection and then strengthen the heat transfer performance in laminar region. By comparison, it is found that the experimental result follows the trend of laminar convective heat transfer correlations derived from traditional working medium, however, the traditional correlations cannot describe the molten salt adequately. Therefore, based on the experimental results and existing correlations, an improved correlation composed of forced convection term and pure natural convection term is proposed, and shows a good agreement with the experiment data with deviations less than ±15%.

Applied Thermal Engineering, 2017, **125**: 995

Preparation and Characterization of Vanadium Carbide Coating on 3Cr13 Steel by Thermal Diffusion Process with Fluoride Salt Bath

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Huang Hefei Li Zhijun Li Xiaoli

Key words FLiNaK, thermal diffusion carbide coating process, 3Cr13 stainless steel, VC coatings

Vanadium carbide (VC) coatings were prepared on 3Cr13 stainless steel using FLiNaK salts through thermal diffusion carbide coating process (TD) for different time. The morphology, composition, hardness and growth kinetics of the VC coatings were investigated by scanning electron microscope (SEM), X-ray diffractometer (XRD), Vickers indenter, electronic probe microanalysis (EPMA) and energy dispersive X-ray spectrometry (EDX). Results show that the VC coatings of 3~5 μm in thickness form on the surface of 3Cr13 stainless steel. The coatings are petal-shaped and contain traces of Si and Fe. The average hardness of the VC coating is up to 32220 MPa and there is a parabola relationship between the thickness of the coatings and the

treatment time. VC coatings are covered by rimous SiO_2 phases with the thickness of hundreds of nanometers. The cracks of SiO2 phases result from the tensile stress during the cooling process, which derive from the different thermal expansivity between VC coating and SiO2 phase. The present study also indicates the potential application of FLiNaK salts in TD process.

Rare Metal Materials and Engineering, 2017, **46**(7): 2028

DEM-CFD simulation of modular PB-FHR core with two-grid method

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Key words PB-FHR, Pebble flow, DEM-CFD, Two-grid approach

For designing and optimizing the reactor core of modular pebble-bed fluoride salt-cooled high-temperature reactor (PB-FHR), it is of importance to simulate the coupled fluid and particle flow due to strong coolant–pebble interactions. Computational fluid dynamics and discrete element method (DEM) coupling approach can be used to track particles individually while it requires a fluid cell being greater than the pebble diameter. However, the large size of pebbles makes the fluid grid too coarse to capture the complicated flow pattern. To solve this problem, a two-grid approach is proposed to calculate interphase momentum transfer between pebbles and coolant without the constraint on the shape and size of fluid meshes. The solid velocity, fluid velocity, fluid pressure and void fraction are mapped between hexahedral coarse particle grid and fine fluid grid. Then the total interphase force can be calculated independently to speed up computation. To evaluate suitability of this two-grid approach, the pressure drop and minimum fluidization velocity of a fluidized bed were predicted, and movements of the pebbles in complex flow field were studied experimentally and numerically. The spouting fluid through a central inlet pipe of a scaled visible PB-FHR core facility was set up to provide the complex flow field. Water was chosen as liquid to simulate the molten salt coolant, and polypropylene balls were used to simulate the pebble fuels. Results show that the pebble flow pattern captured from experiment agrees well with the simulation from two-grid approach, hence the applicability of the two-grid approach for the later PB-FHR core design.

Nuclear Science and Techniques, 2017, **28**(7): 100

Microstructure and local strains in GH3535 alloy heat affected zone and their influence on the mechanical properties

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Key words EBSD, Twinning, Dislocations, Nickel based superalloys, Welding, Hardening

GH3535 alloy plates were welded by Gas Tungsten Arc Welding in order to study the evolution of microstructure and mechanical properties in the heat-affected zone (HAZ). Our results suggest that welding thermal cycles induced the morphology evolution of M_6C carbides from block to eutectic near the fusion line in the HAZ. Electron backscatter diffraction (EBSD) results show that significant amounts of plastic strains occurred in the HAZ after welding. In addition, local coherent twin boundaries (Σ3) and dislocations were observed to decrease with the distance from the fusion line. Mechanical tests indicate that the hardness, yield strength and ultimate strength in HAZ are higher than those in base metal, and their values decrease with the distance from the fusion line. However, the elongation increases as the strengths decrease. The higher strength and lower elongation in the HAZ are mainly attributed to residual strains with the function of strain-hardening. Moreover, the change of Σ3 boundary which is in good agreement with that of elongation suggests a positive influence on the plastic deformation.

Materials Science and Engineering: A , 2017, **699**: 48

Convective heat transfer characteristics in the laminar and transition region of molten salt in concentric tube

Chen YS Zhu HH Tian J Fu Y Tang ZF Wang NX

Key words Molten salt, Laminar flow, Transition flow, Heat exchanger, Heat transfer correlation

Convective heat transfer performances of molten salt for laminar and transition flow in concentric tube are experimentally investigated using molten salt as the hot fluid flowing through the inner concentric tube within the range of Reynolds number 300–10,000 and Prandtl number 11–27. Heat transfer coefficients of tube side molten salt are calculated using Wilson plots and the

heat transfer characteristics are studied by comparing with the traditional correlations. The results show that the laminar flow heat transfer coefficients of molten salt are higher than that of pure forced flow due to natural convection. In the transition region, the transition point to transition flow is expedited to critical Reynolds number down to 1800–2000 due to the effect of natural convection, which might increase the mean value of Nusselt number in low-Reynolds-number transition regime up to 1.3 times than that value predicted by Modified Petukhov correlation. Finally, based on the model of Churchill and Usagi, an overall correlated equation for all Re and Pr is proposed to predict the heat transfer characteristics for laminar and transition regimes. The correlated equation shows good agreement with the experiment data and higher accuracy than prior expressions for the restricted ranges of Re and Pr.

Applied Thermal Engineering, 2017, **117**: 682

Microstructure and mechanical properties of UNS N10003 alloy welded joints

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Li Zhijun Li Zhong Zhou Xingtai

Key words Nickel based alloy, Welding, M6C, Mechanical performance, Strengthening mechanism

Microstructure and mechanical performance of the welded joints of UNS N10003 alloy have been investigated in this work. Primary precipitates in base metal and eutectic precipitates in Heat Affected Zone (HAZ) and weld metal have been characterized and identified as M6C type. The hardness value of HAZ (Eutectic zone) is significantly higher than the rest of joint, including weld and base metal. Tensile tests suggested the welded joints possess a very stable mechanical performance at elevated temperature from 650 °C to 725 °C. Moreover all the tensile samples were fractured in base metal, indicating that the eutectic carbides have no adverse effects on the short-time mechanical performance of joint. The fine carbides, acting as dispersion strengthening in weld metal, are main contribution to enhance the hardness and strength of weld. The good mechanical performance of HAZ is ascribed to the presence of eutectic carbides and twins.

Materials Science and Engineering: A, 2017, **682**: 168

Evaluation on Microstructure and Mechanical Properties of Welded Joints by GMAW in UNS N10003 Alloy

Yu Kun Jiang Zhenguo Shi Xianwu Li Chaowen
Chen Shuangjian Li Zhijun Tao Wang Zhou Xingtai

Key words UNS N10003 alloy, GMAW, Microstructure, Mechanical properties

UNS N10003 alloy is a primary material of the Thorium Molten Salt Reactor (TMSR) in China that is a suitable candidate reactor of the Generation IV nuclear reactors. Gas metal arc welding (GMAW) is more effective than gas tungsten arc welding (GTAW) which is usually used to weld nickel-base alloys. In order to improve welding efficiency, it is necessary to weld nickel-base alloys using GMAW. The purpose of this work is to evaluate effect of GMAW on microstructure evolution and mechanical properties in UNS N10003 alloy. The results of microstructure showed that the sound welded joint without hot cracking can be obtained, although quantities of M_6C-γ eutectic phases with large size were precipitated in fusion zone (FZ) and transformed in heat affected zone (HAZ) because of element segregation. The results of microhardness test indicated that there was no softened zone in the welded joint. The results of tensile test at room temperature and high temperature showed that the short-term time-independent strength was not damaged by the formation of large M_6C-γ eutectic phases.

Proceedings of The ASME Pressure Vessels And Piping Conference, 2017, **6B**: UNSP V06BT06A019

An insight into the effects of B-site transition metals on the activity, activation effect and stability of perovskite oxygen electrodes for solid oxide electrolysis cells

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Fan Chou Chen Xinbing Liu Yihui

Key words Solid oxide electrolysis cells, Oxygen electrode, Perovskite, Activity, Stability

Here, effects of B-site transition metals (TMs) in the $(La_{0.6}Sr_{0.4})XO_{3-\delta}$ (X = Mn, Fe, Co) perovskite structure on the activity and stability of the oxygen electrodes during high temperature electrolysis are discussed to provide a deep understanding of the phenomena observed for different oxygen electrodes under anodic polarizations. Performance and stability of the electrodes vary significantly at 800 °C as the TMs changed from Mn to Fe and Co, which is attributed to the different ionic conductivities and surface chemistry of the materials that have a strong dependence

on the valence state and electronic structure of TMs. Under an anodic current passage of 200 mA cm^{-2} at 800 °C, electrode polarization resistance (RE) and overpotential (η) of the $(La_{0.6}Sr_{0.4})MnO_{3-\delta}$ (LSM) electrode decrease significantly by 1.75 Ω cm^2 and 101 mV during the 1200 min test, compared with the constant values of R_E and η for the $(La_{0.6}Sr_{0.4})FeO_{3-\delta}$ (LSF) and $(La_{0.6}Sr_{0.4})CoO_{3-\delta}$ (LSC) electrodes, an indication of the influence of B-site TMs on the electrode performance and stability. Most serious degradation is observed at the $(La_{0.6}Sr_{0.4})MnO_{3-\delta}$ electrode due to the electrode detachment arising from the accelerated SrO surface segregation and related disintegration of LSM particles near the electrode/electrolyte interface.

Journal of Power Sources, 2017, **363**: 470

Thermodynamic modeling of the $Ca(NO_3)_2$-MNO_3 (M: alkali metal) systems

Li Xiang　Wang Kun　Shen Miao　Wu Zhu　Xie Leidong

Key words　Molten salts, Thermodynamics, Phase equilibria, Energy storage

This work presents a thermodynamic evaluation of the $Ca(NO_3)_2$-MNO_3 (M: Li, Na, K, Rb, Cs) binary systems using the CALPHAD approach. The required Gibbs energy of liquid $Ca(NO_3)_2$ is missing in the literature and has been successfully evaluated in the present work with a fusion enthalpy of 23849 J mol^{-1} . The substitutional solution model can thus be employed to describe the $Ca(NO_3)_2$-base liquid phase. All the intermediate compounds are treated to be stoichiometric and their Gibbs energies comply with the Neumann-Kopp rule. Empirical functions relating mixing enthalpies to ionic parameters are employed to predict the corresponding values of binary melts which are used as input data to assist in parameters optimization for the liquid phases. The final calculated results show good agreement with most of the experimental and predicted data

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CALPHAD: Computer Coupling of Phase Diagrams and Thermochemistry, 2017, **59**: 90

Probing the Influence of Acidity and Temperature to Th(Ⅳ) on Hydrolysis, Nucleation, and Structural Topology

Lin Jian　Qie Meiying　Zhang Linjuan　Wang Xiaomei　Lin Yuejian　Liu Wei　Bao Hongliang　Wang Jianqiang

Systematic control of the molar ratio between thorium hydroxides and selenic acid and their reaction temperature under hydrothermal conditions results in four novel thorium-based selenate complexes, namely, $[Th_8O_4(OH)_8(SeO_4)_6(H_2O)_{16}]\cdot(SeO_4)_2\cdot 13H_2O$ (**Th-1**),

$[Th_8O_4(OH)_8(SeO_4)_8(H_2O)_{13}]\cdot 7H_2O$ (**Th-2**), $Th(OH)_2(SeO_4)H_2O$ (**Th-3**), and $Th_3(SeO_4)_6(H_2O)_6\cdot 2.5H_2O$ (**Th-4**), as well as the thorium mixed selenite selenate compound $Th(SeO_3)(SeO_4)$ (**Th-5**). Smaller $[H_2SeO_4]$/[Th(IV)] ratio or lower temperature give rise to the formation of octameric $[Th_8(\mu_3\text{-}O)_4(\mu_2\text{-}OH)_8]^{16+}$ cores in **Th-1**/**Th-2** and infinite $[Th(\mu_2\text{-}OH)_2H_2O]^{2+}$ chains in **Th-3**, respectively. Increasing the $[H_2SeO_4]$/[Th(IV)] ratio or elevating the temperature generates a microporous (11.3 Å voids) open-framework **Th-4**, a monomeric thorium species without oxo/hydroxyl ligands, and a three-dimensional thorium structure **Th-5**. Formation of these compounds suggests that variables including acidity and temperature play a critical role in the hydrolysis and oligomerization of Th^{IV} ions. Increasing acidity limits the deprotonation of water molecules and formation of nucleophilic hydroxo/oxo-aquo Th species, and high temperature appears to suppress the olation/oxolation hydrolysis reactions, which in both ways limit the formation of the thorium oligomers.

Inorganic Chemistry, 2017, **56**(22): 14198

A perspective on hydrogen production *via* high temperature steam electrolysis

Chen Xinbing Guan Chengzhi Xiao Guoping
Peng Cheng Wang JianQiang

Science China Chemistry, 2017, **60**(11): 1379

Thermodynamic modeling of the GdF_3-MF (M: Li, K, Rb, Cs) systems

Li Xiang Wang Kun Xie Leidong

Key words Phase equilibria, Thermodynamic properties, Ionic parameter

The phase equilibria and thermochemical data for the GdF_3-MF (M: Li, K, Rb, Cs) binary systems were critically evaluated and optimized based upon the CALPHAD approach. Two kinds of models like associated and substitutional solution were used to describe the liquid phase where cations were apt to form short range order (SRO) and random mixing, respectively. All the intermediate compounds were treated as stoichiometric of which Gibbs energies comply with the Neumann-Kopp rule. Model parameters optimization for respective phases was conducted by the least squares minimization procedure with required input data available from experimental measurements and empirical predictions (ionic parameter function). Satisfactory agreements

between all calculated results and experimental & predicted data were achieved which demonstrates that thermodynamic databases for the GdF_3-MF (M: Li, K, Rb, Cs) binary systems were ultimately derived in the present work allowing safe extrapolation into multicomponent system for guiding relative industrial applications.

Fluid Phase Equilibria, 2017, **449**: 18

Thermodynamic description of the MCl_2-$ThCl_4$ (M: Mg, Ca, Sr, Ba) systems

Xie Mengya Li Xiang Ding Yaping Zhang Guoxin

Key words Thermodynamics, Molten salt, Phase diagram

The phase equilibria for the MCl_2-$ThCl_4$(M: Mg, Ca, Sr, Ba) binary systems were critically evaluated and optimized based upon the CALPHAD approach. The substitutional solution model(SSM) was used to describe the liquid phase. All the intermediate compounds were treated as stoichiometric compounds of which Gibbs energies comply with the Neumann-Kopp rule. Thermodynamic model parameters optimization for respective phases was conducted by the least squares minimization procedure with required input data available from experimental measurements. Satisfactory agreements between all calculated results and experimental data were achieved which demonstrates that thermodynamic databases for the MCl_2-$ThCl_4$(M: Mg, Ca, Sr, Ba) binary systems were ultimately derived in the present work allowing safe extrapolation into multi-component system for guiding relative industrial applications.

Chemical Research in Chinese Universities, 2017, **33**(5): 794

Investigation on molecular structure of molten Li_2BeF_4 (FLiBe) salt by infrared absorption spectra and density functional theory (DFT)

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Zhang Peng Liu Hongtao Yao Side
Xie Leidong Hou Huiqi

Key words Infrared absorption spectra, High temperature, Density functional theory, Li_2BeF_4

FLiBe ($2LiF\text{-}BeF_2$) molecular structure was investigated by infrared (IR) absorption spectroscopy combined with density functional theory (DFT) calculations. An instrument was designed and implemented to obtain the in situ IR absorption spectra of molten FLiBe salt. IR absorption spectrum of molten FLiBe salt was obtained at 600 °C and the spectra assignment were aided with the density functional theory (DFT) calculations, which indicated that liquid FLiBe salt can form fluoberyllate of $[BeF_4]^{2-}$. The IR spectrum of FLiBe powder acquired at room temperature furthers to imply that $[BeF_4]^{2-}$ was formed and combined with two Li^+ to make neutral molecule of Li_2BeF_4. Based on the geometry optimization, absorption peaks were also assigned and detailed vibration information was supplied.

Journal of Molecular Liquids, 2017, **242**: 1052

Insight into the Role of Metal–Oxygen Bond and O 2p Hole in High-Voltage Cathode $LiNi_xMn_{2-x}O_4$

Liu Hengjie Zhou Jing Zhang Linjuan Hu Zhiwei
Kuo Changyang Li Jiong Wang Yu Tjeng Liu Hao
Pi Tun-Wen Tanaka Arata Song Li
Wang JianQiang Zhang Shuo

The role of transition-metal d and ligand p hybridization continues to be of immense interest in Li-ion battery cathode, and yet it is still poorly understood. Using combined experimental and theoretical soft X-ray absorption spectroscopic study and density functional theory calculation, we investigated the fundamental electronic structure of the high-voltage spinel $LiNi_xMn_{2-x}O_4$. An oxygen-participating charge rebalance between manganese and nickel ions was found; that is, the content of O 2p holes close to the Fermi level increases along with the increasing Ni content. Moreover, these unstable oxygen holes primarily congregate around the redox active dopants. The underlying mechanism accounting for this charge-compensated occurrence is the reverse of two bonding levels when manganese ions are oxidized from +3 to +4 states. On the basis of these new findings, we further exposed the role of oxygen in electrochemical performance. First, oxygen ions afford the charge variation together with the cations during Li insertion/deinsertion process. Second, the O 2p holes can largely screen the strong electrostatic repulsion between Mn^{4+} and Li^+ ions to effectively enhance the rate capacity. Lastly, the excessive amount of O 2p holes is disadvantageous to the thermal stability associated with the O_2 evolution. Also, we point out that O 2p holes concentration can be modified by the metal–oxygen bonding character, and the "charge-transfer energy" is a crucial point for designing high-capacity positive electrodes for Li-ion battery.

Journal of Physical Chemistry C, 2017, **121**(30): 16079

Identification of Superoxide O_2^- during Thermal Decomposition of Molten KNO_3-$NaNO_2$-$NaNO_3$ Salt by Electron Paramagnetic Resonance and UV-Vis Absorption Spectroscopy

Liu Shuting Su Tao Zhang Peng Fei Zejie) Liu Hongtao

Key words Superoxide, Decomposition of heat transfer salt, High temperature UV-visible, Electron paramagnetic resonance

On account of excellent thermal physical properties, molten nitrates/nitrites salt has been widely employed in heat transfer and thermal storage industry, especially in concentrated solar power system. The thermal stability study of molten nitrate/nitrite salt is of great importance for this system, and the decomposition mechanism is the most complicated part of it. The oxide species O_2^{2-} and O_2^- were considered as intermediates in molten KNO_3-$NaNO_3$ while hard to been detected in high temperature molten salt due to their trace concentration and low stability. In this work, the homemade *in situ* high temperature UV-Vis instrument and a commercial electron paramagnetic resonance were utilized to supply evidence for the formation of superoxide during a slow decomposition process of heat transfer salt (HTS, 53 wt% KNO_3/40 wt% $NaNO_2$/7 wt% $NaNO_3$). It is found that the superoxide is more easily generated from molten $NaNO_2$ compared to $NaNO_3$, and it has an absorption band at 420–440 nm in HTS which red shifts as temperature increases. The band is assigned to charge-transfer transition in NaO_2 or KO_2, responsible for the yellow color of the molten nitrate/nitrite salt. Furthermore, the UV absorption bands of molten $NaNO_2$ and $NaNO_3$ are also obtained and compared with that of HTS.

Chinese Journal of Chemical Physics, 2017, **30**(4): 372

Adsorption of uranium (VI) onto amidoxime-functionalized ultra-high molecular weight polyethylene fibers from aqueous solution

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Bao HongLiang Guan ChengZhi Jin Chan Wang JianQiang

Key words Uranium; Adsorption; Kinetics; Isotherms; Sintering

Amidoxime-functionalized ultra-high molecular weight polyethylene fibers (UHMWPEF-AO) were used to absorb uranium U(VI) from aqueous solutions. In this paper, we study effects of pH,

initial U(VI) concentration, contact time, and temperature on U(VI) adsorption by UHMWPEF-AO. The adsorption process agrees well with pseudo-second-order and Langmuir model. UHMWPEF-AO exhibits excellent adsorptive performance for U(VI) with a maximum adsorption capacity of 176.12 mg/g at pH 4 and 298 K. The structures of UHMWPEF-AO and U(VI)-loaded UHMWPEF-AO are characterized by FT-IR and nano-CT. U(VI)-loaded UHMWPEF-AO is sintered after adsorption process to recycle absorbed U(VI). Powders collected after sintering process are examined by scanning electron microscopy and X-ray diffraction. These results indicate that UHMWPEF-AO is a promising candidate to remove U(VI) from uranium aqueous solutions.

Nuclear Science and Techniques, 2017, **28**(7): 94

A Breakthrough Efficiency of 19.9% Obtained in Inverted Perovskite Solar Cells by Using an Efficient Trap State Passivator Cu(thiourea)I

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Bao Hongliang Sun Weihai Li Yunlong Gu Feidan
Wang Jianqiang Liu Zhiwei Bian Zuqiang Huang Chunhui

It is extremely significant to study the trap state passivation and minimize the trap states of perovskite to achieve high-performance perovskite solar cells (PSCs). Here, we have first revealed and demonstrated that a novel p-type conductor Cu(thiourea)I [Cu(Tu)I] incorporated in perovskite layer can effectively passivate the trap states of perovskite via interacting with the under-coordinated metal cations and halide anions at the perovskite crystal surface. The trap state energy level of perovskite can be shallowed from 0.35–0.45 eV to 0.25–0.35 eV. In addition, the incorporated Cu(Tu)I can participate in constructing the p–i bulk heterojunctions with perovskite, leading to an increase of the depletion width from 126 to 265 nm, which is advantageous for accelerating hole transport and reducing charge carrier recombination. For these two synergistic effects, Cu(Tu)I can play a much better role than that of the traditional p-type conductor CuI, probably due to its identical valence band maximum with that of perovskite, which enables to not only lower the trap state energy level to a greater extent but also eliminate the potential wells for holes at the p–i heterojunctions. After optimization, a breakthrough efficiency of 19.9% has been obtained in the inverted PSCs with Cu(Tu)I as the trap state passivator of perovskite.

Journal of the American Chemical Society, 2017, **139**(22): 7504

Investigating the influence of F^- on U^{4+} in molten $LiCl–KCl–UF_4$ system and electro-deposition of U

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Jiang Feng Wang Xianbin Yu Gong
Long Dewu Li Qingnuan

Key words F- influence, Uranium ion, LiCl-KCl molten salt, Spent fuel

Electrochemical behaviors of U^{4+} in $LiCl–KCl–UF_4$ eutectic and deposition of U metal were investigated. It was found that the presence of F^- has influence on the diffusion of U^{3+} and U^{4+} as comparing to data obtained in pure chloride molten salts. Electrochemical deposition of U was carried out by using pulse current electrolysis. Characterization results indicate that U metal was obtained at the cathode, implying U metal can be directly deposited from $LiCl–KCl–UF_4$ eutectic in this case and the extractive ratio is calculated to be 98%. Our results demonstrate feasible separation of U from $LiCl–KCl–UF_4$ molten salt by electrochemical method.

Journal of Radioanalytical and Nuclear Chemistry, 2017, **312**(3): 479

Thermodynamic reevaluation and experimental validation of the $CsNO_3$-KNO_3-$NaNO_3$ system and its subsystems

An Xuehui Zhang Peng Cheng Jinhui
Chen Shuanglin Wang Jianqiang

Key words Thermal energy storage, Nitrate, Calphad, Phase diagram

Phase equilibria and thermodynamic properties of the $CsNO_3$-KNO_3-$NaNO_3$ system and its three subsys-tems were optimized thermodynamically and validated experimentally. The liquid and end solid solution phases of the KNO_3-$NaNO_3$ and $CsNO_3$-KNO_3 systems were modeled using the substitutional solution and compound energy formalism models, respectively. The $CsNO_3$-KNO_3-$NaNO_3$ ternary system was described thermodynamically based on the self-consistent thermodynamic parameters of the three binary systems. A set of thermodynamic parameters was obtained to reproduce the available information on the thermodynamic properties and phase equilibria. Melting temperature, enthalpy, and specific heat capacity of a eutectic sample were determined using differential scanning calorimetry(DSC). The results show a good consistency with the calculated results, suggesting the reliability of the current thermodynamic database. This work is useful for the construction of multicomponent nitrates and to provide guidance for the development of new medium for thermal energy storage.

Chemical Research in Chinese Universities, 2017, **33**(1): 122

Simulation study of slow extraction for the Shanghai Advanced Proton Therapy facility

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Key words Slow extraction, Accelerator model, Spill ripple, Particle beam therapy, Synchrotron

The Shanghai Advanced Proton Therapy facility employs third-integer slow extraction. In order to achieve accurate treatment, high-quality spill is needed. Therefore, parameters that may affect slow extraction should be investigated by simulation. A computer model of the synchrotron operation slow extraction was constructed with MATLAB®. By simulating the motion of the circulating protons, we could quantify the influence of machine and initial beam parameters on properties of the extracted beam, such as ripple, uniformity, stability, on- and off-time of the spill and spill width in the synchrotron. Suitable design parameters including the horizontal tunes, power supply ripple, longitudinal RF cavity voltage, RF-KO and the chromaticities were determined.

Nuclear Science and Techniques, 2017, **28**(9): 120

Low emittance lattice design with Robinson wiggler in the arc section

Tian ShunQiang Zhang QingLei Zhang ManZhou Wang Kim Jiang BoCheng

Key words Emittance reduction, Damping partition number, Synchrotron light source

Beam emittance reduction is an effective method to increase the brightness of a synchrotron light source. Robinson wiggler can play a role in the beam emittance reduction by increasing the horizontal damping partition number. A replacement of the quadrupoles in the arc section with short combined function dipoles will construct a single-periodic Robinson wiggler in the SSRF storage ring. This scheme provides a lower beam emittance, without occupying any straight section. Detailed analysis is presented in this paper.

Nuclear Science and Techniques, 2017, **28**(1): 9

Investigation on demagnetization of $Nd_2Fe_{14}B$ permanent magnets induced by irradiation

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Wang Guanghong Xia Xiaobin

Key words Demagnetization, $Nd_2Fe_{14}B$, FLUKA, Radiation damage, Microstructure evolution, Ar ion irradiation

$Nd_2Fe_{14}B$ is an important component of insertion devices, which are used in synchrotron radiation sources, and could be demagnetized by irradiation. In the present study, the Monte Carlo code FLUKA was used to analyze the irradiation field of $Nd_2Fe_{14}B$, and it was confirmed that the main demagnetization particle was neutron. $Nd_2Fe_{14}B$ permanent magnet samples were irradiated by Ar ions at different doses to simulate neutron irradiation damage. The hysteresis loops were measured using a vibrating sample magnetometer, and the microstructure evolutions were characterized by transmission electron microscopy. Moreover, the relationship between them was discussed. The results indicate that the decrease in saturated magnetization is caused by the changes in microstructure. The evolution of single crystals into an amorphous structure is the reason for the demagnetization phenomenon of $Nd_2Fe_{14}B$ permanent magnets when considering its microscopic structure.

Nuclear Instruments and Methods in Physics Research Section B: Beam Interactions with Materials and Atoms, 2017, **413**: 48

Eddy current effects in a high field dipole

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Zhang JiDong Ouyang LianHua Li Rui Li DeMing

Key words Eddy current, Time delay, Magnetic field measurement, Dipole, Field control

Eddy currents produced by a time-varying magnetic field will introduce time delay and thus affect field quality. This effect leads to drifting of the beam position over time, especially for a compact synchrotron. Simulations and measurements of different dipoles have been performed, to investigate the time delay and field quality. The simulations are conducted using OPERA software. The measurements are conducted using a long coil and Hall sensor. All results show that the magnetic field deviation is up to 0.4% for the dipole with stainless steel endplates. The simulations show that the main sources of eddy current are the field saturation effect and the field component B_z, introduced by the bedstead-type coil. Field correction using a power supply is adopted to reduce the deviation to less than 0.02%.

Nuclear Science and Techniques, 2017, **28**(12): 173

Development of a Superconducting Undulator Prototype at the SSRF

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Sun Sen Cui Jian Zhang Wei Wang Li
Zhou Qiaogen Yin Lixin

Key words Synchrotron radiation, undulators, cryogenics, superconducting magnets

Development of a 50-period superconducting undulator prototype is underway at the Shanghai Synchrotron Radiation Facility. The prototype is composed of magnetic system, cooling system, and cryostat. The SCU magnet system has a period length of 16 mm and a magnetic gap of 9.5 mm. The coils are wound with NbTi/Cu conductors. The design operation current is 400 A to produce a peak field on axis of 0.67 T. The cooling system includes four cryocoolers and independent cooling circuits for magnet and the beam vacuum chamber. The manufacturing of the magnet and beam vacuum chamber is in progress. The cooling test of the cryostat was performed using a dummy load. Stand-alone test of the prototype is planned in December 2016. Installation into the storage ring is scheduled in July 2017.

IEEE Transactions on Applied Superconductivity, 2017, **27**(4): 4100304

Low energy analysis techniques for CUORE

CUORE Collaboration

CUORE is a tonne-scale cryogenic detector operating at the Laboratori Nazionali del Gran Sasso (LNGS) that uses tellurium dioxide bolometers to search for neutrinoless double-beta decay of ^{130}Te. CUORE is also suitable to search for low energy rare events such as solar axions or WIMP scattering, thanks to its ultra-low background and large target mass. However, to conduct such sensitive searches requires improving the energy threshold to 10 keV. In this paper, we describe the analysis techniques developed for the low energy analysis of CUORE-like detectors, using the data acquired from November 2013 to March 2015 by CUORE-0, a singletower prototype designed to validate the assembly procedure and new cleaning techniques of CUORE. We explain the energy threshold optimization, continuous monitoring of the trigger efficiency, data and event selection, and energy calibration at low energies in detail. We also present the low energy background spectrum of CUORE-0 below 60 keV. Finally, we report the sensitivity of CUORE to WIMP annual modulation using the CUORE-0 energy threshold and background, as well as an estimate of the uncertainty on the nuclear quenching factor from nuclear recoils inCUORE-0

The European Physical Journal C, 2017, **77**(12): 857

Coherent diffractive photoproduction of ρ^0 mesons on gold nuclei at 200 GeV/nucleon-pair at the Relativistic Heavy Ion Collider

STAR Collaboration

The STAR Collaboration reports on the photoproduction of $\pi^+\pi^-$ pairs in gold-gold collisions at a center-of-mass energy of 200 GeV/nucleon-pair. These pion pairs are produced when a nearly real photon emitted by one ion scatters from the other ion.

We fit the $\pi^+\pi^-$ invariant-mass spectrum with a combination of ρ^0 and ω resonances and a direct $\pi^+\pi^-$ continuum. This is the first observation of the ω in ultraperipheral collisions, and the first measurement of ρ−ω interference at energies where photoproduction is dominated by Pomeron exchange. The ω amplitude is consistent with the measured $\gamma p \rightarrow \omega p$ cross section, a classical Glauber calculation, and the $\omega \rightarrow \pi^+\pi^-$ branching ratio. The ω phase angle is similar to that observed at much lower energies, showing that the ρ−ω phase difference does not depend significantly on photon energy.

The ρ^0 differential cross section dσ/dt exhibits a clear diffraction pattern, compatible with scattering from a gold nucleus, with two minima visible. The positions of the diffractive minima agree better with the predictions of a quantum Glauber calculation that does not include nuclear shadowing than with a calculation that does include shadowing.

Physical Review C, 2017, **96**(5): 054904

Bulk properties of the medium produced in relativistic heavy-ion collisions from the beam energy scan program

STAR Collaboration

We present measurements of bulk properties of the matter produced in Au+Au collisions at $\sqrt{S_{NN}}$=7.7,11.5,19.6,27, and 39 GeV using identified hadrons ($\pi^{\pm}$, $K^{\pm}$, p, and $\bar{p}$) from the STAR experiment in the Beam Energy Scan (BES) Program at the Relativistic Heavy Ion Collider (RHIC). Midrapidity (|y|<0.1) results for multiplicity densities dN/dy, average transverse momenta <pT>, and particle ratios are presented. The chemical and kinetic freeze-out dynamics at these energies are discussed and presented as a function of collision centrality and energy. These results constitute the systematic measurements of bulk properties of matter formed in heavy-ion collisions over a broad range of energy (or baryon chemical potential) at RHIC.

Physical Review C, 2017, **96**(4): 044904

Scalar field quasinormal frequencies of Reissner–Nordström black hole surrounded by quintessence by using the continued fraction method

Wu Chen

Key words Scalar perturbation, dark energy, quasinormal modes

We evaluate the quasinormal modes of massless scalar field around Reissner–Nordström black hole surrounded by a static and spherically symmetric quintessence using the continued fraction method. The appropriate Frobenius series for three special cases of the quintessence parameter $\epsilon=-1/3,-2/3\epsilon=-1/3,-2/3$ and $-1-1$ are derived successfully. We show the variation of quasinormal frequencies with charge of the black hole and the quintessential parameters. The numerical results show that quintessence field decreases oscillation frequencies of all angular momentum ll modes and increases the damping time of $l>0l>0$ modes.

International Journal of Modern Physics D, 2017, **26**(10)1750111:

The projected background for the CUORE experiment

CUORE Collaboration

The Cryogenic Underground Observatory for Rare Events (CUORE) is designed to search for neutrinoless double beta decay of ^{130}Te with an array of 988 TeO^2 bolometers operating at temperatures around 10 mK. The experiment is currently being commissioned in Hall A of Laboratori Nazionali del Gran Sasso, Italy. The goal of CUORE is to reach a 90% C.L. exclusion sensitivity on the ^{130}Te decay half-life of 9×10^{25} years after 5 years of data taking. The main issue to be addressed to accomplish this aim is the rate of background events in the region of interest, which must not be higher than 10^{-2} counts/keV/kg/year. We developed a detailed Monte Carlo simulation, based on results from a campaign of material screening, radioassays, and bolometric measurements, to evaluate the expected background. This was used over the years to guide the construction strategies of the experiment and we use it here to project a background model for CUORE. In this paper we report the results of our study and our expectations for the background rate in the energy region where the peak signature of neutrinoless double beta decay of ^{130}Te is expected.

European Physical Journal C, 2017, **77**(8): 543

Measurements of jet quenching with semi-inclusive hadron+jet distributions in Au+Au collisions at $\sqrt{S_{NN}}$ =200 GeV

STAR Collaboration

The STAR Collaboration reports the measurement of semi-inclusive distributions of charged-particle jets recoiling from a high transverse momentum hadron trigger, in central and peripheral Au+Au collisions at $\sqrt{S_{NN}}$ = 200 GeV. Charged jets are reconstructed with the anti-kT algorithm for jet radii R between 0.2 and 0.5 and with low infrared cutoff of track constituents (p_T>0.2 GeV/c). A novel mixed-event technique is used to correct the large uncorrelated background present in heavy ion collisions. Corrected recoil jet distributions are reported at mid-rapidity, for charged-jet transverse momentum $P'^{\mathrm{ch}}_{T,jet}$ < 30 GeV/c. Comparison is made to similar measurements for Pb+Pb collisions at $\sqrt{S_{NN}}$= 2.76 TeV, to calculations for p+p collisions at s√ = 200 GeV based on the PYTHIA Monte Carlo generator and on a Next-to-Leading Order perturbative QCD approach, and to theoretical calculations incorporating jet quenching. The recoil jet yield is suppressed in central relative to peripheral collisions, with the magnitude of the suppression corresponding to medium-induced charged energy transport out of the jet cone of 2.8±0.2(stat)±1.5(sys) GeV/c, for 10< $P'^{\mathrm{ch}}_{T,jet}$ < 20 GeV/c and R = 0.5. No medium-induced change in jet shape is observed for R< 0.5. The azimuthal distribution of low-$P'^{\mathrm{ch}}_{T,jet}$ recoil jets may be enhanced at large azimuthal angles to the trigger axis, due to scattering off quasi-particles in the hot QCD medium. Measurement of this distribution gives a 90% statistical confidence upper limit to the yield enhancement at large deflection angles in central Au+Au collisions of 50±30(sys)% of the large-angle yield in p+p collisions predicted by PYTHIA.

Physical Review C, 2017, **96**(2): 024905

Energy dependence of J/ψ production in Au + Au collisions at $\sqrt{S_{NN}}$= 39, 62.4 and 200 GeV

STAR Collaboration

The inclusive J/ψ transverse momentum spectra and nuclear modification factors are reported at midrapidity (|y| < 1.0) in Au+Au collisions at $\sqrt{S_{NN}}$ = 39, 62.4 and 200 GeV taken by the STAR experiment. A suppression of J/ψ production, with respect to the production in p + p scaled

by the number of binary nucleon–nucleon collisions, is observed in central Au+Au collisions at these three energies. No significant energy dependence of nuclear modification factors is found within uncertainties. The measured nuclear modification factors can be described by model calculations that take into account both suppression of direct J/ψ production due to the color screening effect and J/ψ regeneration from recombination of uncorrelated charm–anticharm quark pairs

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Physics Letters B, 2017, **771**: 13

Dijet imbalance measurements in Au+Au and pp collisions at $\sqrt{S_{NN}}$=200 GeV at STAR

STAR Collaboration

We report the first dijet transverse momentum asymmetry measurements from Au+Au and pp collisions at RHIC. The two highest-energy back-to-back jets reconstructed from fragments with transverse momenta above 2 GeV/c display a significantly higher momentum imbalance in heavy-ion collisions than in the pp reference. When reexamined with correlated soft particles included, we observe that these dijets then exhibit a unique new feature—momentum balance is restored to that observed in pp for a jet resolution parameter of R=0.4, while rebalancing is not attained with a smaller value of R=0.2.

Physical Review Letters, 2017, **119**(6): 062301

CUORE sensitivity to 0νββ decay

CUORE Collaboration

We report a study of the CUORE sensitivity to neutrinoless double beta (0νββ) decay. We used a Bayesian analysis based on a toy Monte Carlo (MC) approach to extract the exclusion sensitivity to the 0νββ decay half-life ($T^{0\nu}_{1/2}$) at 90%90% credibility interval (CI) – i.e. the interval containing the true value of $T^{0\nu}_{1/2}$ with 90% probability – and the 3 σ discovery sensitivity. We consider various background levels and energy resolutions, and describe the influence of the data division in subsets with different background levels. If the background level and the energy resolution meet the expectation, CUORE will reach a 90% CI exclusion sensitivity of $2 \cdot 10^{25}$year with 3 months, and $9 \cdot 10^{25}$ year with 5 years of live time. Under the same conditions, the discovery sensitivity after 3 months and 5 years will be $7 \cdot 10^{24}$ year and $4 \cdot 10^{25}$ year, respectively.

The European Physical Journal C, 2017, **77**(8): 532

Global Λ hyperon polarization in nuclear collisions

STAR Collaboration

The extreme energy densities generated by ultra-relativistic collisions between heavy atomic nuclei produce a state of matter that behaves surprisingly like a fluid, with exceptionally high temperature and low viscosity. Non-central collisions have angular momenta of the order of 1,000$\hbar$, and the resulting fluid may have a strong vortical structure that must be understood to describe the fluid properly. The vortical structure is also of particular interest because the restoration of fundamental symmetries of quantum chromodynamics is expected to produce novel physical effects in the presence of strong vorticity. However, no experimental indications of fluid vorticity in heavy ion collisions have yet been found. Since vorticity represents a local rotational structure of the fluid, spin–orbit coupling can lead to preferential orientation of particle spins along the direction of rotation. Here we present measurements of an alignment between the global angular momentum of a non-central collision and the spin of emitted particles (in this case the collision occurs between gold nuclei and produces Λ baryons), revealing that the fluid produced in heavy ion collisions is the most vortical system so far observed. (At high energies, this fluid is a quark–gluon plasma.) We find that Λ and $\overline{\Lambda}$ hyperons show a positive polarization of the order of a few per cent, consistent with some hydrodynamic predictions. (A hyperon is a particle composed of three quarks, at least one of which is a strange quark; the remainder are up and down quarks, found in protons and neutrons.) A previous measurement that reported a null result, that is, zero polarization, at higher collision energies is seen to be consistent with the trend of our observations, though with larger statistical uncertainties. These data provide experimental access to the vortical structure of the nearly ideal liquid created in a heavy ion collision and should prove valuable in the development of hydrodynamic models that quantitatively connect observations to the theory of the strong force.

Nature, 2017, **548**(7665): 62

Direct virtual photon production in Au+Au collisions at $\sqrt{S_{NN}}$ = 200 GeV

STAR Collaboratio

We report the direct virtual photon invariant yields in the transverse momentum ranges 1<pT<3GeV/c and 5<pT<10GeV/c at mid-rapidity derived from the dielectron

invariant mass continuum region $0.10<M_{ee}<0.28 GeV/c^2$ for 0–80% minimum-bias Au+Au collisions at $\sqrt{S_{NN}}$ =200GeV. A clear excess in the invariant yield compared to the nuclear overlap function T_{AA} scaled p+p reference is observed in the p_T range $1<p_T<3 GeV/c$. For $p_T>6 GeV/c$ the production follows T_{AA} scaling. Model calculations with contributions from thermal radiation and initial hard parton scattering are consistent within uncertainties with the direct virtual photon invariant yield.

Physics Letters B, 2017, **770**: 451

Measurement of D^0 Azimuthal Anisotropy at Midrapidity in Au+Au Collisions at $\sqrt{S_{NN}}$ = 200 GeV

STAR Collaboration

We report the first measurement of the elliptic anisotropy (v2) of the charm meson D^0 at midrapidity (|y|<1) in Au+Au collisions at $\sqrt{S_{NN}}$=200 GeV. The measurement was conducted by the STAR experiment at RHIC utilizing a new high-resolution silicon tracker. The measured D^0 v2 in 0%–80% centrality Au+Au collisions can be described by a viscous hydrodynamic calculation for a transverse momentum (pT) of less than 4 GeV/c. The D^0 v2 as a function of transverse kinetic energy (mT−m0, where mT=$\sqrt{P_T^{2+}m_0^2}$) is consistent with that of light mesons in 10%–40% centrality Au+Au collisions. These results suggest that charm quarks have achieved local thermal equilibrium with the medium created in such collisions. Several theoretical models, with the temperature-dependent, dimensionless charm spatial diffusion coefficient ($2\pi TD_s$) in the range of ∼2–12, are able to simultaneously reproduce our D^0 v2 result and our previously published results for the D^0 nuclear modification factor.

Physical Review Letters, 2017, **118**(21): 212301

The CUORE cryostat and its bolometric detector

CUORE Collaboration

Key words Calorimeters, Cryogenic detectors, Cryogenics and thermal models, Double-beta decay detectors

CUORE is a cryogenic detector that will be operated at LNGS to search for neutrinoless double beta decay ($0\nu\beta\beta$) of ^{130}Te. The detector installation was completed in summer 2016. Before the installation, several cold runs were done to test the cryogenic system performance. In the last

cold run the base temperature of 6.3 mK was reached in stable condition. CUORE-0, a CUORE prototype, has proven the feasibility of CUORE, demonstrating that the target background of 0.01 counts/keV/kg/y and the energy resolution of 5 keV are within reach.

Journal of Instrumentation, 2017, **12**: C02055

Measurement of the two-neutrino double-beta decay half-life of ^{130}Te with the CUORE-0 experiment

CUORE Collaboration

We report on the measurement of the two-neutrino double-beta decay half-life of ^{130}Te with the CUORE-0 detector. From an exposure of 33.4 kg year of TeO2, the half-life is determined to be $T^{2\nu}_{1/2}$=[8.2±0.2(stat.) ±0.6 (syst.)]×10^{20}year. This result is obtained aftera detailed reconstruction of the sources responsible for the CUORE-0 counting rate, with a specific study of those con-tributing to the ^{130}Te neutrinoless double-beta decay regionof interest

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The European Physical Journal C, 2017, **77**(1): 13

Charge-Dependent Directed Flow in Cu+Au Collisions at $\sqrt{S_{NN}}$ =200 GeV

STAR Collaboration

We present the first measurement of charge-dependent directed flow in Cu+Au collisions at $\sqrt{S_{NN}}$=200 GeV. The results are presented as a function of the particle transverse momentum and pseudorapidity for different centralities. A finite difference between the directed flow of positive and negative charged particles is observed that qualitatively agrees with the expectations from the effects of the initial strong electric field between two colliding ions with different nuclear charges. The measured difference in directed flow is much smaller than that obtained from the parton-hadron-string-dynamics model, which suggests that most of the electric charges, i.e., quarks and antiquarks, have not yet been created during the lifetime of the strong electric field, which is of the order of, or less than, 1 fm/c.

Physical Review Letters, 2017, **118**(1): 012301

Mean free path and shear viscosity in central ^{129}Xe+^{119}Sn collisions below 100 MeV/nucleon

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Lopez O Veselsky M

Thermal and transport properties of hot nuclear matter formed in central ^{129}Xe+^{119}Sn collisions at the Fermi energy are investigated using the isospin-dependent quantum molecular dynamical model. Temperature (T), average density (ρ), chemical potential (μ), mean momentum (P), shear viscosity (η), and entropy density (s) are obtained from the phase-space information. The mean free path (λ_{nn}) and the in-medium nucleon-nucleon cross section (σ_{nn}) in the highest compressible stage at different incident energies are deduced and compared with the experimental results from Phys. Rev. C **90**, 064602 (2014). The result shows that λ_{nn} and σ_{nn} have the same trend and similar values as the experimental results when the beam energy is greater than 40 MeV/nucleon at maximum compressed state. Furthermore, the derived shear viscosity over entropy density (η/s) shows a decreasing behavior to a saturated value around $\frac{3}{4\pi}$ as a function of incident energy.

Physical Review C, 2017, **96**(6): 064604

Revisiting directed flow in relativistic heavy-ion collisions from a multiphase transport model

Guo ChongQiang Zhang ChunJian Xu Jun

We have revisited several interesting questions on how the rapidity-odd directed flow is developed in relativistic ^{197}Au+^{197}Au collisions at $\sqrt{S_{NN}}$=200 and 39 GeV based on a multiphase transport model. As the partonic phase evolves with time, the slope of the parton directed flow at midrapidity region changes from negative to positive as a result of the later dynamics at 200 GeV, while it remains negative at 39 GeV due to the shorter life time of the partonic phase. The directed flow splitting for various quark species due to their different initial eccentricities is observed at 39 GeV, while the splitting is very small at 200GeV. From a dynamical coalescence algorithm with Wigner functions, we found that the directed flow of hadrons is a result of competition between the coalescence in momentum and coordinate space as well as further modifications by the hadronic rescatterings.

The European Physical Journal A, 2017, **53**(12): 1

Electromagnetic field effects on nucleon transverse momentum for heavy ion collisions around 100 A MeV

Deng XianGai Ma YuGang

Key words Heavy ion collision, Electromagnetic field, Transverse momentum

With taking electromagnetic field into account for the transport model of Boltzmann-Uehling-Uhlenbeck, electromagnetic effects are studied for $^{208}Pb+^{208}Pb$ collisions around 100A MeV. Electromagnetic field evolution during the collisions was estimated. It was found that the electric field has an obvious effect on the transverse momentum (p_T) spectra of nucleons during heavy ion collisions, and leads to different minimum position for the peak of p_T spectra of nucleons versus beam energy when the electric field is switched on. For the magnetic field, it affects the z-axis direction distributions of nucleons for central heavy ion collisions at lower energy.

Nuclear Science and Techniques, 2017, **28**(12): 182

Measurements of the total cross section of ^{nat}Be with thermal neutrons from a photo-neutron source

Liu LX Wang HW Ma YG Cao XG Cai XZ Chen JG Zhang GL Han JL Zhang GQ Hu JF Wang XH Li WJ Yan Z Fu HJ

Key words Neutron total cross section, Natural beryllium, Digital-signal-processing, Time-of-flight, Geant4

The total neutron cross sections of natural beryllium in the neutron energy region of 0.007 to 0.1 eV were measured by using a time-of-flight (TOF) technique at the Shanghai Institute of Applied Physics (SINAP). The low energy neutrons were obtained by moderating the high energy neutrons from a pulsed photo-neutron source generated from a 16 MeV electron linac. The time dependent neutron background component was determined by employing the 12.8 cm boron-loaded polyethylene (PEB) (5% w.t.) to block neutron TOF path and using the Monte Carlo simulation methods. The present data was compared with the fold Harvey data with the response function of the photo-neutron source (PNS, phase-1). The present measurement of total cross section of ^{nat}Be for thermal neutrons based on PNS has been developed for the acquisition of nuclear data needed for the Thorium Molten Salt Reactor (TMSR).

Nuclear Instruments and Methods in Physics Research Section B: Beam Interactions with Materials and Atoms, 2017, **410**: 158

Dark Matter Results from 54-Ton-Day Exposure of PandaX-II Experiment

PandaX-II Collaboration

We report a new search for weakly interacting massive particles (WIMPs) using the combined low background data sets acquired in 2016 and 2017 from the PandaX-II experiment in China. The latest data set contains a new exposure of 77.1 live days, with the background reduced to a level of 0.8×10^{-3} evt/kg/day, improved by a factor of 2.5 in comparison to the previous run in 2016. No excess events are found above the expected background. With a total exposure of 5.4×10^{4} kg day, the most stringent upper limit on the spin-independent WIMP-nucleon cross section is set for a WIMP with mass larger than 100 GeV/c^2, with the lowest 90% C.L. exclusion at 8.6×10^{-47} cm^2 at 40 GeV/c^2.

Physical Review Letters, 2017, **119**(18): 181302

Simulating spin dynamics with spin-dependent cross sections in heavy-ion collisions

Liu Xing Huang Gang Hu KuanKan Sheng Nan
Tian Chuanshan Shen Y. Ron Wen YuChieh
Shi Guosheng Fang Haiping

We have incorporated the spin-dependent nucleon-nucleon cross sections into a Boltzmann-Uehling-Uhlenbeck transport model for the first time, using the spin-singlet and spin-triplet nucleon-nucleon elastic scattering cross sections extracted from the phase-shift analyses of nucleon-nucleon scatterings in free space. We found that the spin splitting of the collective flows is not affected by the spin-dependent cross sections, justifying it as a good probe of the in-medium nuclear spin-orbit interaction. With the in-medium nuclear spin-orbit mean-field potential that leads to local spin polarization, we found that the spin-averaged observables, such as elliptic flows of free nucleons and light clusters, becomes smaller with the spin-dependent differential nucleon-nucleon scattering cross sections.

Journal of Physical Chemistry C, 2017, **122**(16): 9111

Effects of hadronic mean-field potentials on Hanbury-Brown–Twiss correlations in relativistic heavy-ion collisions

Zhang ChunJian Xu Jun

With the parameters fitted by the particle multiplicity, the energy density at chemical freeze-out, and the charged particle elliptic flow, we have studied the effects of the hadronic mean-field potentials on the Hanbury-Brown and Twiss (HBT) correlation in relativistic heavy-ion collisions based on a multiphase transport model. The hadronic mean-field potentials are found to delay the emission time of the system and lead to large HBT radii extracted from the correlation function. Effects on the energy dependence of $R_o^2 - R_s^2$ and R_o/R_s as well as the eccentricity of the emission source are discussed. The HBT correlations can also be useful in understanding the mean-field potentials of protons, kaons, and antiprotons as well as baryon-antibaryon annihilations.

Physical Review C, 2017, **96**(4): 044907

Chemical freeze-out in relativistic heavy-ion collisions

Xu Jun Ko CheMing

One surprising result in relativistic heavy-ion collisions is that the abundance of various particles measured in experiments is consistent with the picture that they reach chemical equilibrium at a temperature much higher than the temperature they freeze out kinetically. Using a multiphase transport model to study particle production in these collisions, we find, as an example, that the effective pion to nucleon ratio, which includes those from resonance decays, indeed changes very little during the evolution of the hadronic matter from the chemical to the kinetic freeze-out, and it is also accompanied by an almost constant specific entropy. We further use a hadron resonance gas model to illustrate the results from the transport model study.

Physics Letters B, 2017, **772**: 290

Collective Flows of $^{16}O+^{16}O$ Collisions with α-Clustering Configurations

Guo ChenChen He WanBing Ma YuGang

The main purpose of the present work is to discuss whether or not the collective flows in heavy-ion collision at the Fermi energy can be taken as a tool to investigate the cluster configuration in light nuclei. In practice, within an extended quantum molecular dynamics model, four α-clustering (linear chain, kite, square and tetrahedron) configurations of ^{16}O are employed in the initialization, $^{16}O+^{16}O$ around the Fermi energy (40–60 MeV/nucleon) with impact parameter 1–3 fm are simulated, and the directed and elliptic flows are analyzed. It is found that collective flows are influenced by the different α-clustering configurations, and the directed flow of free protons is more sensitive to the initial cluster configuration than the elliptic flow. Nuclear reaction at the Fermi energy can be taken as a useful way to study cluster configuration in light nuclei.

Chinese Physics Letters, 2017, **34**(9): 092101

Nuclear cluster structure effect on elliptic and triangular flows in heavy-ion collisions

Zhang S Ma YG Chen JH He WB Zhong C

The initial geometry effect on collective flows, which are inherited from initial projectile structure, is studied in relativistic heavy-ion collisions of $^{12}C+^{197}Au$ by using a multiphase transport model (AMPT). Elliptic flow (v_2) and triangular flow (v_3) which are significantly resulted from the chain and triangle structure of ^{12}C with three-α clusters, respectively, in central $^{12}C+^{197}Au$ collisions are compared with the flow from the Woods-Saxon distribution of nucleons in ^{12}C. v3/v2 is proposed as a probe to distinguish the pattern of α-clustered ^{12}C. This study demonstrates that the initial geometry of the collision zone inherited from nuclear structure can be explored by collective flow at the final stage in heavy-ion collisions.

Physical Review C, 2017, **95**(6): 064904

Alpha-clustering effects on $^{16}O(\gamma,np)^{14}N$ in the quasi-deuteron region

Huang BoSong Ma YuGang He WanBin

Photonuclear reaction in the quasi-deuteron regime has been investigated in an extended Quantum Molecular Dynamics model at a photon energy of 70-120 MeV. Particularly, the reaction channel of $^{16}O(\gamma,np)^{14}N$ is focused where ^{16}O is considered as having different α-clustering configurations as well as regular spherical structure. Because of three-body decay from the above photonuclear reaction, we can investigate many observables including the recoil momentum, missing energy, pair momentum/energy and opening angle of ejected neutron and proton, hyper-angle and hyper-radius distributions, etc. These quantitative results demonstrate an obvious difference among different initial configurations of ^{16}O, which can be attributed to the spatial-momentum correlation of a neutron-proton pair inside the nucleus. The results illustrate that photonuclear reaction is a good tool to explore different α-clustering structures.

The European Physical Journal A, 2017, **53**(6): 119

A Photonuclear Reaction Model Based on IQMD in Intermediate-Energy Region

Huang BoSong Ma YuGang

A photonuclear reaction transport model based on an isospin-dependent quantum molecular dynamics model (IQMD) is presented in the intermediate energy region, which is named as GiQMD in this study. Methodology to simulate the course of the photonuclear reaction within the IQMD frame is described to study the photoabsorption cross section and π meson production, and the simulation results are compared with some available experimental data as well as the Giessen Boltzmann–Uehling–Uhlenbeck model

Chinese Physics Letters, 2017, **34**(7): 072401

Isovector dipole resonance and shear viscosity in low energy heavy-ion collisions

Guo CQ Ma YG He WB Cao XG Fang DQ
Deng XG Zhou CL

The ratio of shear viscosity over entropy density in low energy heavy-ion collision has been calculated by using the Green-Kubo method in the framework of an extended quantum molecular dynamics model. After the system almost reaches a local equilibration for a head-on $^{40}Ca+^{100}Mo$ collision, thermodynamic and transport properties are extracted. Meanwhile, the isovector giant dipole resonance (IVGDR) of the collision system also is studied. By the Gaussian fits to the IVGDR photon spectra, the peak energies of the IVGDR are extracted at different incident energies. The result shows that the IVGDR peak energy has a positive correlation with the ratio of shear viscosity over entropy density. This is a quantum effect and indicates a difference between nuclear matter and classical fluid.

Physical Review C, 2017, **95**(5): 054622

Investigation of giant dipole resonances in heavy deformed nuclei with an extended quantum molecular dynamics model

Wang SS Ma YG Cao XG He WB Kong HY Ma CW

The deformation evolution of giant dipole resonance (GDR), in the chains of Sm and Nd isotopes, are investigated in the framework of an extended quantum molecular dynamics (EQMD) model. The mass number dependence of resonance peak position (E_m) in the major and minor axis directions of deformed nuclei as well as the difference ΔEm between them are described in detail. The correlation between the splitting ($\Delta E_m/\overline{E_m}$) of the GDR spectra and the deformation (β_2) is further studied. The results confirm that $\Delta E_m/\overline{E_m}$ is proportional to β_2. By comparing the calculation with the experimental data on photon absorption cross section σ_γ, it shows that the EQMD model can quite well reproduce the shape of GDR spectra from spherical to prolate shape. The GDR shapes in ^{134}Sm, ^{136}Sm, ^{138}Sm, ^{130}Nd, ^{132}Nd, and ^{134}Nd are also predicted. In addition, the symmetry energy coefficient (E_{sym}) dependence of GDR spectra of ^{150}Nd is also discussed. It is found that the calculated GDR spectrum in the EQMD model is perfectly consistent with the experimental results when E_{sym} equals 32 MeV.

Physical Review C, 2017, **95**(5): 054615

Production of light nuclei and hypernuclei at High Intensity Accelerator Facility energy region

Liu Peng Chen Jin-Hui Ma Yu-Gang Zhang Song

Key words Heavy-ion accelerator facility; Hyperon; Hypernuclei; Coalescence; Light nuclei

Heavy-ion collisions are powerful tools for studying hypernuclear physics. We develop a dynamical coalescence model coupled with an ART model (version 1.0) to study the production rates of light nuclear clusters and hypernuclei in heavy-ion reactions, for instance, the deuteron (d), triton (t), helium (^{3}He), and hypertriton (${}^{3}_{\Lambda}H$) in minimum bias (0–80% centrality) ^{6}Li + ^{12}C reactions at beam energy of 3.5A GeV. The penalty factor for light clusters is extracted from the yields, and the distributions of θ angle of particles, which provide direct suggesetions about the location of particle detectors in the near future facility—High Intensity heavy-ion Accelerator Facility (HIAF) are investigated. Our calculation demonstrates that HIAF is suitable for studying hypernuclear physics.

Nuclear Science and Techniques, 2017, **28**(4): 55

Constraining simultaneously nuclear symmetry energy and neutron-proton effective mass splitting with nucleus giant resonances using a dynamical approach

Kong HaiYun Xu Jun Chen LieWen
Li BaoAn Ma YuGang

With a newly improved isospin- and momentum-dependent interaction and an isospin-dependent Boltzmann-Uehling-Uhlenbeck transport model, we have investigated the effects of the slope parameter L of the nuclear symmetry energy and the isospin splitting of the nucleon effective mass m^*_{n-p} =(m^*_n− m^*_p)/m on the centroid energy of the isovector giant dipole resonance and the electric dipole polarizability in ^{208}Pb. With the isoscalar nucleon effective mass m^*_s =0.7m constrained by the empirical optical potential, we obtain a constraint of L=64.29±11.84(MeV) and m^*_{n-p} = (−0.019±0.090)δ, with δ being the isospin asymmetry of nuclear medium. With the isoscalar nucleon effective mass m^*_s =0.84m extracted from the excitation energy of the isoscalar giant quadruple resonance in 208Pb, we obtain a constraint of L =53.85±10.29(MeV) and m^*_{n-p}= (0.216±0.114)δ.

Physical Review C , 2017, **95**(3): 034324

Photonuclear reaction as a probe for α-clustering nuclei in the quasi-deuteron region

Huang BS Ma YG He WB

Photon-nuclear reaction in a transport model frame, namely an extended quantum molecular dynamics model, has been realized at the photon energy of 70–140 MeV in the quasi-deuteron regime. For an important application, we pay a special focus on photonuclear reactions of $^{12}C(\gamma,np)^{10}B$ where ^{12}C is considered as different configurations including α clustering. Obvious differences for some observables have been observed among different configurations, which can be attributed to spatial-momentum correlation of a neutron-proton pair inside nucleus, and therefore it gives us a sensitive probe to distinguish the different configurations including α clustering with the help of the photonuclear reaction mechanism.

Physical Review C , 2017, **95**(3): 034606

Medium effect on the nuclear modification factor of protons and pions in intermediate-energy heavy ion collisions

Lv M Ma YG Chen JH Fang DQ Zhang GQ

Nuclear modification factors R_{cp} of protons and pions are investigated by simulating Au+Au collisions from 0.8A to 1.8A GeV in a framework of an isospin-dependent quantum molecular dynamics (IQMD) model. The R_{cp} of protons rise with an increase in the transverse particle momentum pT at different beam energies owing to radial flow and the multiple-collision effect. The rate of increase of R_{cp} is suppressed at higher beam energies. While the R_{cp} of pions display weaker pT dependence. By changing the in-medium nucleon-nucleon cross section, the R_{cp} of protons change a lot, while the R_{cp} of pions do not. In addition, by deactivating the NΔ→NN and πN→Δ channels, the R_{cp} of protons change slightly in their increasing rates compared with the “original” case (with these two channels). However, the R_{cp} of pions is shifted down for the “no NΔ→NN” case and has an inverse trend for the “no πN→Δ” case. Based on these observations, we argue that the observable R_{cp} is a suitable tool to better distinguish in-medium effects of protons and pions.

Physical Review C , 2017, **95**(2): 024614

Alignment calibration and performance study of the STAR PXL detector

Ma Long Dong Xin Qiu Hao
Margetis Spiros Ma YuGang

Key words Alignment calibration; Heavy flavor tracker; STAR

We report in this paper the alignment calibration of the STAR pixel detector (PXL) prototype for the RHIC 2013 run and performance study of the full PXL detector installed and commissioned in the RHIC 2014 run. PXL detector is the innermost two silicon layers of the STAR heavy flavor tracker aiming at high-precision reconstruction of secondary decay vertex of heavy flavor particles. To achieve the physics goals, the calibration work was done on the detector with high precision. A histogram-based method was successfully applied for the alignment calibration, and the detector efficiency after alignment was studied using both p+pp+p collision data and cosmic ray data.

Nuclear Science and Techniques, 2017, **28**(2): 25

Giant dipole resonance in proton capture reactions using an extended quantum molecular dynamics model

Wang K Ma YG Zhang GQ Cao XG
He WB Shen WQ

Proton capture reaction is an important process concerning the astrophysical origin of the elements. In present work, we focus on giant dipole resonance (GDR) in proton capture reactions, such as ^{11}B(p,γ)^{12}C, ^{27}Al(p,γ)^{28}Si, ^{39}K(p,γ)^{40}Ca, and ^{67}Co(p,γ)^{68}Ni in a framework of an extended quantum molecular dynamics model. The systematic properties of GDR parameters including the peak energy, the strength, and full width at half maximum (FWHM) have been studied. The dependence of FWHM on temperature has also been discussed. Some comparisons with experimental data have been presented.

Physical Review C , 2017, **95**(1): 014608

Beta-decay study of T_z = - 2 proton-rich nucleus ^{24}Si

Sun LJ Xu XX Fang DQ Lin CJ Wang JS Li ZH
Wang YT Li J Yang L Ma NR Wang K Zang HL
Wang HW Li C Shi CZ Nie MW Li XF Li H
Ma JB Ma P Jin SL Huang MR Bai Z Wang JG
Yang F Jia HM Zhang HQ Liu ZH Bao PF Wang DX
Yang YY Zhou YJ Ma WH Chen J Ma YG
Zhang YH Zhou X Xu HS Xiao GQ Zhan WL

β -decay spectroscopy on a T_z = - 2 proton-rich nucleus ^{24}Si was performed. The decay scheme of ^{24}Si was reconstructed by the β -delayed γ -ray and proton measurements. Two β branches to the bound 1_1^+ and 1_2^+ states in ^{24}Al were observed for the first time. The observation of the allowed transition firmly established the spin-parity assignment for the 1_2^+ states. The branching ratios to the 1_1^+ and 1_2^+ states were determined to be 31(4)% and 23.9(15)%, respectively. The branching ratios to three unbound states in ^{24}Al including a new level at 6.735MeV were also determined for the first time. The level structure of ^{24}Al was compared with its mirror nucleus ^{24}Na . The Thomas-Ehrman shift on the 1_2^+ state indicates *s* -wave dominance in the state as well as a characteristic behavior of the weakly bound *s* -wave proton in ^{24}Al .

Physical Review C , 2017, **95**(1): 014314

Reconstructed jets in a multi-phase transport model

Ma GuoLiang

Key words jet energy loss, transport model, QGP

With a framework of a multiphase transport model, we studied various of properties of fully reconstructed jets, including dijet asymmetry, jet shape, jet fragmentation function, jet azimuthal anisotropy, and overall momentum balance of dijet events. Our studies concentrate on the stage evolution of these full jet observables in heavy-ion collisions. We demonstrate that the medium modification effect on these observables mainly arises from strong interactions between jet and partonic matter, with further slight modifications from hadronization and hadronic rescatterings. Our model results provide a dynamical understanding of jet transport process in high-energy heavy-ion collisions.

Nuclear and Particle Physics Proceedings, 2017, **289**: 363

Measurement of D^*-meson triggered correlations in p+p collisions at RHIC

Ma Long STAR Collaboration

Key words STAR, heavy flavor, D meson, azimuthal correlation

We report the preliminary results of the azimuthal correlations between $D^{*\pm}$ mesons and charged hadrons (D^*-h) measured by the STAR experiment in proton+proton collisions at $\sqrt{s}$=500 GeV. Results at mid-rapidity in the transverse-momentum range 8≤ P_T^D ≤20 GeV/c are compared with light hadron triggered correlations (h-h) and PYTHIA predictions. We also present an exploratory study of azimuthal correlations between D^{*+} and D^{*-} mesons in p+p collisions. The prospects of measuring heavy-flavor triggered correlations in heavy-ion collisions at RHIC energies are also discussed.

Nuclear and Particle Physics Proceedings, 2017, **289**: 329

Measurement of bottom contribution to the non-photonic electron production in p+p collisions at STAR

Li Wei STAR Collaboration

We present the STAR preliminary results of the azimuthal correlations between non-photonic electrons and charged hadrons at mid-rapidity in p+p collisions at $\sqrt{s}$= 200 GeV and 500 GeV. The correlation distributions are fitted with PYTHIA templates to extract the relative contribution from bottom decays to non-photonic electrons. This could provide a precise p+p reference for the study of bottom production in heavy-ion collisions at RHIC.

Journal of Physics: Conference Series, 2017, **779**: 012053

Ω and ϕ in Au + Au collisions at $\sqrt{s_{NN}}$ =200 and 11.5 GeV from a multiphase transport model

Ye YJ Chen JH Ma YG Zhang S Zhong C

Key words multi-strangeness particles, AMPT, RHIC

Within the framework of a multiphase transport model, we study the production and properties of Ω and ϕ in Au + Au collisions with a new set of parameters for $\sqrt{s_{NN}}$ =200 GeV and with the

original set of parameters for $\sqrt{s_{NN}}$ =11.5 GeV . The AMPT model with string melting provides a reasonable description at $\sqrt{s_{NN}}$ =200 GeV , while the default AMPT model describes the data well at $\sqrt{s_{NN}}$ =11.5 GeV . This indicates that the system created at top RHIC energy is dominated by partonic interactions, while hadronic interactions become important at lower beam energy, such as $\sqrt{s_{NN}}$ =11.5 GeV . The comparison of $N(\Omega^{+}+\Omega^{-})/[2N(\phi)]$ ratio between data and calculations further supports the argument. Our calculations can generally describe the data of nuclear modification factor as well as elliptic flow.

Chinese Physics C, 2017, **41**(8): 084101

Measurement of the cross section and longitudinal double-spin asymmetry for dijet production in polarized pp collisions at $\sqrt{s_{NN}}$ =200 GeV

STAR Collaboration

We report the first measurement of the longitudinal double-spin asymmetry A_{LL} for midrapidity dijet production in polarized pp collisions at a center-of-mass energy of $\sqrt{s_{NN}}$ =200 GeV. The dijet cross section was measured and is shown to be consistent with next-to-leading order (NLO) perturbative QCD predictions. A_{LL} results are presented for two distinct topologies, defined by the jet pseudorapidities, and are compared to predictions from several recent NLO global analyses. The measured asymmetries, the first such correlation measurements, support those analyses that find positive gluon polarization at the level of roughly 0.2 over the region of Bjorken-x>0.05.

Physical Review D, 2017, **95**(7): 071103

Cyclic thermal characterization of a molten-salt packed-bed thermal energy storage for concentrating solar power

Zhao Bingchen Cheng Maosong Liu Chan Dai Zhimin

Key words Concentrating solar power, Packed-bed thermal energy storage, Molten-salt, Encapsulated phase change material, Cyclic thermal characterization, Numerical analysis

Molten-salt packed-bed thermocline thermal energy storage (TES) is identified to be a cost-competitive TES type for concentrating solar power (CSP). The present study reveals the system-level cyclic thermal characteristics of the molten-salt packed-bed TES with typical

configurations on two levels of investigation, based on a one-dimensional enthalpy-method dispersed-concentric (D-C) model. Firstly, a three-stage operation scheme is proposed to evaluate the thermal performance of the introduced partial charge cycles and the subsequent full charge cycles, under ideal operating conditions. The 'partial charge effect' of the packed-bed TES is identified by evaluating the variations in thermocline development and energy storage/release capacity. The results show that the introduced partial charge cycles can generally lead to a thermocline degradation, and then impact the energy store/release capacity in the subsequent full charge cycles. The configurations containing encapsulated PCMs are of greater resistance and stronger recoverability to the variation in energy storage/release capacity. Then the study is extended to investigate the thermal performance of a 100 MWe CSP plant integrated with a well-sized packed-bed TES system, over a 14-day practical operation based on variable energy collections. Deviations between the designed and practical energy store/release capacity of the systems are evaluated. The results indicate that of the sensible-heat and the single-layered latent-heat packed-bed TES present significant shortages in energy storage capacity during the operation, which can lead to energy collection discards. Overall, the obtained results present a new perspective to evaluate the availability of the packed-bed TES system for CSP plants.

Applied Energy, 2017, **195**: 761

A Wind Power Plant with Thermal Energy Storage for Improving the Utilization of Wind Energy

Liu Chang　Cheng MaoSong　Zhao BingChen　Dai ZhiMin

Key words　wind power plant (WPP), thermal energy storage (TES), district heating (DH), wind power rejection, Modelica

The development of the wind energy industry is seriously restricted by grid connection issues and wind energy generation rejections introduced by the intermittent nature of wind energy sources. As a solution of these problems, a wind power system integrating with a thermal energy storage (TES) system for district heating (DH) is designed to make best use of the wind power in the present work. The operation and control of the system are described in detail. A one-dimensional system model of the system is developed based on a generic model library using the object-oriented language Modelica for system modeling. Validations of the main components of the TES module are conducted against experimental results and indicate that the models can be used to simulate the operation of the system. The daily performance of the integrated system is analyzed based on a seven-day operation. And the influences of system configurations on the performance of the

integrated system are analyzed. The numerical results show that the integrated system can effectively improve the utilization of total wind energy under great wind power rejection.

Energies, 2017, **10**(12): 2126

Treatment of radioactive spent extraction solvent by supercritical water oxidation

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Chen Kun Qiao Yanbo He Liubin Qian Zhenghua
Liu Xueyang Li Zheng Xia Xiaobin

Key words Supercritical water oxidation, Distribution, Spent extraction solvent, Radionuclide

Radioactive spent extraction solvent was treated by supercritical water oxidation. In this work, influences of reaction conditions on total organic carbon (TOC) removal, the volume percentage of CO_2 yielded, and the distributions of radionuclides in gas, liquid and solid phase have been investigated. The results show that the TOC removal and the volume percentage of CO_2 would be increased up to above 99% under optimal conditions. More than 88% of thorium and 67% of uranium were precipitated in solid phase, the rest remained in the liquid effluent, and no thorium and uranium were detected in gas phase.

Journal of Radioanalytical and Nuclear Chemistry, 2017, **314**(2): 1169

Design of PC-based quantitative split charging device for hydrogen isotope elemental gases

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Wang Yu Liu Wei

Key words Hydrogen isotopes, Split charging, LabVIEW

A quantitative split charging device for hydrogen isotope elemental gases in the operation ranges of 10^{-5} Pa − 6 bar, 15–40 °C, and 10–500 sccm, controlled by a personal computer (PC) on the workbench of LabVIEW software, was carefully designed and constructed. In the device, volumetric charging mode and flow-controller charging mode can be adopted according to the molar quantity of split charging. The leakage rate and the quantitative split charging accuracy of the set-up were evaluated systemically. According to the experimental results of quantitative split

charging from our device and mass comparator, this apparatus is well designed and assembled, and can guarantee 0.001 g quantitative split charging accuracy in the two charging modes.

International Journal of Hydrogen Energy, 2017, **42**(29): 18484

Source apportionment of carbonaceous particulate matter during haze days in Shanghai based on the radiocarbon

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Feng Jialiang Zhang Yihua Xiao Detao Liu Wei

Key words Radiocarbon, Contemporary emissions, Haze days, Carbonaceous particulate matter

To estimate the sources of carbonaceous particulate matter, ^{14}C and biomass-burning marker (levoglucosan) were measured in the form of organic carbon (OC) and elemental carbon (EC) in $PM_{2.5}$ that was collected in five different functional districts of Shanghai during winter 2013. Spatial variations of the contemporary proportion among different districts were evident. The results of levoglucosan in Xujiahui (XH) and Chongming (CM) agreed well with those of ^{14}C. The results indicate that environmental protection policies should vary for functional districts within the same city to account for their different sources of emissions.

Journal of Radioanalytical and Nuclear Chemistry, 2017, **313**(1): 145

Effects of alloying substitutions on the anti-disproportionation behavior of ZrCo alloy

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Qian Yuan Zeng Youshi Wu Xiaoling Qiu Jie
Yin Huiqin Liu Wei Li Yan

Key words Tritium storage, First-principles study, ZrCo alloy, ZrCoH3, 8e site, Hydrogen-induced, disproportionation

We perform first-principles calculations to investigate the effects of alloying substitutions (i.e. Ti, Hf, Sc, Fe, Ni and Cu) on hydrogen-induced disproportionation of ZrCo alloy. H at the 8e site of $ZrCoH_3$ (H(8e)) plays the key role in the disproportionation process. It is found that H(8e) prefers to form strong covalent-like binding with the neighboring Co and its substitute elements, which is distinctly different from H at the $4c_2$ and $8f_1$ sites. Alloying substitutions can restrain or accelerate the disproportionation by influencing the Zr—H(8e) bond length and the size of the 8e

site. Judged from this, the anti-disproportionation ability of these alloying substitutions is identified. Our results of Ti, Hf, Sc, Fe and Ni are in good agreement with the previous experimental results. It is also predicated that Cu can accelerate hydrogen-induced disproportionation of ZrCo alloy.

International Journal of Hydrogen Energy, 2017, **42**(24): 15782

Theoretical study of the interaction between hydrogen and 4d alloying atom in nickel

Liu WenGuan Qian Yuan Zhang DongXun Han XingBo Chu XinXin Zeng YouShi Bao GuangLiang Wang GuangHua Wu ShengWei Liu Wei

Key words Hydrogen, Tritium, Transition metal, Nickel, First-principles calculation

In order to investigate the tritium behaviors in Hastelloy N alloy in molten salt reactor, first-principles calculations are used to study the interaction between hydrogen and 4*d* transition metal alloying atom in nickel-based alloy. The interaction energies between 4*d* elements and H are calculated. Atomic size effects and electron distribution effects are analyzed. The hydrogen–4*d* interactions are compared with the hydrogen–3*d* interactions calculated in our previous work.

Nuclear Science and Techniques, 2017, **28**(6): 82

Extraction of lanthanide ions with N,N,N′,N′-tetrabutyl-3-oxa-diglycolamide from nitric acid media

Peng XiuJing Cui Yu Ma JiFei Li Yulan Sun GuoXin

Key words Lanthanide ions, Extraction, N,N,N'N'-tetrabutyl-3-oxa-diglycolamide, Nitric acid, Toluene

Extractability and extraction mechanism of lanthanide ions were investigated by using a new extractant, *N*,*N*,*N*′,*N*′-tetrabutyl-3-oxa-diglycolamide (TBDGA), in toluene from nitric acid media. The effects of HNO_3 and TBDGA concentrations, and temperature, on extraction of lanthanide ions were studied. Stoichiometries of the main extracted species were HNO_3·TBDGA and $M(NO_3)_3$·3TBDGA (M = Er, Dy, Tb, Gd, La, Ce, Nd, Sm and Eu). The extracted species for metal ions were established to be ionic complex. In this complex, nitrate anion was not coordinated to the central ion. The extraction pattern increased gradually across the lanthanide ions series, showing

enhanced affinity of TBDGA toward heavy lanthanide ions. Thermodynamic parameters were investigated for the exothermic extraction reaction.

Nuclear Science and Techniques, 2017, **28**(6): 87

A theoretical study of the effects of sp-elements on hydrogen in nickel-based alloys

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Han Xingbo Chu Xinxin Yin Huiqin Yang Guo
Wang Guanghua Wu Shengwei Liu Wei

Key words Hydrogen, Sp-elements, Nickel-based alloy, First-principles calculation

By using first-principles calculations, we present a theoretical study of the interactions between hydrogen (H) and sp-elements from the 3rd, 4th and 5th period (Al, Si, P, S, Ga, Ge, As, Se, In, Sn, Sb and Te) in nickel-based alloy. The interactions between H and sp-atom are evaluated by the calculated interaction energy. Judged by the interaction energy, H is repelled by all these elements (except S) in nickel-based alloy. The atomic and electronic structures are analyzed. Especially, the interaction energy is found to be closely related with the electronic structure and electronegativity. The larger the electronegativity of the sp-elements, the weaker the H-sp bond. The weaker H-sp bond results in the more positive interaction energy and the repulsion to H. Particularly, for the cases of S and Se, the long H—S and H—Se distances can largely relieve the strain effect induced by the insertion of the H atom, thus decrease the repulsion to H. The interaction energy for S is even reduced to a negative value, which means that H is attracted in the Ni—S—H system. Our work presents a fundamental understanding of the effects of the sp-elements on H in nickel-based alloys systematically.

Computational Materials Science, 2017, **128**: 37

Analysis of atmospheric pollutant metals by laser ablation inductively coupled plasma mass spectrometry with a radial line-scan dried-droplet approach

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Li Yulan Yao Jian Wang Guanghua Ma Jifei Liu Wei

Key words LA-ICP-MS, Atmospheric samples, Quantification, Filters, Pollutant metals

A novel method has been improved for analyzing atmospheric pollutant metals (Be, Mn, Fe, Co, Ni, Cu, Zn, Se, Sr, Cd, and Pb) by laser ablation inductively coupled plasma mass spectrometry.

In this method, solid standards are prepared by depositing droplets of aqueous standard solutions on the surface of a membrane filter, which is the same type as used for collecting atmospheric pollutant metals. Laser parameters were optimized, and ablation behaviors of the filter discs were studied. The mode of radial line scans across the filter disc was a representative ablation strategy and can avoid error from the inhomogeneous filter standards and marginal effect of the filter disc. Pt, as the internal standard, greatly improved the correlation coefficient of the calibration curve. The developed method provides low detection limits, from 0.01 $ng \cdot m^{-3}$ for Be and Co to 1.92 $ng \cdot m^{-3}$ for Fe. It was successfully applied for the determination of atmospheric pollutant metals collected in Lhasa, China. The analytical results showed good agreement with those obtained by conventional liquid analysis. In contrast to the conventional acid digestion procedure, the novel method not only greatly reduces sample preparation and shortens the analysis time but also provides a possible means for studying the spatial distribution of atmospheric filter samples.

Spectrochimica Acta Part B: Atomic Spectroscopy, 2017, **138**: 18

Synchrotron radiation X-ray powder diffraction techniques applied in hydrogen storage materials - A review

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Han Xingbo Jin Huiming Wang Yu Liu Yi Wu Changle

Key words Synchrotron radiation, X-ray powder diffraction, Hydrogen storage materials, Review

Synchrotron radiation is an advanced collimated light source with high intensity. It has particular advantages in structural characterization of materials on the atomic or molecular scale. Synchrotron radiation X-ray powder diffraction (SR-XRPD) has been successfully exploited to various areas of hydrogen storage materials. In the paper, we will give a brief introduction on hydrogen storage materials, X-ray powder diffraction (XRPD), and synchrotron radiation light source. The applications of ex situ and in situ time-resolved SR-XRPD in hydrogen storage materials, are reviewed in detail. Future trends and proposals in the applications of the advanced XRPD techniques in hydrogen storage materials are also discussed.

Progress in Natural Science: Materials International, 2017, **27**(1): 72

Radiolysis products and degradation mechanism studies on di-1-methyl heptyl methyl phosphonate

Li Ruifen Cao Xiaojun Zhao Haogui Liu Chunxia
Li Zheng Wang Jinhua Zhang Lan Li Qinguan

Key words Di-1-methyl heptyl methyl phosphonate, Radiolysis products, Radiolysis mechanism, Structure

Di-1-methyl heptyl methyl phosphonate (DMHMP) is a promising alternative extractant for Th-U fuel reprocessing, in which the irradiation stability of extractant should be systematically studied. In this paper, the radiolysis products of DMHMP were analyzed qualitatively and quantitatively with gas and ion chromatograph, the possible radiolysis mechanism of DMHMP was also concluded. Moreover, the effect of structure on the radiolysis products and irradiation stability of neutral organophosphorus compound extractant was also discussed.

Journal of Radioanalytical and Nuclear Chemistry, 2017, **314**(3): 1715

High-performance functionalized polyethylene fiber for the capture of trace uranium in water

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Zhang Maojiang Wu Guozhong

Key words Uranium, Radiation grafting, Removal efficiency, EXAFS

A new functionalized ultrahigh molecular weight polyethylene-based chelating fiber (UHMWPE-AM) for trace uranium extraction from wastewater was synthesized by preirradiation grafting modification. Adsorption behavior of adsorbent was examined under varying conditions like solution pH, contact time, initial ion concentration and adsorbent dose. The results showed the maximum removal of U(VI) was 99.7% at pH 4. Adsorption isotherm was in agreement with Langmuir isotherm equation with the maximum monolayer adsorption capacity of 16.56 mg/g, and the pseudo-second-order model can well describe the kinetics process. The dominant coordination mechanism of U(VI) on the UHMWPE-AM fibers was ascribed to inner-sphere surface complexation.

Journal of Radioanalytical and Nuclear Chemistry, 2017, **314**(3): 2393

Reprocessing Th-based spent fuels with di-1-methyl heptyl methyl phosphonate using centrifugal extractors

Li Ruifen Zhao Haogui Liu Chunxia He Shuhua
Li Zheng Li Qingnuan Zhang Lan

Key words DMHMP, Solvent extraction, Th-based spent fuel process, Centrifugal extractor

In this paper, a reprocessing Th-based spent fuels process using di-1-methyl heptyl methyl phosphonate (DMHMP) as extractant was proposed and tested by multistage countercurrent extraction using batch simulation and centrifugal extractors. The analysis results of process samples show that the recovery of Th and U in 1A (co-extraction of Th and U), 1B (separation of Th from U) and 1C (stripping of U from organic to aqueous phase) section was more than 99.8% and 99.9%, respectively. The separation factor of Th from U and U from Th in 1B section was 5.9×10^3 and 7.1×10^3, respectively. Compared with Thorex process using TBP as extractant, the process could be operated under lower acidity and flow ratio of O: A due to the strong extraction ability of DMHMP. Thus, DMHMP would be a promising alternative extractant for Th-based spent fuels process.

Hydrometallurgy, 2017, **174**: 84

Supercritical CO_2 foaming of radiation crosslinked polypropylene/high-density polyethylene blend: Cell structure and tensile property

Yang Chenguang Xing Zhe Zhang Mingxing Zhao Quan
Wang Mouhua Wu Guozhong

Key words Radiation cross-linking, Polypropylene, Supercritical carbon dioxide, Microcellular foams, Tensile property

A blend of isotactic polypropylene (PP) with high-density polyethylene (HDPE) in different PP/HDPE ratios was irradiated by γ-ray to induce cross-linking and then foamed using supercritical carbon dioxide ($scCO_2$) as a blowing agent. Radiation effect on the melting point and crystallinity were analyzed in detail. The average cell diameter and cell density were compared for PP/HDPE foams prepared under different conditions. The optimum absorbed dose for the $scCO_2$ foaming of PP/HDPE in terms of foaming ability and cell structure was 20 kGy. Tensile measurements showed that the elongation at break and tensile strength at break of the crosslinked

PP/HDPE foams were higher than the non-crosslinked ones. Of particular interest was the increase in the foaming temperature window from 4 ℃ for pristine PP to 8–12 ℃ for the radiation crosslinked PP/HDPE blends. This implies much easier handling of $scCO_2$ foaming of crosslinked PP with the addition of HDPE.

Radiation Physics and Chemistry, 2017, **141**: 276

The recovery of uranium from irradiated thorium by extraction with di-1-methyl heptyl methylphosphonate (DMHMP)/*n*-dodecane

Li Ruifen Zhao Haogui Liu Chunxia He Shuhua
Li Zheng Li Qingnuan Zhang Lan

Key words DMHMP, Uranium extraction, EXAFS spectroscopy, Irradiation stability

The process using DMHMP as extractant for the recovery of uranium from irradiated thorium was proposed. Firstly, the process parameters, including concentration of DMHMP, concentratation of HNO_3 in feed, scrub and stripping solution, and phase ratio, were systematically optimized by batch extraction experiment. Then, a batch multistage countercurrent extraction simulation experiment was used to verify and test the process. Finally, the irradiation stability of DMHMP was assessed and compared with TBP. The results indicate that DMHMP is a potential candidate for the separation of U(VI) from bulk Th(IV). Furthermore, the complexes of U(VI) and Th(IV) with DMHMP were also demonstrated.

Separation and Purification Technology, 2017, **188**: 219

Potential application of graphene oxide membranes for removal of Cs(I) and Sr(II) from high level-liquid waste

Ma Fuyin Li Zheng Zhao Haogui Geng Yiyun
Zhou Wei Li Qingnuan Zhang Lan

Key words Graphene oxide membrane, High level-liquid waste, Permeation, Cs(I), Sr(II)

As a new carbon-based membrane material used for ionic and molecular sieving, the graphene oxide (GO) membrane also has potential application in radiochemical separation. In this work, the permeation performances of some typical metallic elements in high level-liquid waste (HLLW) through the ionic sieving 5-μm-thick GO membranes were investigated. It was found that the

permeation rates of ions through GO membranes markedly decreased with the increase of hydrated ionic radii. Cs(I) and Sr(II) permeated through GO membranes quickly, whereas lanthanide ions and actinide ions infiltrated much more slowly, thus providing the feasibility of separation according to the difference of hydrated ionic radii. Moreover, the concentrations of initial metal ions and acidity in feed solutions also had influences on the permeation of ions through GO membranes, and higher initial metal ions and feed solution acidity were favorable to the removal of Cs(I) and Sr(II). The barrier separation test indicated that GO membranes had promising ability for the separation of Cs(I) and Sr(II) from lanthanide and actinide ions due to the difference of hydrated ion radius, and the separation factor of Cs(I)/U(VI) and Sr(II)/U(VI) would reach about 10 and 3 in single penetration. The presented results demonstrated that the membrane separation based on GO membrane would be a promising candidate for the removal of Cs(I) and Sr(II) from HLLW.

Separation and Purification Technology, 2017, **188**: 523

Matrix Infrared Spectra of Manganese and Iron Isocyanide Complexes

Chen Xiuting Li Qingnuan Andrews Lester Gong Yu

Mono and diisocyanide complexes of manganese and iron were prepared via the reactions of laser-ablated manganese and iron atoms with $(CN)_2$ in an argon matrix. Product identifications were performed based on the characteristic infrared absorptions from isotopically labeled $(CN)_2$ experiments as compared with computed values for both cyanides and isocyanides. Manganese atoms reacted with $(CN)_2$ to produce $Mn(NC)_2$ upon $\lambda > 220$ nm irradiation, during which MnNC was formed mainly as a result of the photoinduced decomposition of $Mn(NC)_2$. Similar reaction products FeNC and $Fe(NC)_2$ were formed during the reactions of Fe and $(CN)_2$. All the product molecules together with the unobserved cyanide isomers were predicted to have linear geometries at the B3LYP level of theory. The cyanide complexes of manganese and iron were computed to be more stable than the isocyanide isomers with energy differences between 0.4 and 4 kcal/mol at the CCSD(T) level. Although manganese and iron cyanide molecules are slightly more stable according to the theory, no absorption can be assigned to these isomers in the region above the isocyanides possibly due to their low infrared intensities.

Journal of Physical Chemistry A, 2017, **121**(46): 8835

Preparation of antimicrobial MnO_4^--doped nylon-66 fibers with excellent laundering durability

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Key words Nylon 66 fibers, Irradiation induced graft polymerization, Permanganate ions, Antimicrobial activity, Laundering durability

A highly effective antimicrobial nylon 66 fiber doped with permanganate ions was prepared via a simultaneous irradiation induced graft polymerization. The physicochemical properties of the fibers were carefully characterized by various techniques, including Fourier-transform infrared spectroscopy, scanning electron microscopy, thermogravimetric analysis, and X-ray photoelectron spectroscopy, revealing that permanganate ions (about 1.48 mmol/g) have been successfully loaded onto the surface of the nylon 66 fibers. The antimicrobial activity of the modified nylon 66 fibers against *Staphylococcus aureus* and *Candida albicans* were investigated. Accelerated laundering tests and tensile tests were conducted to access the effect of laundering on the antimicrobial activity and the mechanical property of the modified nylon 66 fibers, respectively. All results indicate that we have prepared a new highly effective antimicrobial nylon 66 fiber (almost a 100% reduction in the number of *S. aureus* and *C. albicans* colonies). Furthermore, the modified nylon 66 fibers are durable, maintaining antimicrobial resistance after 100 commercial or domestic launderings and retaining its excellent mechanical property during preparation and laundering.

Applied Surface Science, 2017, **422**: 1067

Determination of Trace Fission Products Associated with Thorium and HCl Matrix by Inductively Coupled Plasma Mass Spectrometry after Anion Exchange Separation

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Zhang Lan Li Qinnuan

Key words Fission product, thorium, anion exchange, inductively coupled plasma mass spectrometry

For the determination of μg-mg L^{-1} of FPs in 100 g L^{-1} of thorium matrix with HCl medium, a method, including anion-exchange pre-separation, evaporation and inductively coupled plasma

mass spectrometry (ICP-MS) measurement, was developed. The procedure parameters, such as the matrix effect of thorium, the acidity of separation, the elution curve of thorium and FPs and the temperature of evaporation were optimized by batch equilibration, column elution and evaporation experiments. It was found that the average recovery of the FPs was in the range 80 – 110%, and the RSD values were in the range 2 – 15% utilizing prior anion exchange separation of FPs from thorium samples. Furthermore, the detection limit of the method was also investigated.

Analytical Sciences, 2017, **33**(11): 1265

Infrared Spectroscopic and Theoretical Studies on the OMF_2 and OMF (M = Cr, Mo, W) Molecules in Solid Argon

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Group 6 metal oxide fluoride molecules in the form of OMF_2 and OMF (M = Cr, Mo, W) were prepared via the reactions of laser-ablated metal atoms and OF_2 in excess argon. Product identifications were performed by using infrared spectroscopy, $^{18}OF_2$ samples, and electronic structure calculations. Reactions of group 6 metal atoms and OF_2 resulted in the formation of ternary $OCrF_2$, $OMoF_2$, and OWF_2 molecules with C_{2v} symmetry in which the tetravalent metal center is coordinated by one oxygen and two fluorine atoms. Both $OCrF_2$ and $OMoF_2$ are computed to possess triplet ground states, and a closed shell singlet is the ground state for OWF_2. Triatomic OCrF, OMoF, and OWF molecules were also observed during sample deposition. All three molecules were computed to have a bent geometry and quartet ground state. A bonding analysis showed that the OMF_2 molecules have highly ionic M–F bonds. $^3OCrF_2$ and $^3OMoF_2$ have an M–O double bond composed of a σ bond and a π bond. $^1OWF_2$ has an M–O triple bond consisting of a σ bond, a π bond, and a highly delocalized O lone pair forming the other π bond. The M–O bonds in the OMF compounds have triple-bond character for all three metals.

Journal of Physical Chemistry A, 2017, **121**(40): 7603

Coordination Structure and Fragmentation Chemistry of the Tripositive Lanthanide-Thio-Diglycolamide Complexes

Chen Xiuting Li Qingnuan Gong Yu

Tripositive $Ln(TMTDA)_3^{3+}$ complexes (Ln = La–Lu except Pm, TMTDA = tetramethyl 3-thio-diglycolamide) were observed in the gas phase by electrospray ionization of $LnCl_3$ and

TMTDA mixtures. Collision-induced dissociation (CID) was employed to investigate their fragmentation chemistry, which revealed the influence of metal center as well as ligand on the ligated complexes. $Ln(TMTDA)_2(TMTDA\text{-}45)^{3+}$ resulting from $C_{carbonyl}$–N bond cleavage of TMTDA and hydrogen transfer was the major CID product for all $Ln(TMTDA)_3^{3+}$ except $Eu(TMTDA)_3^{3+}$, which predominantly formed charge-reducing product $Eu^{II}(TMTDA)_2^{2+}$ via electron transfer from TMTDA to Eu^{3+}. Density functional theory calculations on the structure of $La(TMTDA)_3^{3+}$ and $Lu(TMTDA)_3^{3+}$ revealed that Ln^{3+} was coordinated by six $O_{carbonyl}$ atoms from three neutral TMTDA ligands, and both complexes possessed C_{3h} symmetry. The S_{ether} atom deviating from the ligand plane was not coordinated to the metal center. On the basis of the CID results of $Ln(TMTDA)_3^{3+}$, $Ln(TMGA)_3^{3+}$, and $Ln(TMOGA)_3^{3+}$, the fragmentation chemistry associated with the ligand depends on the coordination mode, while the redox chemistry of these tripositive ions is related to the nature of both metal centers and diamide ligands.

Journal of Physical Chemistry A, 2017, **121**(49): 9429

Formation and Fragmentation Chemistry of Tripositive $Ln(TMGA)_3^{3+}$ Complexes in the Gas Phase

Chen Xiuting Li Qingnuan Gong Yu

Key words Multiply charged cation, Lanthanide, Glutaramide, Reduction potential, Gas phase

Electrospray ionization (ESI) of $LnCl_3$ (Ln = La-Lu except Pm) and TMGA (tetramethyl glutaramide) mixtures resulted in the formation of gas-phase $Ln(TMGA)_3^{3+}$ complexes, where tripositive lanthanide cation was coordinated by three neutral TMGA ligands. Collision induced dissociation (CID) was employed to investigate the fragmentation chemistry of these tripositive complexes. $Ln(TMGA)_2(TMGA-45)^{3+}$ resulting from $C_{carbonyl}$–N bond cleavage of TMGA and hydrogen transfer is the major CID product for all $Ln(TMGA)_3^{3+}$ except $Eu(TMGA)_3^{3+}$ which predominantly forms divalent $Eu^{II}(TMGA)_2^{2+}$ complex via loss of $TMGA^+$. Analogous $Yb^{II}(TMGA)_2^{2+}$ and $Sm^{II}(TMGA)_2^{2+}$ complexes arising from charge reduction were also observed, in competition with the formation of charge conserving $Yb^{III}(TMGA)(TMGA\text{-}H)^{2+}$ and $Sm^{III}(TMGA)(TMGA\text{-}H)^{2+}$ products. The yield of these charge reducing products follows their reduction potentials in condensed phase. In addition to $Ln(TMGA)_3^{3+}$, tripositive ions such as $Ln(TMGA)_4^{3+}$ and $Ln(TMGA)_2^{3+}$ were experimentally identified as well. While the former was observed along with $Ln(TMGA)_3^{3+}$ during ESI, the latter was observed upon CID of $Ln(TMGA)_3^{3+}$, suggesting two TMGA molecules can stabilize Ln^{3+} in the gas phase.

Journal of the American Society for Mass Spectrometry, 2017, **28**(8): 1696

Preparation of Cu^{2+} -Chitosan Quaternary Ammonium Salt-g-Poly(acrylicacid) with Efficient Antibacterial Activity

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Key words Chitosan quaternary ammonium salt, Cupric ion, Antibacterial property, Acrylic acid

Acrylic acid (AAc) was grafted to chitosan quaternary ammonium salt (HACC) by ammonium persulfate as an initiator. HACC-g-PAAc-Cu^{2+} with efficient antibacterial activity was further prepared through complexation of Cu^{2+} with HACC-g-PAAc. The chemical structure of the grafted HACC was characterized by Fourier transform infrared spectroscopy and proton nuclear magnetic resonance (^{1}H NMR). The capacity of grafted HACC loading Cu^{2+} was determined by ultraviolet-visible spectroscopy(UV-Vis) and thermagravimetric analysis(TGA) . Antimicrobial property of HACC-Cu^{2+} and HACC-g-PAAc-Cu^{2+} against staphylococcus aurous (S. Aurous) and E. coli bacillus were tested. Toxicity for oral intake of mice and coating irritation on rabbit skin of HACC-Cu^{2+} and HACC-g-PAAc-Cu^{2+} were also evaluated. The property of antibacterial and capacity of complexing Cu^{2+} can be improved by grafting of AAc. The molar ratio of Cu^{2+} /HACC increased from 3: 7 before grafting to 1: 1 after graftin . The minimum inhibitory concentration(MIC) of S. Aurous and E. coli bacillus decreased from 60 mg /L to 9. 2 mg /L and 37 mg /L to 6. 3 mg /L. Moreover, HACC-Cu^{2+} and HACC-gPAAc-Cu^{2+} have no toxic ingestion and skin irritation.

Chemical Journal of Chinese Universities-Chinese, 2017, **38**(5): 902

Formation and Characterization of Homoleptic Thorium Isocyanide Complexes

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Homoleptic thorium isocyanide complexes have been prepared via the reactions of laser-ablated thorium atoms and $(CN)_2$ in a cryogenic matrix, and the structures of the products were characterized by infrared spectroscopy and theoretical calculations. Thorium atoms reacted with $(CN)_2$ under UV irradiation to form the oxidative addition product $Th(NC)_2$, which was calculated to have closed-shell singlet ground state with a bent geometry. Further reaction of $Th(NC)_2$ and $(CN)_2$ resulted in the formation of $Th(NC)_4$, a molecule with a tetrahedral geometry. Minor products such as ThNC and $Th(NC)_3$ were produced upon association reactions of CN with

Th and $Th(NC)_2$. Homoleptic thorium cyanide isomers $Th(CN)_x$ (x = 1–4) are predicted to be less stable than the corresponding isocyanides. The C–N stretches of thorium cyanides were calculated to be between 2170 and 2230 cm^{-1} at the B3LYP level, more than 120 cm^{-1} higher than the N–C stretches of isocyanides and with much weaker intensities. No experimental absorptions appeared where $Th(CN)_x$ should be observed.

Inorganic Chemistry, 2017, **56**(9): 5060

The extraction of uranium using graphene aerogel loading organic solution

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Li Qingnuan Zhang Lan

Key words Solvent extraction, Graphene aerogel, Superhydrophobic, Uranium

A new approach for uranium extraction employing graphene aerogel (GA) as a skeleton loading organic solution (GA-LOS) is proposed and investigated. Firstly, the GA with super-hydrophobicity and high organic solution absorption capacity was fabricated by one-step reduction and self-assembly of graphene oxide with ethylenediamine. By adsorbing Tri-n-butyl phosphate (TBP)/n-dodecane solution to prepare GA-LOS, the extraction of U(VI) from nitric acid medium using GA-LOS was investigated and compared with conventional solvent extraction. It is found that the GA-LOS method can provide several advantages over conventional solvent extraction and adsorption due to the elimination of aqueous-organic mixing-separation procedures and easy solid-liquid separation. Furthermore, it also possesses higher extraction capacity (the saturated extraction capacity of GA loading TBP for U(VI) was 316.3 mg g^{-1}) and lower consumption of organic diluents, leading to less organic waste. Moreover, the stability of GA-LOS in aqueous solution and cycling test were also studied, and it shows a remarkable regeneration capability, making it an ideal candidate for metal extraction from aqueous solution.

Talanta, 2017, **166**: 284

More wear-resistant and ductile UHMWPE composite prepared by the addition of radiation crosslinked UHMWPE powder

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Xing Zhe Hu Jiangtao Wang Mouhua Wu Guozhong

Key words applications, crosslinking, friction, irradiation, mechanical properties, wear and

lubrication

Radiation crosslinked ultrahigh molecular weight polyethylene (X-UHMWPE) powder was prepared by γ-ray irradiation under nitrogen atmosphere with a dose of 50–200 kGy at a dose rate of 7 kGy/h and further annealing in vacuum at 120 °C for 4 h. The crosslinked powder was characterized by FT-IR spectroscopy, gel content, and hot-press molding. Then, X-UHMWPE was added to pristine UHMWPE to prepare a composite with 0–25 wt % filler. The morphology, wear resistance, and tensile property of the composite were investigated. Using X-UHMWPE as a filler could sufficiently improve the wear resistance of the composite. Adding 25 wt % X-UHMWPE (dose: 150 kGy) improved wear resistance by 130% and retained approximately 90% tensile strength and 70% ductility. Wear-resistant and ductile UHMWPE composite may be potentially used for artificial joint replacement and engineering devices. The proposed route is useful in fabricating UHMWPE material with excellent comprehensive performance or functional polymer composite.

Journal of Applied Polymer Science, 2017, **134**(13): 44643

Optimization of molar content of amidoxime and acrylic acid in UHMWPE fibers for improvement of seawater uranium adsorption capacity

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Key words Ultra-high molecular weight polyethylene fiber, Amidoxime, Acrylic acid, Seawater, Uranium adsorption

Ultra-high molecular weight polyethylene (UHMWPE) fibrous adsorbents with different molar content of amidoxime (M_{AO}) and acrylic acid (M_{AA}) were prepared by graft polymerization of acrylonitrile (AN) and acrylic acid (AA), followed by amidoximation. Uranium adsorption experiments in both artificial and natural seawater were carried out to investigate the effect of M_{AO} and M_{AA} on the uranium adsorption capacity of UHMWPE fibrous adsorbents. Adsorption results showed that the UHMWPE fibrous adsorbent with M_{AO} = 4.27 and M_{AA} = 4.64 mmol/g-ads exhibited better uranium adsorption capacity in both artificial (7.01 mg-U/g-ads) and natural (0.77 mg-U/g-ads) seawater.

Journal of Radioanalytical and Nuclear Chemistry, 2017, **311**(3): 1771

Electrochemical behavior and electrowinning of uranium(IV) from FLiNaK molten salt

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Gong Yu Li Qingnuan

Key words Uranium, Fluoride, Molten salt, Electrochemical behavior, Electrowinning

The electrochemical behaviors and electrowinning of uranium from LiF–NaF–KF (46.5–11.5–42.0 mol%, FLiNaK) molten salt were investigated. Cyclic voltammetric and chronopotentiometric studies revealed the presence of two steps during the electro-reduction of UF_4 on W electode. U(IV) undergoes a one-electron reduction to form U(III) followed by a three-electron reduction to form U(0). The diffusion coefficient (D) of U(IV) ion was determined to be 1.33×10^{-6} cm^2 s^{-1} at 550 °C. Based on the electrochemical behaviors of U(IV) in FLiNaK melt, pulse current electrolysis was carried out using Ni electrode. The black bulks obtained as electrolysis products were characterized to contain metallic U. Consecutive electrolysis experiments demonstrated up to 74.7% U can be separated from the fluoride melt.

Journal of Radioanalytical and Nuclear Chemistry, 2017, **311**(3): 1891

Application of polyantimonic acid–polyacrylonitrile for removal of strontium(II) from simulated high-level liquid waste

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Key words Polyantimonic acid-polyacrylonitrile, Simulated HLLW, Strontium(II), Adsorption, Removal

Applicability of polyantimonic acid–polyacrylonitrile (PAA–PAN) in 60–150 mesh for removal of strontium(II) from simulated high-level liquid waste (HLLW) was investigated in this paper. The adsorption behavior of Sr(II) and other typical fission products (FPs) onto PAA–PAN was determined by using batch experiments. The results show that PAA–PAN exhibited high adsorption affinity for Sr(II) in HNO_3 medium, and other FPs except for Zr, which could be eluted by $H_2C_2O_4$–HNO_3, were weakly adsorbed on PAA–PAN. Then, a column experiment was performed to remove Sr(II) from simulated HLLW, and it's found that Sr(II) could be effectively transferred onto the PAA–PAN column from HLLW.

Journal of Radioanalytical and Nuclear Chemistry, 2017, **311**(3): 2007

Radiation effects on the foaming of atactic polypropylene with supercritical carbon dioxide

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Key words Polypropylene, Radiation, Cross-linking, Supercritical carbon dioxide, Foaming

Atactic polypropylene (PP) samples with melt flow indices (MFI) of 7.0 g/10 min were irradiated and then foamed with supercritical carbon dioxide ($scCO_2$). A detailed investigation was carried out to understand the effect of radiation on the $scCO_2$ foaming of polypropylene. Variations in the molecular weight, branching degree, crystallinity, and melting and crystallization temperatures of irradiated PP were investigated. The cell diameter, cell density, volume expansion ratio and foaming rate were analyzed in detail under different conditions. It was found that the cell structure of PP foam became more uniform and the foaming temperature window increased to 10 °C. This compares favorably to the 4 °C observed with pristine atactic PP. The best cell morphology was observed at a dose of 30 kGy. The corresponding average diameter and cell density were 16.4μm and 5.7×10^7 cells/cm^3, respectively.

Radiation Physics and Chemistry, 2017, **131**: 35

Di-1-methyl heptyl methylphosphonate (DMHMP): A promising extractant in Th-based fuel reprocessing

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Li Zheng Li Qingnuan Zhang Lan

Key words DMHMP, Physical property, Solvent extraction, Thorium-based fuel reprocessing

In this paper, the physical properties of tri-*iso*-amyl phosphate (TiAP), tri-*sec*-butyl phosphate (TsBP) and di-1-methyl heptyl methyl phosphonate (DMHMP) were studied and compared with tri-*n*-butyl-phosphate (TBP). Furthermore, the extraction behaviors of U(VI), Th(IV), nitric acid and fission products, and the extraction capacity of Th(IV) in different extractants were also investigated. The results indicated that the physical and extraction properties of DMHMP were better than that of other extractants and it is more appropriate to be used in thorium-based fuel reprocessing. A thorium-uranium co-decontamination process using DMHMP as extractant was proposed, optimized and verified by multistage countercurrent extraction using batch simulation and centrifugal extractors. By comparison with conventional Thorex process using TBP as extractant, it is found that DMHMP is more promising in thorium-based fuel reprocessing.

Separation and Purification Technology, 2017, **173**: 105

Electrochemical Behavior of Graphite Anode in LiF-NaF-KF Eutectic with YF_3

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Key words FLiNaK, graphite anode, electrolysis, current density, anode potential

The electrode reactions and electrolysis process of graphite anode were investigated in LiF-NaF-KF (FLiNaK, 46.5-11.5-42.0 mol%) eutectic with YF_3 at 823 K. Two different types of reactions were observed on graphite anode. The graphite was oxidized to carbon mono- and dioxide in a potential range of 0–2 V (*vs.* Ni^{2+}/Ni, similarly hereinafter), and carbon fluorides were generated when the potential fell into 6–8 V. In addition, some fluoride products could be reduced at about −0.22 V during reverse cyclic voltammetry scan, which has never been reported. Anode potential fluctuation was found between 6 and 8 V during galvanostatic electrolysis due to the formation of gaseous products as well as change of anode surface area and current density. Both Raman and X-ray photoelectron spectroscopy were employed to probe the chemical states of fluorination/oxidation products on graphite anode after electrolysis. The formation of fluorocarbon species is responsible for the disorder on graphite surface.

Electrochimica Acta, 2017, **225**: 392

Pyrohydrolysis of SmF_3 in moist air

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Key words SmF_3, Pyrohydrolysis, Thermogravimetry, Reaction mechanism, Kinetics

In order to prove the feasibility of pyrohydrolysis method of fluorides in TMSR spent fuel reprocessing, pyrohydrolysis behavior and reaction mechanism of neutron poison represented by SmF_3 in moist air, have been studied by means of thermogravimetric analysis (TG). Then, reaction products in solid state were characterized by means of XRD and SEM. The results indicated that SmF_3 began to hydrolyze in 773 K. Two definite breaks on TG curves were correlated to the conversions of SmF_3 into SmOF and SmOF into Sm_2O_3, respectively. Through the simulation calculation, we found that the two stages of the reaction can both meet the second-order reaction kinetics, and their corresponding activation energies are 60.2 and 31.2 kJ/mol, respectively. From the results of dynamics simulation, the rate equation obeyed the phase boundary rate law, which

was expressed by $[1 - (1-x)^{1/3}] = kt$. Further studies indicated that the rate-determining step was the surface reaction control, and the shrinking core model was applied to describe the mechanism. These results showed that pyrohydrolysis method of fluorides could be used for fuel reprocessing due to its unique reaction mechanism.

Journal of Fluorine Chemistry, 2017, **193**: 106

The evaporation behaviors of rare-earth-doped FLiNaK melts during low-pressure distillation

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Key words Molten salt, Low pressure distillation, Decontamination factor, Rare earth fluoride

Low pressure distillation of FLiNaK containing rare earth fluorides was carried out to investigate evaporation behaviors of FLiNaK as well as decontamination of rare earth fluorides. Evaporation rate of NdF_3–FLiNaK increased with rising temperature. Decontamination factors (DFs) of six rare earth elements were around 10^3 and 10^4 except europium due to the formation of EuF_2. A higher DF of europium up to 1.4×10^3 was obtained upon the addition of oxidant CeF_4. A hundred-gram scale experiment on FLiNaK containing NdF_3 and EuF_3 was performed, with a recovery ratio of 94.2% and the DF of europium to 2.4×10^3 at 900 °C.

Journal of Radioanalytical and Nuclear Chemistry, 2017, **311**(1): 637

Radiation-induced graft polymerization for the preparation of a highly efficient UHMWPE fibrous adsorbent for Cr(VI) removal

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Key words UHMWPE fiber, Radiation-induced graft polymerization, Cr(VI) adsorption, Reusable fibrous adsorbent

A novel fibrous adsorbent containing amine and quaternary ammonium groups was prepared by radiation-induced graft of glycidyl methacrylate (GMA) onto ultra-high molecular

weight polyethylene (UHMWPE) fiber and further modifying with triethylenetetramine (TETA) and glycidyl trimethylammonium chloride (GTA). The ATR-IR spectra and SEM observation demonstrated that amine and quaternary ammonium groups were immobilized onto the surface of UHMWPE fiber. The principal factors affecting the adsorption of Cr(VI) ions have been investigated including pH of the aqueous solution, contact time, temperature and coexisting anions. This novel fibrous adsorbent could effectively adsorb Cr(VI) in the range of pH 1–9, and the maximum adsorption capacity reached 295 mg/g at pH 3 and 25 °C based on the Langmuir isotherm. It was found that adsorption equilibrium could be achieved within 2 h for initial Cr(VI) of 100 mg/L, following the pseudo-second order model. The effect of coexisting anions (including SO_4^{2-}, $H_2PO_4^-$, $NO_3^-$and Cl^-) on the uptake of Cr(VI) was investigated in detail. Additionally, the adsorption saturated fiber could be regenerated by soaking in 0.5 mol/L NaOH solution, and the adsorption performance of this adsorbent could be maintained at 90% after eight cycles of adsorption-desorption. ATR-IR and XPS analysis revealed that Cr(VI) ions were adsorbed on the fiber adsorbent through ion exchange mechanism.

Radiation Physics and Chemistry, 2017, **130**: 92

An efficient tank size estimation strategy for packed-bed thermocline thermal energy storage systems for concentrated solar power

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Key words　Concentrated solar power, Thermal energy storage in a packed-bed, 1-D enthalpy-based model, Tank size estimation strategy

Thermocline storage in a packed-bed is considered as a promising thermal energy storage (TES) method that achieves cost reduction with respect to current concentrated solar power (CSP) plants. Several parametric studies investigated thermal performances of different types of packed-bed thermocline TES systems, and cost analyses and dimension design studies were conducted based on this. However, parametric studies typically involve high computing costs for a dimension design, and results obtained by correlation fitting suffer from a relative lack of accuracy. The main objective of the present study involves directly determining the tank size of a packed-bed thermocline TES system to satisfy certain design requirements of a CSP plant without requiring parametric studies. In order to achieve this goal, a one-dimensional enthalpy-based dispersion-concentric (D-C) model is developed and validated to investigate the periodic thermal behavior of the system. An efficient tank size estimation strategy is proposed based on the periodic

thermal performance of the system. The strategy is used to size four different packed-bed thermocline TES types under two exemplary operating conditions. The results reveal that tank size estimation strategy is independent of initial conditions, and that it is self-convergent, involves cost saving in terms of computing costs, is generally applicable, and can provide guidelines for the design of a TES system for CSP plants.

Solar Energy, 2017, **153**: 104

Growth and Scintillation Properties of GdI_3: Ce Crystal

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Huang YueFeng Xu JiaYue Ren GuoHao

Key words GdI_3: 2%Ce crystal, Bridgman method, scintillation property

Gadolinium iodide doped with Cerium (GdI_3: 2%Ce) and undoped gadolinium iodide (GdI_3) crystals were grown by vertical Bridgman method with sealed quartz crucible. Crystal ingots with dimension of ϕ15 mm×20 mm were cut and polished to be plates of 12 mm×10 mm×2.5 mm and 11 mm×8 mm×2.5 mm. GdI_3: 2%Ce without crack and inclusion were encapsulated for all the measurements. X-ray diffraction analysis shows that the Ce^{3+}-doped GdI_3 and undoped GdI_3 crystal have the same structure. X-ray and ultraviolet excited luminescence spectra of GdI_3: 2%Ce present broad emission bands peaking at 520 nm and 550 nm, respectively, which correspond to 5d-4f transition luminescence of Ce^{3+}. Three peaks located at 262, 335 and 440 nm can be observed in excitation spectra when photoluminescence is monitored at 550 nm. The GdI_3: 2%Ce crystal presents an excellent energy resolution of 3.4% and decay time of (58±3) ns under excitation of 662 keV gamma-rays from ^{137}Cs source. The results show the GdI_3: 2%Ce crystal is a promising scintillator for gamma ray and neutron detection.

Journal of Inorganic Materials, 2017, **32**(4): 346

Radionuclides in primary coolant of a fluoride salt-cooled high-temperature reactor during normal operation

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He ZhaoZhong Chen Kun

Key words Source term, FHR, Primary coolant, Fick's law, Diffusion

The release of fission products from coated particle fuel to primary coolant, as well as the activation of coolant and impurities, were analysed for a fluoride salt-cooled high-temperature

reactor (FHR) system, and the activity of radionuclides accumulated in the coolant during normal operation was calculated. The release rate (release fraction per unit time) of fission products was calculated with STACY code, which is modelled mainly based on the Fick's law, while the activation of coolant and impurities was calculated with SCALE code. The accumulation of radionuclides in the coolant has been calculated with a simplified model, which is generally a time integration considering the generation and decay of radionuclides. The results show that activation products are the dominant gamma source in the primary coolant system during normal operation of the FHR while fission products become the dominant source after shutdown. In operation condition, health-impacts related nuclides such as ^{3}H, and ^{14}C originate from the activation of lithium and coolant impurities including carbon, nitrogen, and oxygen. According to the calculated effective cross sections of neutron activation, ^{6}Li and ^{14}N are the dominant ^{3}H production source and ^{14}C production source, respectively. Considering the high production rate, ^{3}H and ^{14}C should be treated before being released to the environment.

Nuclear Science and Techniques, 2017, **28**(3): 41

Thermal performance analysis of a thermocline thermal energy storage system with FLiNaK molten salt

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A thermocline thermal storage unit with a heat transfer fluid (HTF) of high-temperature molten salt is considered as one of the most promising methods of thermal storage due to its lower cost and smaller size. The main objective of this work is to analyze the transient behavior of the available molten salt FLiNaK used as the HTF in heat transfer and heat storage in a thermocline thermal energy storage (TES) system. Thermal characteristics including temperature profiles influenced by different inlet velocities of HTF and different void fractions of porous heat storage medium are analyzed. The numerical investigation on the heat storage and heat transfer characteristics of FLiINaK has been carried out. A comparison between two different molten salts, FLiNaK and Hitec, has been explored in this paper with regards to their charging and discharging operations. The results indicate the system with FLiNaK has a greater energy storage capability, a shorter charging time and a higher output power. The numerical investigation reveals heat storage and heat transfer characteristics of the thermocline TES system with FLiNaK, and provide important references for molten salt selection of the TES system in the future.

IOP Conference Series:　Earth and Environmental Science, 2017, **52**: 012039

Neutronics physics analysis of a large fluoride-salt-cooled solid-fuel fast reactor with Th-based fuel

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Key words Fluoride salts, Thorium cycle, Fast reactor, Core characteristics, Equilibrium

Fast reactors based on thorium fuel have enhanced inherent safety. Fluoride salt performs well as a coolant in high-temperature nuclear systems. In this paper, we present a reference core for a large fluoride-salt-cooled solid-fuel fast reactor (LSFR) using thorium–uranium fuel cycle. Neutronics physics of the LSFR reference core is investigated with 2D and 3D in-core fuel management strategy. The design parameters analyzed include the fuel volume fraction, power density level and continuous removal of fission products with 3D fuel shuffling that obtains better equilibrium core performance than 2D shuffling. A self-sustained core is achieved for all cases, and the core of 60% fuel volume fraction at 50 MW/m^3 power density is of the best breeding performance (average breeding ratio 1.134). The LSFR core based on thorium fuel is advantageous in its high discharge burn-up of 20–30% fissions per initial heavy metal atom, small reactivity swing over the whole lifetime (to simplify the reactivity control system), the negative reactivity temperature coefficient (intrinsically safe for all cases) and accepted cladding peak radiation damage. The LSFR reactor is a good alternative option for the deployment of a self-sustained thorium-based nuclear system.

Nuclear Science and Techniques, 2017, **28**(11): 158

The feasibility research of thorium breeding using fluoride salt as a fast reactor coolant

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Cai Xiangzhou Xu Hongjie

Key words Fluoride salts, Coolant selection, Neutron balance, Thorium cycle, Fast reactor

Breeder reactors are considered as a unique tool for fully exploiting natural resources. Fast breeder reactors based on thorium fuel can enhance inherent safety. Fluoride salt has good performance as a coolant in high-temperature nuclear systems. However, there is some doubt about the fuel breeding ability using fluoride salt coolant for fast spectrum due to its moderating ability. The aim of this study was to choose a proper fluoride salt mixture for Liquid-salt-cooled Solid-fuel Fast Reactor (LSFR) based on thorium-uranium fuel and give parametric studies to provide a design window for flexible self-sustaining core design. Infinite assembly model was used to

analyze the salt selection from five candidate fluorides for fast spectrum as coolant. Combining neutron balance analysis with linear least squares fitting method based on 0D model, parametric studies at the neutron balance equation unique solution with burn-up for several parameters such as fuel volume fraction, removing fission gases process, total neutron losses and power density were presented in this paper. It was found that BeF_2-NaF was a promising coolant in the five candidate fluoride salt mixture. This study proved that the design of a self-sustaining core for fluoride-salt-cooled fast breeder based on thorium fuel is achievable. A design window was found in the definition of a self-sustaining core for various fuel volume fractions and neutron loss fractions. Core design and fuel management strategy will be given in future.

Progress in Nuclear Energy, 2017, **101**: 199

Transition toward thorium fuel cycle in a molten salt reactor by using plutonium

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Chen JinGen

Key words Molten salt reactor, Thorium fuel cycle, Plutonium, Reprocessing

The molten salt reactor (MSR), as one of the Generation IV advanced nuclear systems, has attracted a worldwide interest due to its excellent performances in safety, economics, sustainability, and proliferation resistance. The aim of this work is to provide and evaluate possible solutions to fissile ^{233}U production and further the fuel transition to thorium fuel cycle in a thermal MSR by using plutonium partitioned from light water reactors spent fuel. By using an in-house developed tool, a breeding and burning (B&B) scenario is first introduced and analyzed from the aspects of the evolution of main nuclides, net ^{233}U production, spectrum shift, and temperature feedback coefficient. It can be concluded that such a Th/Pu to Th/^{233}U transition can be accomplished by employing a relatively fast fuel reprocessing with a cycle time less than 60 days. At the equilibrium state, the reactor can achieve a conversion ratio of about 0.996 for the 60-day reprocessing period (RP) case and about 1.047 for the 10-day RP case. The results also show that it is difficult to accomplish such a fuel transition with limited reprocessing (RP is 180 days), and the reactor operates as a converter and burns the plutonium with the help of thorium. Meanwhile, a pre-breeding and burning (PB&B) scenario is also analyzed briefly with respect to the net ^{233}U production and evolution of main nuclides. One can find that it is more efficient to produce ^{233}U under this scenario, resulting in a double time varying from about 1.96 years for the 10-day RP case to about 6.15 years for the 180-day RP case.

Nuclear Science and Techniques, 2017, **28**(10): 152

Evaluation of the fraction of delayed photoneutrons for TMSR-SF1

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Key words Photoneutron, Effective delayed neutron fraction, TMSR-SF1

The 10 MW_{th} solid-fueled thorium molten salt reactor (TMSR-SF1) is a FLiBe salt-cooled pebble bed reactor to be deployed in 5–10 years, designed by the TMSR group. Due to a large amount of beryllium in the core, the photoneutrons are produced via (γ, n) reactions. Some of them are generated a long time after the fission event and therefore are considered as delayed neutrons. In this paper, we redefine the effective delayed neutrons into two fractions: the delayed fission neutron fraction and the delayed photoneutron fraction. With some reasonable assumptions, the inner product method and the *k*-ratio method are adopted for studying the effective delayed photoneutron fraction. In the *k*-ratio method, the Monte Carlo code MCNP6 is used to evaluate the effective photoneutron fraction as the ratio between the multiplication factors with and without contribution of the delayed neutrons and photoneutrons. In the inner product method, with the Monte Carlo and deterministic codes together, we use the adjoint neutron flux as a weighting function for the neutrons and photoneutrons generated in the core. Results of the two methods agree well with each other, but the *k*-ratio method requires much more computing time for the same precision.

Nuclear Science and Techniques, 2017, **28**(9): 135

Development of a GPU-accelerated 3D neutron dynamics code for PB-FHR

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Key words PB-FHR, 3D neutron dynamics, GPU-accelerated, Fine mesh, Conjugate gradient method, Preconditioner

Pebble bed fluoride-salt cooled high temperature reactor (PB-FHR) is a kind of novel nuclear energy systems, combining advanced techniques such as coated particle fuel and molten-salt coolant to achieve better safety and economy performance. The compact core of a PB-FHR is geometrically complicated due to the randomly-packed pebble bed with fuel motion in a complex core chamber, which yields a highly detailed core-modeling for accurate neutron dynamics analysis. Three-dimensional fine mesh finite volume method is expected to achieve better accuracy because

of its strong geometry adaptability in detailed core-modeling, but is much more time-consuming compared to other methods such as coarse mesh nodal method. A GPU-accelerated 3D fine mesh neutron dynamics code (GAND) is developed, using conjugate gradient method (CG) to solve the time-dependent multi-group neutron diffusion equations in r-z-θ coordinates. The GAND code is verified by a cylindrical reactor benchmark with good agreement, and is preliminarily applied to a PB-FHR core in both static and transient analysis. Speed-up ratio and other performance of GAND code using different equation preconditioners is studied, a best speed-up ratio of 21.65 has been achieved using Neumann polynomials-preconditioned CG.

Nuclear Engineering and Design, 2017, **320**: 88

A specialized code for operation transient analysis and its application in fluoride salt-cooled high-temperature reactors

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Key words FHR, Simulation, Pebble bed, Transient analysis

Fluoride salt-cooled high-temperature reactors (FHRs) include many attractive features, such as high temperature, large heat capacity, low pressure and strong inherent safety. Transient characteristics of FHR are particularly important for evaluating its operation performance. Thus, a specialized code OCFHR (operation and control analysis code of FHR) issued to study an experimental FHR's operation behaviors. The geometric modeling of OCFHR is based on one-dimensional lumped parameter method, and some simplifications are taken into consideration during simulation due to the existence of complex structures such as pebble bed, intermediate heat exchanger (IHX), air radiator (AR) and multiply channels. A point neutron kinetics model is developed, and neutron physics calculation is needed to provide some key inputs including axial power density distribution, reactivity coefficients and parameters about delayed neutron precursors. For analyzing the operational performance, five disturbed transients are simulated, involving reactivity step insertion, variations of coolant mass flow rate of primary loop and intermediate loop, adjustment of air inlet temperature and mass flow rate of air cooling system. Simulation results indicate that inherent self-stability of FHR restrains severe consequences under above transients, and some dynamic features are observed, such as large negative temperature feedbacks, remarkable thermal inertia and high response delay.

Nuclear Science and Techniques, 2017, **28**(8): 119

Influences of ^{7}Li enrichment on Th–U fuel breeding for an Improved Molten Salt Fast Reactor (IMSFR)

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Chen JinGen Xu HongJie

Key words IMSFR, ^{7}Li enrichment, Thorium, Fuel breeding

The molten salt fast reactor (MSFR) shows great promise with high breeding ratio (BR), large negative temperature coefficient of reactivity, high thermal–electric conversion efficiency, inherent safety, and online reprocessing. Based on an improved MSFR optimized by adding axial fertile salt and a graphite reflector, the influences of ^{7}Li enrichment on Th–U breeding are investigated, aiming to provide a feasible selection for the molten salt with high fissile breeding and a relatively low technology requirement for ^{7}Li concentration. With the self-developed molten salt reactor reprocessing sequence based on SCALE6.1, the burn-up calculations with online reprocessing are carried out. Parameters are explored including BR, ^{233}U production, double time (DT), spectrum, ^{6}Li inventory, neutron absorption, and the tritium production. The results show that the ^{7}Li enrichment of 99.95% is appropriate in the fast fission reactor. In this case, BR above 1.10 can be achieved for a long time, corresponding to the ^{233}U production of 130 kg per year and DT of 36 years. After 80 years' operation, the tritium production for 99.5% is only about 7 kg, and there is no obvious increase compared to that for 99.9995%.

Nuclear Science and Techniques, 2017, **28**(7): 97

Impact of photoneutrons on reactivity measurements for TMSR-SF1

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Key words TMSR-SF1, Delayed photoneutrons, Coupled neutron-photon point kinetics, Reactivity measurement

The solid-fueled thorium molten salt reactor (TMSR-SF1) is a 10 MW_{th} test reactor design to be deployed in 5–10 years by the TMSR group. Its design combines coated particle fuel and molten FLiBe coolant for great intrinsic safety features and economic advantages. Due to a large amount of beryllium in the coolant salt, photoneutrons are produced by (γ, n) reaction, hence the increasing fraction of effective delayed neutrons in the core by the photoneutrons originating from the long-lived fission products. Some of the delayed photoneutron groups are of long lifetime, so a direct effect is resulted in the transient process and reactivity measurement. To study the impact of

photoneutrons for TMSR-SF1, the effective photoneutron fraction is estimated using *k*-ratio method and performed by the Monte Carlo code (MCNP5) with ENDF/B-VII cross sections. Based on the coupled neutron–photon point kinetics equations, influence of the photoneutrons is analyzed. The results show that the impact of photoneutrons is not negligible in reactivity measurement. Without considering photoneutrons in on-line reactivity measurement based on inverse point kinetics can result in overestimation of the positive reactivity and underestimation of the negative reactivity. The photoneutrons also lead to more waiting time for the doubling time measurement. Since the photoneutron precursors take extremely long time to achieve equilibrium, a "steady" power operation may not directly imply a "real" criticality.

Nuclear Science and Techniques, 2017, **28**(6):

Projector Augmented Wave Method Incorporated into Gauss-Type Atomic Orbital Based Density Functional Theory

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The Projector Augmented Wave (PAW) method developed by Blöchl is well recognized as an efficient, accurate pseudopotential approach in solid-state density functional theory (DFT) calculations with the plane-wave basis. Here we present an approach to incorporate the PAW method into the Gauss-type function (GTF) based DFT implementation, which is widely used for molecular quantum chemistry calculations. The nodal and high-exponent GTF components of valence molecular orbitals (MOs) are removed or pseudized by the ultrasoft PAW treatment, while there is elaborate transparency to construct an accurate and well-controlled pseudopotential from all-electron atomic description and to reconstruct an all-electron form of valence MOs from the pseudo MOs. The smoothness of the pseudo MOs should benefit the efficiency of GTF-based DFT calculations in terms of elimination of high-exponent primitive GTFs and reduction of grid points in the numerical quadrature. The processes of the PAW method are divided into basis-independent and -dependent parts. The former is carried out using the previously developed PAW libraries libpaw and atompaw. The present scheme is implemented by incorporating libpaw into the conventional GTF-based DFT solver. The details of the formulations and implementations of GTF-related PAW procedures are presented. The test calculations are shown for illustrating the performance. With the near-complete GTF basis at the cc-pVQZ level, the total energies obtained using our PAW method with suited frozen core treatments converge to those with the conventional all-electron GTF-based method with a rather small absolute error.

Journal of Chemical Theory and Computation, 2017, **13**(7): 3236

Effect of Cr contents on the diffusion behavior of Te in Ni-based alloy

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Qiu Jie Liu Min Li Zhijun

Key words Te, Ni-Cr alloy, Diffusion, Gibbs free energy, Intergranular embrittlement

The embrittlement of Ni-based structural alloys caused by fission production Te is one of the major challenges for molten salt reactors. It has been reported that solution element Cr can prevent the situation of intergranular cracks caused by Te. However, there is no detailed mechanism explanation on this phenomenon. In this study, the effect of Cr on Te diffusion in Ni-Cr binary system was investigated by diffusion experiments at 800 °C for 100 h. Results show that Te reacts with the alloy mainly forming Ni_3Te_2, and strip shaped Cr_3Te_4 is only found on the surface of Ni-15%Cr alloy. According to the discussion of thermodynamic chemical reaction process, Cr_3Te_4 exhibits the best stability and preferential formation compound in Te/Ni–Cr system as its Gibbs free energy of formation is the lowest. With the increase of Cr content in the alloy, the diffusion depth of Te along grain boundaries significantly decreases. Moreover, the formation process of reaction product and diffusion process are described. The diffusion of Te can be suppressed by high content of Cr in Ni-Cr alloy due to the formation of Cr_3Te_4 and thus the grain boundary is protected from Te corroding.

Journal of Nuclear Materials, 2017, **497**: 101

Behaviors of fine (IG-110) and ultra-fine (HPG-510) grain graphite irradiated by 7 MeV Xe^{26+} ions

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Zhang Can Song JinLiang Lei GuanHong Zhou XingTai
Xia HuiHao Huai Ping

Key words Molten salt reactor, Graphite, Ion irradiation, Raman spectra, Hardness and Young's modulus

Developing a molten salt reactor needs molten salt–impermeable nuclear graphite. Ultra-fine grain graphite is a good choice as it is better in permeability than fine grain graphite. In this paper, ultra-fine grain graphite (HPG-510) and fine grain graphite (IG-110) samples are irradiated at room temperature by 7 MeV Xe ions to doses of 1×10^{14}–5×10^{15} ions/cm^2. Scanning electron

microscopy, transmission electron microscopy (TEM), Raman spectroscopy and nano-indentation are used to study the radiation-induced changes. After irradiation of different doses, all the HPG-510 samples show less surface fragment than the IG-110 samples. The TEM and Raman spectra, and the hardness and modulus characterized by nano-indentation, also indicate that HPG-510 is more resistant to irradiation.

Nuclear Science and Techniques, 2017, **28**(10): 144

Infiltration of graphite by molten 2LiF–BeF_2 salt

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Zhang Can Wang Xue Song Jinliang
Huai Ping Zhou Xingtai

With the aim of developing neutron moderator and neutron reflector materials for fluoride-salt-cooled high-temperature reactors (FHRs), static infiltration tests were performed on graphite materials in molten 2LiF–BeF_2 (FLiBe) salt, which is a potential primary coolant, at 700 °C and various pressures. The weight gain ratios of four grades (NBG-18, IG-110, NG-CT-10, and NG-CT-50) of graphite after infiltration were measured to determine their infiltration curves. The threshold pressure for FLiBe salt infiltration for the ultrafine-grained graphite (NG-CT-50) was greater than 600 kPa and much higher than those of the other three grades (medium-grained/fine-grained graphites), indicating that this graphite grade more probably resists salt infiltration in FHRs than other grades of graphite. However, if the threshold pressure is exceeded, it has the highest potential capacity for infiltrated salt over the pressures tested. The four grades were also characterized using mercury intrusion porosimetry. It was found that the infiltration curves of these two unwetting liquids were very similar. Scanning electron microscopy characterization showed that the FLiBe salt was distributed relatively uniformly in all four grades, indicating the presence of interconnected networks of open pores throughout the samples. X-ray diffraction patterns showed that infiltration test at high pressure led to an improved structural order and a decreased d-spacing in graphite.

Journal of Materials Science, 2017, **52**(19): 11346

Novel 3D metallic boron nitride containing only sp^2 bonds

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Key words boron nitride, stability, metallicity, DFT calculations

As the closest isoelectronic analogue of carbon, boron nitride (BN) shares a similar structure with carbon from 1D nanotubes, 2D nanosheets, and 3D diamond structures. However, most BN

structures are insulators, which limits their application. In this work, under the inspiration of the sp^2 hybridized carbon honeycomb, we propose a hexagonal phase of BN consisting of only sp^2 bonds, which exhibits intriguingly intrinsic metallicity. First-principles calculations confirm that this phase is both thermally and dynamically stable. Moreover, the calculations on the band structure, partial density states and electron localization function suggest that the metallic behavior is attributable to the delocalized B-2p electrons, leading to second-neighbor interaction between the p*z* states of sp^2-bonded B atoms in adjacent layers. Our findings not only enrich the BN allotrope family with 3D structures but also stimulate further experimental interest in applications of metallic BN in electronic devices.

Journal of Physics D: Applied Physics, 2017, **50**(38): 385302

High temperature in-situ synchrotron-based XRD study on the crystal structure evolution of C/C composite impregnated by FLiNaK molten salt

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Yang Xinmei Xia Huihao Yan Long Tsang Derek K. L.
Huai Ping Zhou Xingtai

An *in-situ* real-time synchrotron-based grazing incidence X-ray diffraction was systematically used to investigate the crystal structural evolution of carbon fiber reinforced carbon matrix (C/C) composite impregnated with FLiNaK molten salt during the heat-treatment process. It was found that the crystallographic thermal expansion and contraction rate of interlayer spacing d_{002} in C/C composite with FLiNaK salt impregnation is smaller than that in the virgin sample, indicating the suppression on interlayer spacing from FLiNaK salt impregnated. Meanwhile the crystallite size L_{C002} of C/C composite with FLiNaK salt impregnation is larger than the virgin one after whole heat treatment process, indicating that FLiNaK salt impregnation could facilitate the crystallization of C/C composite after heat treatment process. This improved crystallization in C/C composite with FLiNaK salt impregnation suggests the synthetic action of the salt squeeze effect on crooked carbon layer and the release of internal residual stress after heating-cooling process. Thus, the present study not only contribute to reveal the interaction mechanism between C/C composite and FLiNaK salt in high temperature environment, but also promote the design of safer and more reliable C/C composite materials for the next generation molten salt reactor.

Scientific Reports, 2017, **7**: 10673

First-principles study of helium clustering at initial stage in ThO_2

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Key words first-principles study, thorium dioxide, helium cluster, defective properties

The clustering behavior of helium atoms in thorium dioxide has been investigated by first-principles calculations. The results show that He atoms tend to form a cluster around an octahedral interstitial site (OIS). As the concentration of He atoms in ThO_2 increases, the strain induced by the He atoms increases and the octahedral interstitial site is not large enough to accommodate a large cluster, such as a He hexamer. We considered three different Schottky defect (SD) configurations (SD_1, SD_2, and SD_3. When He atoms are located in the SD sites, the strain induced by the He atoms is released and the incorporation and binding energies decrease. The He trimer is the most stable cluster in SD_1. Large He clusters, such as a He hexamer, are also stable in the SDs.

Chinese Physics B, 2017, **26**(9): 097101

First-principles study of fission product stability and clustering in ThO_2

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Ren, Cui-Lan Huai, Ping

Key words Thorium dioxide, First-principles study, Fission product, Defective properties

The stability and clustering behavior of fission products (Zr, Mo, Ru, and Rh) in thorium dioxide have been investigated by density functional theory. The calculations were performed considering the possible insertion sites in ThO_2, including interstitial sites, thorium vacancies, oxygen vacancies, the oxygen–thorium divacancy, and three types of Schottky defect. The thorium vacancy is the most energetically favorable trap site for all of these fission products. Zr and Mo can exist as oxide precipitates whereas Rh and Ru tend to form metallic clusters in ThO_2. Moreover, Ru and Rh dimers are the most stable clusters in the Schottky defect in ThO_2, suggesting that metal clusters in ThO_2 may be formed of these dimers trapped in Schottky defects.

Computational Materials Science, 2017, **137**: 186

Evaluating Young's modulus of porous nuclear graphite by a novel multi-scale method

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Nuclear graphite has served as neutron moderator, reflector and structural material in various nuclear reactors due to its excellent irradiation performance and mechanical properties at high temperature. However, the microstructure of nuclear graphite contains over 10% porosity by volume. During the lifetime of reactors, the porosity of nuclear graphite will be increased due to the irradiation-induced volume changes and/or radiolytic oxidation. Consequently, it is important to predict the effect of porosity on the mechanical properties of nuclear graphite. In this paper, a novel multi-scale method was used to study the effect of porosity on Young's modulus. Numerical results suggested that Young's modulus versus porosity can be predicted by the Knudsen law. Then, the influence of different pore distributions on Young's modulus was analysed. Finally, Young's modulus with different pore sizes and the effect of pore shape were studied. And a relationship between decay coefficients in the Knudsen law and the pore shape ratios was found.

Journal of Materials Science, 2017, **52**(18): 10959

First-principles prediction of interstitial carbon, nitrogen, and oxygen effects on the helium behavior in nickel

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Huang HeFei Yin YaRu Zhang Wei Lumpkin Gregory
Huai Ping Zhu ZhiYuan

The effects of interstitial carbon, nitrogen, and oxygen (C/N/O) on the helium behavior in nickel are studied by using first-principles calculations. The interstitial C/N/O changes the occupying priority of helium to the first nearest neighbor Oct-site, which is related to local strain effect and chemical bonding between helium and its adjacent atoms. Both binding energy calculation and diffusion property analysis confirm that the interstitial C/N/O can trap helium in nickel. Moreover, with lower binding energy and larger trapping radii to helium, the interstitial oxygen has significant effect on helium trapping compared with that of nitrogen and carbon. With more helium aggregating at vacancy, the C/N/O would also trap smaller helium clusters and repel larger ones, indicating that the interstitial C/N/O could disperse helium bubbles and further inhibit their growth in nickel. This work helps to understand the helium embrittlement resistant mechanisms of the initial nucleation sites for second phase nanoparticles in nickel-based alloys.

Journal of Applied Physics, 2017, **122**(6): 065901

Effect of Mg on the Microstructure and Corrosion Resistance of the Continuously Hot-Dip Galvanizing Zn-Mg Coating

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Xing Hui Shu Da Sun Baode Wang Jun

Key words continuously hot-dip galvanizing, Zn-Mg coating, TEM, corrosion resistance

The microstructure of continuously hot-dip galvanizing Zn-Mg coating was investigated in order to obtain the mechanism of the effects of Mg on the corrosion resistance. In this paper, the vertical section of the Zn-0.20 wt % Al-Mg ternary phase diagram near the Al-low corner was calculated. The results indicates that the phase composition of the Zn-0.20 wt % Al-Mg ternary phase diagram near the Al-low corner is the same as Zn-Mg binary phase diagram, suggesting Al in the Zn-Mg (ZM) coatings mainly concentrates on the interfacial layer between the coating and steel substrate. The microstructure of continuously hot-dip galvanizing ZM coatings with 0.20 wt % Al containing 1.0–3.0 wt % Mg was investigated using tunneling electron microscopy (TEM). The morphology of Zn in the coating changes from bulk to strip and finally to mesh-like, and the $MgZn_2$ changes from rod-like to mesh-like with the Mg content increasing. Al in the ZM coatings mainly segregates at the Fe_2Al_5 inhibition layer and the Mg added to the Zn bath makes this inhibition layer thinner and uneven. Compared to GI coating, the time of the first red rust appears increases by more than two-fold and expansion rate of red rust reduces by more than four-fold in terms of salt spray experiment. The ZM coating containing 2.0 wt % Mg has the best corrosion resistance. The enhanced corrosion resistance of ZM coatings mainly depends on different corrosion products.

Materials, 2017, **10**(8): 980

Effects of SO_4^{2-} ions on the corrosion of GH3535 weld joint in FLiNaK molten salt

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Chen Huaican Ai Hua Yu Guojun
Wang Jianqiang Zhou Xingtai

Key words Molten salt, FLiNaK, Corrosion, SO_4^{2-} ions, Weld joint, Ni-based alloy

The present work studied the impact of SO_4^{2-} ions on the corrosion behaviors of GH3535 weld joint in FLiNaK molten salt. The concentration of SO_4^{2-} ions in the FLiNaK molten salt was controlled by adjusting the quantity of Na_2SO_4 added into the salt. Results indicate that the

SO_4^{2-} ions in the FLiNaK salt speed up the corrosion rate remarkably by promoting the dissolution of Cr from the alloy matrix into the salt. With the concentration of SO_4^{2-} ions in the FLiNaK salt increases from 100 ppm to 1000 ppm, the weight losses and the Cr depletion layer depths of the corroded specimens increase linearly. Even in the case of the heavy corrosion attack caused by the SO_4^{2-} ions, the corrosion performance is similar between the base zone and fusion zone in the GH3535 weld joint. It is demonstrated that the structural diversity caused by the welding process has little impact on the corrosion performances of GH3535 alloy in FLiNaK molten salt.

Journal of Nuclear Materials, 2017, **492**: 122

First-principles study of noble gas stability in ThO_2

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Wang ChangYing Guo YongLiang Ren CuiLan Huai Ping

Key words Thorium dioxide, Defective properties, Noble gas, First-principles study

The stability of noble gases (He, Ne, Ar, Kr and Xe) in thorium dioxide is studied by means of density functional theory. The computations are performed considering insertion sites of ThO_2, including the interstitial sites, the thorium vacancies, the oxygen-thorium di-vacancy and three types of Schottky defects. Our results show that there is an approximately linear relation between the energies and the atomic radii. As the size of the noble gas atom increases, the noble gas atoms energetically prefer to incorporate into large vacancy defects rather than into interstitial positions. Moreover, the binding energy of Kr or Xe interstitial in a Schottky defect is larger than the formation energy of a Schottky defect, suggesting the Schottky defects are thermodynamically favorable in the presence of these noble gas atoms. The charged defects are also considered for noble gas atoms trapped in Th and O vacancies.

Journal of Nuclear Materials, 2017, **490**: 181

First-principles investigation on the geometries, stabilities and defective properties of fluoride surfaces

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Shao Kuan Zhang Wei Dai Jianxing Huai Ping

Key words Metal fluoride, First-principles, Surface property, Density functional calculation

From first-principles calculations, we perform a systematic study of the stoichiometric surface morphology of NaF, MgF_2 and CaF_2 and the associated stability, charge transfer and defective

properties. Given the geometries of their low index surfaces, it is found that the surfaces with the lowest surface energies for NaF, MgF_2, and CaF_2 are (1 0 0), (1 1 0) and (1 1 1) surfaces, respectively. The dependence of surface energies, electrostatic potentials and effective charges on the slab thickness is discussed. Moreover, we demonstrate the broken bond model, which is based on the covalent interactions, is also suitable for ionic fluoride crystals after modification. By setting a fitting parameter *k* around 0.5, the estimated surface energies are close to the ones by slab modeling for all the 10 surfaces considered in this work.

Computational Materials Science, 2017, **133**: 159

Pressure-induced structural transformations and polymerization in ThC_2

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Ren Cuilan Sun Baoxing Huai Ping Xie Ruobing
Ke Xuezhi Zhu Zhiyuan Xu Hongjie

Thorium-carbon systems have been thought as promising nuclear fuel for Generation IV reactors which require high-burnup and safe nuclear fuel. Existing knowledge on thorium carbides under extreme condition remains insufficient and some is controversial due to limited studies. Here we systematically predict all stable structures of thorium dicarbide (ThC_2) under the pressure ranging from ambient to 300 GPa by merging *ab initio* total energy calculations and unbiased structure searching method, which are in sequence of C2/c, C2/m, Cmmm, Immm and P6/mmm phases. Among these phases, the C2/m is successfully observed for the first time via *in situ* synchrotron XRD measurements, which exhibits an excellent structural correspondence to our theoretical predictions. The transition sequence and the critical pressures are predicted. The calculated results also reveal the polymerization behaviors of the carbon atoms and the corresponding characteristic C-C bonding under various pressures. Our work provides key information on the fundamental material behavior and insights into the underlying mechanisms that lay the foundation for further exploration and application of ThC_2.

Scientific Reports, 2017, **7**: 45872

The Effect of Milling Time on the Microstructural Characteristics and Strengthening Mechanisms of NiMo-SiC Alloys Prepared via Powder Metallurgy

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Key words powder metallurgy, DPS strengthening, spark plasma sintering, transmission electron microscopy, electron backscatter diffraction, molten salt reactor

A new generation of alloys, which rely on a combination of various strengthening mechanisms, has been developed for application in molten salt nuclear reactors. In the current study, a battery of dispersion and precipitation-strengthened (DPS) NiMo-based alloys containing varying amounts of SiC (0.5–2.5 wt %) were prepared from Ni-Mo-SiC powder mixture via a mechanical alloying (MA) route followed by spark plasma sintering (SPS) and rapid cooling. Neutron Powder Diffraction (NPD), Electron Back Scattering Diffraction (EBSD), and Transmission Electron Microscopy (TEM) were employed in the characterization of the microstructural properties of these in-house prepared NiMo-SiC DPS alloys. The study showed that uniformly-dispersed SiC particles provide dispersion strengthening, the precipitation of nano-scale Ni_3Si particles provides precipitation strengthening, and the solid-solution of Mo in the Ni matrix provides solid-solution strengthening. It was further shown that the milling time has significant effects on the microstructural characteristics of these alloys. Increased milling time seems to limit the grain growth of the NiMo matrix by producing well-dispersed Mo_2C particles during sintering. The amount of grain boundaries greatly increases the Hall–Petch strengthening, resulting in significantly higher strength in the case of 48-h-milled NiMo-SiC DPS alloys compared with the 8-h-milled alloys. However, it was also shown that the total elongation is considerably reduced in the 48-h-milled NiMo-SiC DPS alloy due to high porosity. The porosity is a result of cold welding of the powder mixture during the extended milling process.

Materials, 2017, **10**(4): 389

Probing Chemical Bonding and Electronic Structures in ThO^- by Anion Photoelectron Imaging and Theoretical Calculations

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Fei Zejie Tang Zichao Liu Hongtao

Because of renewed research on thorium-based molten salt reactors, there is growing demand and interest in enhancing the knowledge of thorium chemistry both experimentally and theoretically. Compared with uranium, thorium has few chemical studies reported up to the present. Here we report the vibrationally resolved photoelectron imaging of the thorium monoxide anion. The electron affinity of ThO is first reported to be 0.707 ± 0.020 eV. Vibrational frequencies of the ThO molecule and its anion are determined from Franck–Condon simulation. Spectroscopic evidence is obtained for the two-electron transition in ThO^-, indicating the strong electron correlation among the $(7s_\sigma)^2(6d_\delta)^1$ electrons in ThO^- and the $(7s_\sigma)^2$ electrons in ThO. These findings are explained by using quantum-chemical calculations including spin–orbit coupling, and the chemical bonding of gaseous ThO molecules is analyzed. The present work will enrich our understanding of bonding capacities with the 6d valence shell.

Journal of Physical Chemistry A, 2017, **121**(10): 2108

The influence of FLiNaK salt impregnation on the mechanical properties of a 2D woven C/C composite

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Key words 2D woven C/C composite, Mechanical property, Molten salt, Impregnation, X-ray computed tomography

Impregnating of molten LiF-NaF-KF salt (LiF-NaF-KF: 46.5–11.5-42 mol%, FLiNaK) into a 2D woven C/C composite was performed at 650 °C under different pressure. The weight gain and mechanical properties change of the 2D woven C/C composite after FLiNaK salt impregnation were measured. The FLiNaK salt distribution into the 2D woven C/C composite was observed by X-ray computed tomography (X-ray CT) and scanning electron microscopy. The results showed that the weight gain of the 2D woven C/C composite increased with increasing impregnating pressure. In X-ray CT images, FLiNaK salt was distributed into the open pores and fissures among

fiber bundles and neighboring plies. The interlaminar shear strength, compressive strength, and flexural strength of the 2D woven C/C composite increased with the increase of weight gain. The influence of FLiNaK salt impregnation on the mechanical properties was attributed to the coupling effect of re-densification of FLiNaK salt impregnation and residual stress formed in 2D woven C/C composite.

Journal of Nuclear Materials, 2017, **485**: 74

First-Principles Study of Vacancies in Ti_3SiC_2 and Ti_3AlC_2

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Hou Yu-Yang Tang Jun Dai Jian-Xing Ren Cui-Lan
Zhang Wei Huai Ping

Key words MAX phases, vacancies, diffusion barrier, density functional theory

MAX phase materials have attracted increased attention due to their unique combination of ceramic and metallic properties. In this study, the properties of vacancies in Ti_3AlC_2 and Ti_3SiC_2, which are two of the most widely studied MAX phases, were investigated using first-principles calculations. Our calculations indicate that the stabilities of vacancies in Ti_3SiC_2 and Ti_3AlC_2 differ greatly from those previously reported for Cr_2AlC. The order of the formation energies of vacancies is $V_{Ti(a)} > V_{Ti(b)} > V_C > V_A$ for both Ti_3SiC_2 and Ti_3AlC_2. Although the diffusion barriers for Ti_3SiC_2 and Ti_3AlC_2 are similar (~0.95 eV), the properties of their vacancies are significantly different. Our results show that the vacancy–vacancy interaction is attractive in Ti_3AlC_2 but repulsive in Ti_3SiC_2. The introduction of V_{Ti} and V_C vacancies results in the lattice constant *c* along the [0001] direction increasing for both Ti_3SiC_2 and Ti_3AlC_2. In contrast, the lattice constant *c* decreases significantly when V_A are introduced. The different effect of V_A on the lattice constants is explained by enhanced interactions of nearby Ti layers.

Materials, 2017, **10**(2): 103

On the origin of strengthening mechanisms in Ni-Mo alloys prepared via powder metallurgy

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Thorogood Gordon J. Huang Hefei Zhou Xingtai

Key words Powder metallurgy, DPS strengthening, Spark plasma sintering, Transmission electron microscopy, Electron backscatter diffraction, Molten salt reactor

A new class of materials, which rely on the dispersion strengthening of SiC particles in addition to precipitation strengthening by nano-precipitates is being developed for the application

in molten salt nuclear reactors. A battery of dispersion and precipitation strengthened (DPS) NiMo-based alloys containing varying amount of SiC (0.5–2.5 wt.%) was prepared via a mechanical alloying (MA) route followed by spark plasma sintering (SPS), rapid cooling, high-temperature annealing and water quenching. Lab X-ray Diffraction (XRD), Electron Back Scattering Diffraction (EBSD), and Transmission Electron Microscopy (TEM) were employed in the microstructural characterization of this new type of alloys. It is shown that the NiMo matrix of these alloys is effectively reinforced by dispersion of SiC from the initial powder mixture and nano-Ni_3Si precipitates, which precipitated during the sintering/annealing process. Furthermore, the matrix is strengthened by solid-solution of Mo in Ni. As a result, these newly developed NiMo alloys take advantage of dispersion, precipitation and solid solution strengthening, which leads to their superior mechanical properties.

Materials & Design, 2017, **113**: 223

Theoretical study of the substitutional solute effect on the interstitial carbon in nickel-based alloy

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The carbon binding in nickel-based alloy with 3d, 4d and 5d transition metal solutes is investigated by using first-principles methods. The first nearest neighbor carbon exhibits repulsive behaviors with most metals except Cr element, which are analyzed from both mechanical and chemical aspects. It shows that the size factor from metal solute is one of the main reasons affecting 1NN carbon–metal binding. Further electronic structures analysis shows that the hybridization of C $2p_z$–M $3d_z^2$ states plays an important role in C–M bonding. The introduced vacancy enhances carbon bonding to most metal solutes through local strain change and charge redistribution. Among all the metal solutes, Cr shows its affinity to carbon which coincides with the previous experimental observation that chromium carbides are commonly precipitated in nickel-based alloys. The present study helps to understand the carbon–metal solute interaction in nickel-based alloys.

RSC Advances, 2017, **7**(33): 20567

Diffusion of tellurium at nickel grain boundaries: a first-principles study

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The knowledge of the behavior of Te in nickel grain boundaries (GB) is of significant importance for the application of nickel alloys in molten salt reactors. The atomic structures, stabilities, segregation behaviors and diffusion barriers of Te are studied for the bulk, surfaces and four kinds of GBs of nickel. Our first-principles calculations indicate the segregation of Te is most favorable at Σ = 5 (021) GB and the weakest at Σ = 3 (111) GB. The diffusion barriers of Te increase in sequence: Σ = 11 (11$\bar{3}$), Σ = 9 (221), Σ = 3 (111) and Σ = 5 (021). The calculated diffusion barrier of Te on Σ = 11 (11$\bar{3}$) is 0.35 eV lower than in the bulk, indicating a fast diffusion of Te along this GB. We also consider the effect of strain on the diffusion and find it to be sensitive to the different GB types. When the tensile strain is up to 4%, the diffusion barriers of Te are lowered by 0.51 eV and 0.15 eV for Σ = 5 (021) and Σ = 11 (11$\bar{3}$), respectively. In contrast, this effect for Σ = 3 (111) is negligible.

RSC Advances, 2017, **7**(14): 8421

Effects of Cr^{3+} on the corrosion of SiC in LiF–NaF–KF molten salt

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Liu Hongtao Wang Jianqiang

Key words Ceramic, Molten Salts, XPS, Raman spectroscopy, Reactor conditions, High temperature corrosion

Effects of Cr^{3+} on the corrosion of SiC in LiF–NaF–KF molten salt were investigated. Results reveal that Cr^{3+} can drive the corrosion of SiC. Thickness of the corroded region induced by Cr^{3+} is greater than 12 μm for 400 h, while the corroded region induced by pure salt is ~2.5 μm. Corrosion induced by Cr^{3+} should be attributed to the reactions of Cr^{3+} with SiC. Cr^{3+} reacts with SiC to form Cr_3C_2, Cr_7C_3, and graphitic carbon in the corroded region of SiC, which results in the dissolution of element Si from SiC into the salt.

Corrosion Science, 2017, **114**: 96

The Fabrication of Multifunctional SLIPS Films by Electrospinning

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Key words anti-wetting, electrospun films, multifunctional films, omniphobic films

The pitcher plant has inspired anti-wetting coatings. However, it is still a challenge to create oleophobic surfaces that repel non-polar liquids due to their low surface tension. Here we develop an effective strategy to fabricate multifunctional fibrous films by electrospinning polyvinylidene fluoride (PVDF) and polyvinyl acetate (PVAc) polymers. The as-prepared multifunctional films combined the Janus behavior with hydrophobicity on the upper side and thermally adhesive properties on the lower side. By spraying with lubricant, a pitcher-plant-like omniphobic surface has been prepared, which exhibited excellent anti-wetting properties against water, low surface tension and complex fluids. Furthermore, the transparency of the film has been greatly enhanced after lubrication, which was suitable for glass-based anti-fouling materials or coatings.

ChemNanoMat, 2017, **3**(12): 869

Stretchable Ionic-Liquid-Based Gel Polymer Electrolytes for Lithium-Ion Batteries

Guan Jipeng Li Yongjin Li Jingye

Stretchable cross-linked gel polymer electrolytes (C-GPEs) have been fabricated through electron-beam irradiation (EBI) of poly(vinylidene fluoride-*co*-hexafluoropropylene) [P(VDF-*co*-HFP)]/triallyl isocyanurate (TAIC) blend films followed by adsorption of the ionic liquid 1-ethyl-3-methylimidazolium bis(trifluoromethylsulfonyl)imide ([EMIm][TFSI]). It was found that polymer films containing 5 wt % cross-linker exhibit an excellent IL uptake value of 3.0 when irradiated at 75 kGy. The prepared C-GPEs have a high ion conductivity of 1.4 mS/cm at room temperature compared with a value of 0.7 mS/cm for P(VDF-*co*-HFP)/IL (1/3, m/m) blend gel. Morphological measurements indicate interconnected nanoporous structures in the films that can provide effective channels for ion immigration. Moreover, the C-GPEs show a high tensile strength of 10.6 MPa and an excellent elasticity, with almost full strain recovery after 100% stretch. In a $LiFePO_4$/C-GPE/Li half-cell, the C-GPEs exhibit high electrochemical stability. Therefore, we consider that the prepared C-GPEs might have a potential application in flexible or/and stretchable energy storage devices.

Industrial & Engineering Chemistry Research, 2017, **56**(44): 12456

Green and efficient synthesis of an adsorbent fiber by preirradiation-induced grafting of PDMAEMA and its Au(III) adsorption and reduction performance

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Zhang Bowu Wang Ziqiang Yu Ming Shen Rongfang
Ma Hongjuan Li Jingye

Key words adsorption, aqueous solutions, precious metal, radiation-induced graft polymerization

N,*N*-Dimethylamino ethyl methacrylate (DMAEMA) is covalently bonded on a commercial polyethylene-coated polypropylene skin-core structure fiber (PE/PP) in aqueous and MeOH/H_2O solutions by a one-step green reaction using radiation-induced graft polymerization. The effects of the absorbed dose and solvent system on grafting yield are investigated, while the chemical and physical properties of the functionalized fiber are also evaluated. The fiber with a D_g of 51.6% exhibited good adsorption capacity of Au(III) ions over a large range of concentrations (from 10 to 2.5 g L^{-1}) in both batch and flow-through adsorption tests. The highest capacity of Au was 949.3 mg g^{-1}. After elution, the adsorbents can be reused without any further regeneration for at least five adsorption-desorption cycles. Additionally, the fibers show high selectivity for Au(III). The distribution coefficient of Au(III) is 10^4 to 10^5 times higher than that for Cu(II), Fe(III), Ni(II), and Pb(II) even at 100 times lower Au(III) concentration compared to the co-existing metal ion concentration. This study provides an effective and novel approach for gold recovery from aqueous solutions.

Journal of Applied Polymer Science, 2017, **134**(25): 44955

Radiation graft of acrylamide onto polyethylene separators for lithium-ion batteries

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Li LinFan Li JingYe

Key words Lithium-ion battery, Polyethylene, Acrylamide, Irradiation graft, Separator

To improve the affinity between separators and electrolyte in lithium-ion battery, microporous polyethylene (PE) separator was grafted of polyacrylamide (PAAm) by radiation. Chemical structure of the PAAm-grafted PE separators (denoted as PE-g-PAAm) was characterized by Fourier transform infrared spectroscopy and X-ray photoelectron spectroscopy. Properties of the

pristine PE and PE-g-PAAm were tested by scanning electron microscope, liquid electrolyte uptake and lithium-ion conductivity. Electrochemical performances of the grafted PE separators (up to 0.76×10^{-3} S/cm of ionic conductivity at room temperature) were much better than pristine PE, and performance of the battery with the grafted separator behaved better than with the virgin PE separator, under the same condition (assembled in Ar-filled glove box).

Nuclear Science and Techniques, 2017, **28**(6): 77

Amidoxime-based adsorbents prepared by cografting acrylic acid with acrylonitrile onto HDPE fiber for the recovery of uranium from seawater

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Wang MouHua Shen RongFang Guo XiaoJing
Wang YinNing Li JingYe Wu GuoZhong

Key words Radiation-induced grafting, Amidoxime, Acrylonitrile, Uranium, Selectivity

An amidoxime-based polymeric adsorbent was prepared by pre-irradiation grafting of acrylonitrile and acrylic acid onto high-density polyethylene fibers using electron beams, followed by amidoximation. Quantitative recovery of uranium was investigated by flow-through experiment using simulated seawater and marine test in natural seawater. The maximum amount of uranium uptake was 2.51 mg/g-ads after 42 days of contact with simulated seawater and 0.13 mg/g-ads for 15 days of contact with natural seawater. A lower uranium uptake in marine test can be attributed to the short adsorption time and the contamination of marine microorganisms and iron. However, the high selectivity toward uranium against vanadium may be beneficial to harvest uranyl ion onto adsorbents and the economic feasibility for recovery of uranium from seawater.

Nuclear Science and Techniques, 2017, **28**(4): 45

Preparation of Dynamic Superhydrophobic Cotton Fabric *via* Radiation-induced Graft Polymerization

Li Jingye Wang Ziqiang Yu Ming

Key words Dynamic superhydrophobic, Radiation-induced graft polymerization, Cotton fabrics, Sliding angle

With cotton fabrics as substrates, *γ*-ray irradiation was used to initiate the graft polymerization of lauryl methacrylate (LMA), to attach polystyrene (PS) nanospheres to the cotton fabrics in by

covalent bonding *via* the grafted chains, form a nano-scale coarse structure with low surface energy on the surface of cotton fabrics, and obtain dynamic superhydrophobic cotton fabrics with a low water droplet sliding angle. The grafting kinetics was studied and the degree of grafting (DG) increased regularly with the increasing of the concentration of the monomer. Therefore the DG could be controlled by changing the conditions of the graft polymerization. Fourier transform infrared spectroscopy (FTIR) analyses were carried out on the cotton fabrics after the graft and the results confirmed the presence of PS nanospheres and grafted PLMA chains on the modified cotton fabrics. Scanning electron microscopy (SEM) analysis showed that the attachment of the PS nanospheres onto the cotton fabrics led to the formation of a nanoscale coarse structure on the surface of the cotton fibers. The contact angle of water droplet on the modified cotton fabric was higher than 150°, which demonstrated that the modified cotton fabrics were superhydrophobic. Relative to the cotton fabrics solely grafted with LMA, the PS nanospheres-decorated cotton fabrics had a significantly reduced water droplet sliding angle, and possessed dynamic superhydrophobicity. This should be attributed to the "lotus effect" of the surface of the modified cotton fabrics containing low surface energy and regular nano-scale roughness structure formed by the attachment of PS nanospheres. The softness of the cotton fabrics was characterized through the measurements of their flexural rigidity before and after their modification. The results showed that radiation-induced graft polymerization of LMA and the immobilization of PS nanospheres did not influence the wearability of the cotton fabrics, as it did not have a significant effect on their softness.

Acta Polymerica Sinica, 2017, (2): 315

Uranium Adsorption Tests of Amidoxime-Based Ultrahigh Molecular Weight Polyethylene Fibers in Simulated Seawater and Natural Coastal Marine Seawater from Different Locations

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Li Rong Pang Lijuan Ma Hongjuan Li Jingye
Wu Guozhong Lu Shuimiao Wang Deli

Uranium recovery from seawater was investigated in simulated seawater in the laboratory and in natural seawater from the coasts of China with different amidoxime-based (AO) ultrahigh molecular weight polyethylene (UHMWPE) fibers. The capacities of adsorbents AO-UHMWPE-1 and -2 were 4.54 and 2.41 mg U/g-adsorbent, respectively, after 24 h of adsorption in the simulated seawater with 330 ppb U. Their capacities were 2.93 and 1.95 mg U/g-adsorbent, respectively, after 42 days of adsorption in simulated seawater flow-through experiments with 3.3 ppb U. However,

because of sediment and marine organism contamination, the capacities were 0.25 and 0.04 mg U/g-adsorbent, respectively, after 68 days of adsorption in natural seawater in Xiamen. The capacity of AO-UHMWPE-7 was 1.41 mg U/g-adsorbent after 15 days of adsorption in natural seawater in Daishan. The average capacity of AO-UHMWPE-7 was 1.50 mg U/g-adsorbent, which was 18 times greater than that for V after 15 days of adsorption in natural seawater in Daishan. Results indicated that there were many factors affecting the adsorption capacity of uranium. In addition to the character of the adsorbent, including degree of grafting, functional group density, and AO conversion ratio, the marine hydrological conditions, such as temperature, flow velocity, turbidity, etc., are also crucially important for uranium extraction from seawater.

Industrial & Engineering Chemistry Research, 2017, **56**(4): 1103

Poly (vinylidene fluoride) dielectric composites with both ionic nanoclusters and well dispersed graphene oxide

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Key words Nanostructured dielectric composites, Ionic liquid, Graphene oxide nanosheet, Nanoclusters, Electron beam irradiation

Nanostructured polymeric dielectric composites, based on poly (vinylidene fluoride) (PVDF), graphene oxide (GO), and an ionic liquid (IL), 1-vinyl-3-ethylimidazolium tetrafluoroborate ([VEIM] [BF_4]), denoted as Nano-PVDF/IL/GO, were fabricated through casting method, electron beam (EB) irradiation and microphase separation processes. Through the strategy, GO nanosheets were dispersed homogeneously in PVDF matrix and the organic nanoclusters formed by microphase separation of IL grafted PVDF (PVDF-*g*-IL) chain segments tended to adhere onto the surface of GO nanosheets. The Nano-PVDF/IL/GO composites displayed a drastic reduction in dc conductivity compared with PVDF/GO and PVDF/IL/GO composites because of impeding the direct contact between GO nanosheets by the nanoclusters. Furthermore, the mircocapacitors between the adjacent GO nanosheets and nanoclusters contributed the increase of dielectric constant. At the same time, the dielectric loss from the current leakage of GO nanosheets was almost fully eliminated due to the strong interfacial bonding between polymer matrix and fillers which restrained the formation of conductive network. Therefore, we proposed an effective strategy for using the organic nanoclusters to modify the inorganic conductive fillers and impeding the formation of conductive network in the dielectric materials, which paves new possibility to prepare polymer nanocomposites with both high dielectric constant and low dielectric loss.

Composites Science and Technology, 2017, **138**: 98

Preparation of freestanding graphene-based laminar membrane for clean-water intake *via* forward osmosis process

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Zhao Hongwei Li Jingye

Here, a facile strategy is reported to prepare thin freestanding graphene oxide (GO) laminar membranes through thermally-induced chemical cross-linking process. The resultant freestanding cross-linked GO (F-CGO) membranes show controllable inter-laminar distance and hydraulic stability in aqueous media. Semi-permeability tests through a forward osmosis (FO) system show that the water permeation rate of the F-CGO membranes is up to 35.5 L m^{-2} h^{-1} when the draw solution is 2.0 mol L^{-1} NaCl solution. This value is much higher than that of standing cross-linked GO (S-CGO) membranes, which indicates that the internal concentration polarization (ICP) effect has been alleviated by the F-CGO membrane. Furthermore, clean-water was taken in from various wastewaters, but without any detectable residual pollutants by using the F-CGO membrane as a separator. This work demonstrates that the F-CGO membrane is promising for water purification applications through the FO process, especially for portable water purification systems utilized during emergency situations.

RSC Advances, 2017, **7**(3): 1326

Temperature dependence of nickel ion irradiation damage in GH3535 alloy weld metal

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Key words GH3535 alloy, Ion irradiation, Microstructural evolution, Irradiation hardening, Temperature effect

Bulk samples of the GH3535 alloy weld metal have been characterized by transmission electron microscopy, X-ray diffraction and nanoindentation to determine their microstructural evolution and mechanical property changes after 8 MeV Ni^{3+} ions irradiation. The irradiation experiments were carried out at room temperature and 600 °C, and the ion fluences correspond to a calculated peak damage dose of 0.5, 2 and 12 dpa, respectively. TEM results show the formation of

solute clusters or dislocation loops with a number density of approximately 5–14 × 10^{22} m^{-3} and sizes between 3 and 10 nm at room temperature due to irradiation induced defects and their evolution. Moreover, the peak shift with increasing ion dose observed in XRD diffraction patterns reveals the lattice distortion induced by ion irradiation. As far as the case of high temperature irradiation, several solute clusters with the same size were observed, whereas the number density was smaller than that of the former case. The calculated indentation values in irradiated samples were found to be much higher in comparison to the unirradiated one, indicating the dose dependent effect of irradiation on hardness. However, in the case of the ion irradiation at 600 °C, the hardness value of samples was significantly decreased. The relationship between ion irradiation induced microstructural evolution and the changes in the mechanical properties of this weld metal is discussed in the context of ion dose and irradiation temperature.

Journal of Nuclear Materials, 2017, **497**: 108

Raman spectra and modulus measurement on the cross section of proton-irradiated graphite

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Wang Yongqi Li Jianjian Huang Hefei Yan Long
Lei Guanhong Xie Ruobing

Key words Nuclear graphite, Ion irradiation, Raman spectrum, Nano-indentation

A method combining proton irradiation and nano-indentation was explored in this study to measure the modulus of irradiated graphite. A IG-110 graphite sample was irradiated with 2.5-MeV protons to a fluence of 1.2 × 10^{18} ions/cm^2 at room temperature. Proton irradiation produced a damaged layer with a thickness of ~75 μm. A scan of Raman spectrum was performed on cross section of irradiated sample. Analysis of the Raman spectra indicates that the graphite breaks into nano-crystalline graphite at very low dose (0.02–0.04 dpa) during room-temperature irradiation. Nano-indentation tests were performed on the cross section of irradiated sample so that the damage along the loading direction is uniform. Thus, it was able to identify a dpa value for the nano-indentation tests. Using this method, the modulus at 0.015 dpa was deduced to be 2.39 times that of the un-irradiated graphite. The hardness is also more than doubled after irradiation to 0.015 dpa.

Nuclear Instruments and Methods in Physics Research Section B: Beam Interactions with Materials and Atoms, 2017, **412**: 221

Encapsulation of metal-based phase change materials using ceramic shells prepared by spouted bed CVD method

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Lin Jun Zhu Zhiyong

Key words Phase change materials, Encapsulation, Spouted bed CVD method

Metals are promising high-temperature phase change materials (PCMs) with high heat storage density and high heat exchange rate for high high-temperature heat storage. However, encapsulation of metallic PCMs is essential for its practical application owing to its highly corrosive to encapsulation materials and its volume expansion during the phase change. The present study applied spouted bed chemical vapor deposition (CVD) method to encapsulate metallic PCMs. A novel heat storage capsule was developed using iron core encapsulated with porous pyrolytic carbon (PyC) layer, dense PyC layer and dense silicon carbide (SiC) layer in turn from inside to outside. The inner porous PyC layer is used to accommodate the volume expansion of the iron core and the outer dense SiC layer act as package layer and the oxidation resistance layer. The SiC/C-shells/Fe-core capsules could work at a temperature up to 1100 °C and include solid-solid phase change (48.85 J/g, 686 °C) and solid-liquid phase change (128 J/g，1136 °C). It is demonstrated that the SiC/C-shells/Fe-core capsules have several desired characteristics, such as high thermal conductivity and high thermal density, excellent oxidation resistance and good thermal cycling performance.

Solar Energy Materials and Solar Cells, 2017, **17**0: 137

In-core fuel management strategy for the basket-fuel-assembly molten salt reactor

Xue Chun Zhu ZhiYong Zhang HaiQing Lin Jun

Key words BFAMSR, Fuel elements, Fuel management strategy, Loading pattern

Molten salt reactor, with good economics and inherent reliability, is one of the six types of Generation IV candidate reactors. The Basket-Fuel-Assembly Molten Salt Reactor (BFAMSR) is a new concept design based on fuel assemblies composed of fuel pebbles made of TRISO-coated particles. Four refueling patterns, similar to the fuel management strategy for water reactors, are designed and analyzed for BFAMSR in terms of economy and security. The MCNPX is employed to calculate the parameters, such as the total duration time, cycle length, discharge burnup, total discharge quantity of ^{235}U, total discharge quantity of ^{239}Pu, neutron flux distribution and power

distribution. The in–out loading pattern has the highest burnup and duration time, the worst neutron flux and power distribution and the lowest neutron leakage. The out–in pattern possesses the most uniform neutron flux distribution, the lowest burnup and total duration time, and the highest neutron leakage. The out–in partition alternate pattern has slightly higher burnup, longer total duration time and smaller neutron leakage than that of the out–in loading pattern at the cost of sacrificing some neutron flux distribution and power distribution. However, its alternative distribution of fuel elements cut down the refueling time. The low-leakage pattern is the second highest in burnup, and total duration time, and its neutron flux and power distributions are the second most uniform.

Nuclear Science and Techniques, 2017, **28**(9): 130

Characterization the microstructure and defects of matrix graphite irradiated with Xe ions

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Gu BC　Liu B

Key words　Graphite, Irradiation, Defects, Raman, Positron

The matrix graphite of pebble fuel elements was irradiated with 1 MeV Xe ions at room temperature to fluences of 5.8×10^{14} ions/cm^2 and 2.9×10^{15} ions/cm^2, respectively. The microstructure and defects of matrix graphite samples were characterized by using scanning electron microscopy (SEM), Raman spectroscopy and slow positron beam techniques. The SEM result reveals that hundred-nanometer sized pores appear at the surface after irradiation and the density of pore increases with fluence. Raman results show that D peak (1350 cm^{-1}) and G peak (1580 cm^{-1}) are broadened after irradiation. In addition, the G peak position shifts from 1580 cm^{-1} to 1560 cm^{-1} with the linewidth increases from 21 cm^{-1} to 132 cm^{-1}, corresponding to the increase in bond-angle disorder as the matrix graphite transforms from microcrystalline to amorphous carbon(a-C). The slow positron beam study shows that the defects-trapped positron S parameter increases with fluence, suggesting that the vacancy-type defects concentration or size of open volume defects increases. The analysis of Raman and slow positron beam consistently conclude that the reason for the phase transition after irradiation is the increase in irradiation-induced vacancy defects accompanied by the overlap of disordered regions.

Nuclear Instruments and Methods in Physics Research Section B: Beam Interactions with Materials and Atoms, 2017, **406**: 638

Effect of irradiation damage on corrosion of 4H-SiC in FLiNaK molten salt

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Zhao Bin Ji Gengwu Zhang Wei Xie Ruobing Yan Long

Key words SiC, Irradiation, Corrosion, FLiNaK molten salt

The corrosion behavior of 4H-SiC in the FLiNaK molten salt (650 °C), pre-irradiated with 70-keV Si ions to 2.5 dpa at 650 °C, was investigated in order to clarify the effect of irradiation on corrosion. The irradiated region of 4H-SiC is peeled off by the molten salt, and the corrosion depth is nearly consistent with the irradiation damage depth. Molten salt corrosion leads to the loss of Si element and the formation of carbon-rich phase in irradiated 4H-SiC surface. The broken of Si-C bonds induced by irradiation plays a key role in the irradiation-assisted corrosion of SiC.

Corrosion Science, 2017, **125**: 194

PL and ESR study for defect centers in 4H-SiC induced by oxygen ion implantation

Cheng GuoDong Chen Ye Yan Long Shen RongFang

Key words Ion implantation. Electron spin resonance. Photoluminescence. First-principles calculations

Radiation damage in 4*H*-SiC samples implanted by 70 keV oxygen ion beams was studied using photoluminescence and electron spin resonance techniques. ESR peak of g = 2.0053 and two zero-phonon lines were observed with the implanted samples. Combined with theoretical calculations, we found that the main defect in the implanted 4*H*-SiC samples was oxygen-vacancy complex. The calculated defect formation energies showed that the oxygen-vacancy centers were stable in *n*-type 4*H*-SiC. Moreover, the $V_{Si}O_C^0$ and $V_{Si}O_C^{-1}$ centers were optically addressable. The results suggest promising spin coherence properties for quantum information science.

Nuclear Science and Techniques, 2017, **28**(8): 105

The elemental move characteristic of nickel-based alloy in molten salt corrosion by using nuclear microprobe

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Shen Hao Li Yan

Key words Nickel-based alloy, Salt corrosion, Micro-PIXE, Nuclear microprobe

Nickel-based alloys as candidate materials for Thorium Molten Salt Reactor (TMSR), need to be used under high temperature in molten salt environment. In order to ensure the safety of the reactor running, it is necessary to study the elemental move characteristic of nickel-based alloys in the high temperature molten salts. In this work, the scanning nuclear microprobe at Fudan University was applied to study the elemental move. The Nickel-based alloy samples were corroded by molten salt at different temperatures. The element concentrations in the Nickel-based alloys samples were determined by the scanning nuclear microprobe. Micro-PIXE results showed that the element concentrations changed from the interior to the exterior of the alloy samples after the corrosion.

Nuclear Instruments and Methods in Physics Research Section B: Beam Interactions with Materials and Atoms, 2017, **404**: 185

Surface morphology and microstructure evolution of IG-110 graphite after xenon ion irradiation and subsequent annealing

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Yan Long Huang Hefei

Key words Nuclear graphite, Ion irradiation, Anisotropic swelling

IG-110 graphite samples were polished and irradiated with Xe ions at various fluences, then annealed at high temperatures up to 1100 °C. After irradiation, small hills were found on the polished surfaces, indicating an anisotropic swelling induced by irradiation. Around 30% swelling at a fluence of 2×10^{15} ions/cm^2 was characterized using atomic force microscopy. Severe swelling of the graphite crystallites caused stresses between adjacent crystallites, but leaved no intergranular cracks on the polished surface, which was ascribed to irradiation-induced creep of graphite. The pore morphology was affected by the anisotropic swelling. We found many contracted pores but only one expanded pore, indicating a decreased porosity induced by irradiation. After annealing at 1100 °C, TEM characterization showed clearly increased lattice order and decreased width of the

(002) diffraction arc, indicating the annihilation of dislocations and recovery of basal plane rotations. Annealing-induced recrystallization of damaged graphite led to recovery of the crystallites' swelling and many small cracks appearing on the samples' surfaces.

Journal of Nuclear Materials, 2017, **491**: 213

Mesocarbon microbead based graphite for spherical fuel element to inhibit the infiltration of liquid fluoride salt in molten salt reactor

Zhong Yajuan Zhang Junpeng Lin Jun Xu Liujun Zhang Feng Xu Hongxia Chen Yu Jiang Haitao Li Ziwei Zhu Zhiyong Guo Quangui

Mesocarbon microbeads (MCMB) and quasi-isostatic pressing method were used to prepare MCMB based graphite (MG) for spherical fuel element to inhibit the infiltration of liquid fluoride salt in molten salt reactor (MSR). Characteristics of mercury infiltration and molten salt infiltration in MG were investigated and compared with A3-3 (graphite for spherical fuel element in high temperature gas cooled reactor) to identify the infiltration behaviors. The results indicated that MG had a low porosity about 14%, and an average pore diameter of 96 nm. Fluoride salt occupation of A3-3 (average pore diameter was 760 nm) was 10 wt% under 6.5 atm, whereas salt gain did not infiltrate in MG even up to 6.5 atm. It demonstrated that MG could inhibit the infiltration of liquid fluoride salt effectively. Coefficient of thermal expansion (CTE) of MG lies in 6.01×10^{-6} K^{-1} ($\alpha_{/\!/}$) and 6.15×10^{-6} K^{-1} ($\alpha_{\perp}$) at the temperature range of 25–700 °C. The anisotropy factor of MG calculated by CTE maintained below 1.02, which could meet the requirement of the spherical fuel element (below 1.30). The constant isotropic property of MG is beneficial for the integrity and safety of the graphite used in the spherical fuel element for a MSR.

Journal of Nuclear Materials, 2017, **490**: 34

Synthesis of thorium sol for fabricating fuel kernels

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Key words Thorium sol, Sol-gel method, PH, Viscosity, Turbidity, Particle size distribution

To fabricate thorium-based fuel kernel for solid fuel molten salt reactor, a component of tri-structural isotropic fuel particles is mostly based on sol–gel method. The preparation of thorium

sol is an important step for fabrication of thorium-based fuel kernels, such as thorium carbide and thorium oxide. The gel quality affects the gel particle dispersion and the final products. In this work, thorium sols were prepared using $Th(NO_3)_4$ and $NH_3 \cdot H_2O$ by sol–gel method. The effects of thorium concentration, mole ratio of NH_4^+/NO_3^- and reaction temperature on the pH, viscosity, turbidity, particle size and the thorium sol distribution were investigated. The results show that the viscosity and turbidity increased with the NH_4^+/NO_3^- ratio; the turbidity and colloidal particle size increased with the reaction temperature, which affected little the sol viscosity; the sol viscosity increased with the thorium concentration, which virtually did not change the turbidity; and the particle size decreased and the size distribution narrowed with increasing thorium concentration. The sol could be stored at room temperature for one day without significant property changes. Thorium gel spheres of good quality were prepared at 60 °C with the NH_4^+/NO_3^- ratio of 75–85% and the thorium concentration of 1.2–1.4 mol/L.

Nuclear Science and Techniques, 2017, **28**(7): 96

Ion irradiation-induced swelling and hardening effect of Hastelloy N alloy

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The volumetric swelling and hardening effect of irradiated Hastelloy N alloy were investigated in this paper. 7 MeV and 1 MeV Xe ions irradiations were performed at room temperature (RT) with irradiation dose ranging from 0.5 to 27 dpa. The volumetric swelling increases with increasing irradiation dose, and reaches up to 3.2% at 27 dpa. And the irradiation induced lattice expansion is also observed. The irradiation induced hardening initiates at low ion dose (≤1dpa) then saturates with higher ion dose. The irradiation induced volumetric swelling may be ascribed to excess atomic volume of defects. The irradiation induced hardening may be explained by the pinning effect where the defects can act as obstacles for the free movement of dislocation lines. And the evolution of the defects' size and number density could be responsible for the saturation of hardness.

Journal of Nuclear Materials, 2017, **489**: 180

Reactions of Triplet-State Difloxacin with Amino Acids and dGMP: A Laser Flash Photolysis Study

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Ma LiuKui Wei ChiYuan Wang WenFeng

Key words Laser flash photolysis, Difloxacin, Triplet state, Amino acid

The reactions of triplet-state difloxacin (DFX) with various amino acids and deoxyguanylic acid in aqueous media were studied using laser flash photolysis. Tryptophan, tyrosine, cysteine, and 2'-deoxyguanosine-5'-monophosphate (dGMP) were found to completely quench the triplet state of DFX in aqueous solution, the corresponding second-order rate constants being 1.97×10^8, 1.48×10^8, 1.72×10^8, and 6.92×10^7 $dm^3\cdot mol^{-1}\cdot s^{-1}$. The quenching mechanism involves electron transfer to the photoexcited triplet state of DFX from the tryptophan, tyrosine, cysteine, and dGMP moieties, followed by fast protonation of the resulting DFX anion radical.

Acta Physico-Chimica Sinica, 2017, **33**(5): 1051

ERDA, RBS, TEM and SEM characterization of microstructural evolution in helium-implanted Hastelloy N alloy

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Deng Qi Liu Zhe Yang Guo Shi Liqun

Key words Hastelloy N alloy, ERDA, Helium bubbles, Coarsening, Release

Hastelloy N alloy was implanted with 30 keV, 5×10^{16} ions/cm^2 helium ions at room temperature, and subsequent annealed at 600 °C for 1 h and further annealed at 850 °C for 5 h in vacuum. Using elastic recoil detection analysis (ERDA) and transmission electron microscopy (TEM), the depth profiles of helium concentration and helium bubbles in helium-implanted Hastelloy N alloy were investigated, respectively. The diffusion of helium and molybdenum elements to surface occurred during the vacuum annealing at 850 °C (5 h). It was also observed that bubbles in molybdenum-enriched region were much larger in size than those in deeper region. In addition, it is worth noting that plenty of nano-holes can be observed on the surface of helium-implanted sample after high temperature annealing by scanning electron

microscope (SEM). This observation provides the evidence for the occurrence of helium release, which can be also inferred from the results of ERDA and TEM analysis.

Nuclear Instruments and Methods in Physics Research Section B: Beam Interactions with Materials and Atoms, 2017, **399**: 62

Investigation of the damage behavior in CVD SiC irradiated with 70 keV He ions by NEXAFS, Raman and TEM

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Key words NEXAFS, Raman, Irradiation, Amorphization, Stacking faults

Chemical vapor deposited (CVD) SiC was irradiated with 70 keV He ions at room temperature. The damage behavior was investigated by near edge X-ray absorption fine structure (NEXAFS) spectroscopy, Raman spectroscopy and transmission electron microscopy (TEM). NEXAFS spectra at the Si K-edge display the obvious decrease in intensity of crystalline peaks and near disappearance of the peak at 1852 eV, suggesting an increase in crystalline disorder resulting from an increased number of Si vacancies caused by irradiation. Raman spectra show the decomposition of crystalline Si-C bonds and the formation of homonuclear (Si–Si and C ⎯ C) bonds during irradiation. TEM results show the transition from slight disorder to full amorphization with increasing dose. The dose to amorphization (DTA) is estimated to be about 1 dpa. It is also found that high density of stacking faults in CVD SiC may contribute to the enhancement of amorphization resistance compared to single crystal β-SiC.

Journal of the European Ceramic Society, 2017, **37**(4): 1253

Radical-Induced Degradation of Fluoxetine in Aqueous Solution by Pulse and Steady-State Radiolysis Studies

Ji Tian-Yi Liu Yan-Cheng Zhao Jian-Feng Xu Gang Wang Wen-Feng Wu Ming-Hong

Key words Fluoxetine, Pulse radiolysis, Hydroxyl radical, Sulfate radical anion, Degradation

The reactions of the pharmaceutical fluoxetine (FLX) with different radicals were investigated by pulse radiolysis. The reaction of hydroxyl radical (·OH) with FLX formed hydroxylated adduct of the aromatic ring, while oxidation of FLX by sulfate radical anion ($SO_4^{\cdot-}$) formed benzene

radical cation that further reacted with H_2O to yield the ·OH adduct. The determined rate constants of ·OH, hydrated electrons (e_{aq}^-), and $SO_4^{\cdot-}$ with FLX were 7.8×10^9, 2.3×10^9, and 1.1×10^9 mol·L^{-1}·s^{-1}, respectively. In the steady-state radiolysis study, the degradation of FLX in different radiolytic conditions by electron beam irradiation was detected by HPLC and UV-Vis spectra techniques. It was found that FLX concentration decreased by more than 90% in both N_2O and air-saturated solutions after 1.5 kGy irradiation. In contrast, only 43% of FLX was decomposed in N_2-saturated solution containing 0.1 mol·L^{-1} tert-butanol. The degradation rates of FLX in acidic and neutral solutions were higher than those in alkaline solutions. Our results showed that the degradation of FLX is optimal in air-saturated neutral solution, and ·OH-induced degradation is more efficient than $SO_4^{\cdot-}$ oxidation of FLX. The obtained kinetic data and optimal conditions give some hints to understand the degradation of FLX.

Acta Physico-Chimica Sinica, 2017, **33**(4): 823

Structural Phase Transition of ThC Under High Pressure

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Yu Xiaohe Yang Ke Li Nana Yang Wenge Sun Baoxing
Xie Ruobing Xu Hongjie

Thorium monocarbide (ThC) as a potential fuel for next generation nuclear reactor has been subjected to its structural stability investigation under high pressure, and so far no one reported the observation of structure phase transition induced by pressure. Here, utilizing the synchrotron X-ray diffraction technique, we for the first time, experimentally revealed the phase transition of ThC from B1 to P4/nmm at pressure of ~58 GPa at ambient temperature. A volume collapse of 10.2% was estimated during the phase transition. A modulus of 147 GPa for ThC at ambient pressure was obtained and the stoichiometry was attributed to the discrepancy of this value to the previous reports.

Scientific Reports, 2017, **7**: 96

A paramagnetic neutral C_BV_N center in hexagonal boron nitride monolayer for spin qubit application

Cheng GD Zhang YG Yan L Huang HF Huang Q
Song YX Chen Y Tang Z

Key words Qubit, Defect, First-principle calculations, Spin coherence time

First-principles calculations in combination with group theory analyses were employed to study the spin-polarized electronic structures of C_BV_N centers consisting of a nitrogen vacancy and

a substitutional carbon atom in hexagonal boron nitride (*h*-BN) monolayer with different charge states. It is clarified that the paramagnetic neutral C_BV_N center is stable in the *n*-type *h*-BN monolayer. The neutral defect center possesses a triplet (S = 1) ground state and with two spin-conserved optical vertical transition. Its spin coherence time is estimated to be 3.9 ms at T = 0 K by a simple scheme combining the mean-field theory and the first-principles calculations. The results indicate that the neutral C_BV_N center is very suitable for achieving spin qubit.

Computational Materials Science, 2017, **129**: 247

Theory of sulfur-vacancy defect in diamond: a comparable NV^{-1} isoelectronic center

Cheng GD Huang Q Shen YH Huang HF Yan L

Key words Color center, Zero-phonon line, First-principles calculation, Defect levels, Spin coherence time

A color center in diamond which is a comparable NV^{-1} isoelectronic center is predicted based on first-principles electronic structure calculations. The defect consists of a substitutional sulfur and an adjacent carbon vacancy (S-V). We find that the S-V center is optically accessible with two zero-phonon line of about 1.12 and 1.22 eV. The S-V center also shares many of the characteristics of the NV^{-1} center in diamond. A prominent spin coherence time is predicted by combining first-principles calculations and a mean-field theory for spin hyperfine interaction, and is at the same level with that of NV^{-1} center in diamond. Furthermore, the neutral S-V center in diamond provides more degrees of freedom for spin manipulation than the NV^{-1} center in diamond.

Optik, 2017, **136**: 151

Synthesis of a ceria-supported iron-ruthenium oxide catalyst and its structural transformation from subnanometer clusters to single atoms during the Fischer-Tropsch synthesis reaction

Wang Xu Fu XinPu Yu WenZhu Ma Chao
Jia ChunJiang Si Rui

The formation of supported metal/metal oxide single-atom catalysts (SAC), as well as their structural evolution during catalytic reactions have attracted much research interest in the fields of

both inorganic chemistry and catalysis recently. In this work, we report the synthesis of iron (*ca.* 10 at%) oxide catalysts with the doping of a small amount (0.5–0.6 at%) of ruthenium oxide, which have been deposited onto the surface of ceria nanorods by an optimized deposition–precipitation (DP) route. Multiple characterization studies including X-ray diffraction (XRD), high-resolution transmission electron microscopy (HRTEM) and nitrogen adsorption/desorption confirmed the identical structural and textural properties of the ceria support after the DP step. Aberration-corrected high-angle annular dark-field scanning transmission electron microscopy (HAADF-STEM) combined with electron energy loss spectroscopy (EELS) showed the formation of subnanometer iron species in the fresh samples. Furthermore, the X-ray absorption fine structure (XAFS) technique with the help of related data analysis verified the generation of noncrystalline iron oxide clusters predominantly composed of Fe^{3+} ions. Here, the addition of a secondary metal (ruthenium) greatly promoted the dispersion of Fe over the ceria nanorods. After the catalytic reaction of Fischer–Tropsch synthesis (FTS), the transformation from subnanometer iron oxide species to ionic $Fe^{\delta+}$ single atoms has been revealed and confirmed by the corresponding profile fits on the extended X-ray absorption fine structure (EXAFS) spectra. In contrast to the normal coarsening process, the FTS conditions (up to 300 °C, 2 MPa, CO/H_2 = 1/1) did drive the creation of such iron single atoms solely coordinated by oxygen ions.

Inorganic Chemistry Frontiers, 2017, **4**(12): 2059

Effects of Multiple Platinum Species on Catalytic Reactivity Distinguished by Electron Microscopy and X-ray Absorption Spectroscopy Techniques

Nan Bing Hu Xiu-Cui Wang Xu Jia Chun-Jiang
Ma Chao Li Ming-Xing Si Rui

Supported platinum species in the forms of single atoms, ultrafine clusters, and metallic particles have been widely investigated because of their unique catalytic properties in diverse redox reactions. In this work, we used thermally stable ceria–zirconia–lanthana ($Ce_{0.5}Zr_{0.42}La_{0.08}O_x$) as an active oxide support to deposit platinum with different loading amounts from 0.5 to 2 at. % via an incipient wetness impregnation. The as-obtained samples were measured under the methane oxidation reaction conditions with high space velocities up to 100,000 $mL \cdot g^{-1} \cdot h^{-1}$. Here, 1 at. % Pt sample showed the best catalytic performance with a total reaction rate of 1.93 $\mu mol_{CH4} \cdot g_{cat}^{-1} \cdot s^{-1}$ and exclusive platinum rate of 24.4 $mmol_{CH4} \cdot mol_{Pt}^{-1} \cdot s^{-1}$ at 450 °C. Multiple characterization means, especially aberration-corrected high-angle annular dark-field scanning

transmission electron microscopy (HAADF-STEM) and X-ray absorption fine structure (XAFS) with the related profile fittings, were carried out to determine the electronic and local coordination structures of platinum. On the basis of these experimental evidence, we have distinguished the effects of different components and found that platinum oxide clusters (Pt_xO_y) with averaged sizes from subnanometer to 2–3 nm play an essential role for the oxidation of methane. Metallic Pt particles are probably active species, but their large-size characteristics impair the reactivity. However, ionic platinum single atoms may not be appropriate for this catalytic process.

Journal of Physical Chemistry C, 2017, **121**(46): 25805

Ternary organic solar cells: compatibility controls for morphology evolution of active layers

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Yin Jingping Yu Zoukangning Liu Siqi Ma Wei
Zeng Jianrong Chen Yiwang

The fundamental principles of how a third component influences morphology evolution in ternary solar cells remains poorly understood. Here, P3BT, P3HT, and P3OT with different side chain lengths were incorporated into a *p*-DTS(FBTTh$_2$)$_2$: PC$_{71}$BM system to investigate the morphology evolution of films from a single component to binary blend films and from binary to ternary blend films. The compatibility between different components determined the final morphology of active layers during film formation, which could be described by Flory–Huggins parameters calculated through a melting point depression method. P3BT could promote crystallization of *p*-DTS(FBTTh$_2$)$_2$ in ternary blends to afford an optimized morphology, reaching a maximum power conversion efficiency (PCE) of 7.3% after further annealing treatment.

Journal of Materials Chemistry C, 2017, **5**(41): 10801

Investigating microstructure of Longmaxi shale in Shizhu area, Sichuan Basin, by optical microscopy, scanning electron microscopy and micro-computed tomography

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Jin Chan Wang YanFei

Key words Micro-computed tomography, Pore microstructure, Heterogeneity, Matrix layers, Longmaxi shale

Microstructure of shale formation is the key to understanding its petrophysical and chemical properties. Optical microscopy, scanning electron microscopy and micro-computed tomography (μ-CT) have been combined for characterization of microstructure of Longmaxi (LMX) shale from Shizhu area, Sichan Basin. The results indicate that laminated LMX shale consists of mineral matrix-rich layers and organic matter (OM)-rich layers at micrometer scale in two and three dimensions. Mineral matrix layers, mainly consisting of interparticle pores and intraplatelet pores, are approximately parallel to the bedding plane. Pyrite-rich layer, mainly containing intercrystalline pores, shows a strong preferred orientation parallel to the bedding plane. OM-rich layer, mainly containing OM pores, seems to be discontinuous. In addition, intercrystalline pores are enriched in some layers, while OM pores are distributed irregularly in matrix layers. This vertical heterogeneity of pore microscopic structures in LMX shale is of great importance to understand its petrophysical and chemical properties.

Nuclear Science and Techniques, 2017, **28**(11): 163

Improving the efficiency of small-angle x-ray scattering computed tomography using the OSEM algorithm

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Bian Fenggang Xiao Tiqiao

Small-angle x-ray scattering computed tomography (SAXS-CT) is a nondestructive method for the nanostructure analysis of heterogeneous materials. However, the limits of a long data acquisition time and vast amounts of data prevent SAXS-CT from becoming a routine experimental method in the applications of synchrotron radiation. In this study, the ordered subsets expectation maximization (OSEM) algorithm is introduced to improve the efficiency of SAXS-CT. To demonstrate the practicability of this method, a systematic simulation and experiments were carried out. The simulation results on a numerical phantom show that the OSEM-based SAXS-CT can effectively eliminate streaking artifacts and improve the efficiency of data acquisition by at least 3 times compared with the filter backprojection algorithm. By compromising the reconstruction speed and image quality, the optimal reconstruction parameters are also given for the image reconstruction in the OSEM-based SAXS-CT experiments. An experiment on a bamboo sample verified the validity of the proposed method with limited projection data. A further experiment on polyethylene demonstrated that the OSEM-based SAXS-CT is able to reveal the local nanoscale information about the crystalline structure and distributional difference inside the sample. In

conclusion, the OSEM-based SAXS-CT can significantly improve experimental efficiency, which may promote SAXS-CT becoming a conventional method.

Applied Optics, 2017, **56**(30): 8326

Investigation of atom distribution in Mg-9wt.%Al melt using small-angle X-ray scattering and molecular dynamics simulation

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Key words Mg-9wt.%Al, Atom distribution, Molecular dynamics simulation, Small-angle X-ray scattering

Two kinds of atom distribution in Mg-9wt.%Al melt, undissolved particles and atom aggregation, were investigated by synchrotron small-angle X-ray scattering (SAXS) and molecular dynamics simulation, respectively. The SAXS results indicated that no undissolved particles exist in Mg-9wt.%Al melt after short-time equilibration. The simulation results indicated that atom Mg and Al have a tendency to form bonds in Mg-9wt.%Al melt and the sizes of aggregated Al-centred clusters are within the characteristic scale of medium-range order; the degree of atom aggregation in Mg-9wt.%Al melt increases slightly with increasing temperature.

Journal of Non-Crystalline Solids, 2017, **473**: 47

Improved Glass Transition Temperature towards Thermal Stability via Thiols Solvent Additive versus DIO in Polymer Solar Cells

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Key words additives, dynamic mechanical analysis, glass transition temperature, polymer solar cells, thermal stability

The halogen-free solvent additive, 1,4-butanedithiol (BT) has been incorporated into PTB7-Th: $PC_{71}BM$, leading to higher power conversion efficiency (PCE) value as well as substantially

enhanced thermal stability, as compared with the traditional 1,8-diiodooctane (DIO) additive. More importantly, the improved thermal stability after processing with BT contributes to a higher glass transition temperature (T_g) of PTB7-Th, as determined by dynamic mechanical analysis. After thermal annealing at 130 °C in nitrogen atmosphere for 30 min, the PCE of the specimen processed with BT reduces from 9.3% to 7.1%, approaching to 80% of its original value. In contrast, the PCE of specimens processed with DIO seriously depresses from 8.3% to 3.8%. These findings demonstrate that smart utilization of low-boiling-point solvent additive is an effective and practical strategy to overcome thermal instability of organic solar cells via enhancing the T_g of donor polymer.

Macromolecular Rapid Communications, 2017, **38**(20): 1700428

Morphology and structure improvement of the hybrid $CH_3NH_3PbI_3$ perovskite film via external doping

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Ji Gengwu Li Haiyang Jiang Zheng Song Fei

Key words Surface morphology, Perovskites, Thin film, Doping, Methylammonium lead iodide, Guanidinium iodide

The optoelectronic properties of perovskite films are closely related to their quality. Herein, we report the doping of guanidinium iodide ($C(NH_2)_3I$) organic into $CH_3NH_3PbI_3$ perovskite thin films and reveal the enhancement of both morphology and structure of the perovskite films by doping with $C(NH_2)_3I$ in the range of 0 to 25%. Nuclear magnetic resonance is utilized to determine the molecular structure of the synthesized $C(NH_2)_3I$ and grazing-incidence X-ray diffraction is employed to characterize the lattice structure of doped perovskite films. Furthermore, doped $CH_3NH_3PbI_3$ perovskite films with different amounts of $C(NH_2)_3I$ is also investigated by X-ray photoelectron spectroscopy and scanning electron microscopy. It is found that the $C(NH_2)_3I$ dopant mainly assembles on the surface region of the pristine $CH_3NH_3PbI_3$ perovskite film. In the end, 5% $C(NH_2)_3I$ to $CH_3NH_3PbI_3$ perovskite film is found to be the doping ratio resulting in the best film structure and surface morphology.

Thin Solid Films, 2017, **636**: 296

High Extinction Coefficient Thieno[3,4-b]thiophene-Based Copolymer for Efficient Fullerene-Free Solar Cells with Large Current Density

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Yang Chunpeng Li Yonghai Yang Chunming
Xu Jintong Yang Renqiang

A thieno[3,4-*b*]thiophene-based donor polymer PTBTz-2 was employed to construct fullerene-free solar cell with the classical acceptor ITIC. Interestingly, due to the high extinction coefficients and wide absorption for these two materials, the active layer can harvest a larger fraction of the coverage solar spectrum even in ultrathin film. Furthermore, the simultaneous advantages of appropriate cascade energy level, well-balanced hole/electron mobility (μ_h/μ_e = 1.16), and low charge accumulation and recombination, make the PTBTz-2/ITIC-based solar cells exhibit an excellent power conversion efficiency of 10.92% with large short circuit current density of 20.34 mA cm^{-2}. The results indicate that fine-tailored thieno[3,4-*b*]thiophene-based polymers would be another type of promising donor materials, except for widely reported efficient benzo[*d*][1,2,3]triazole (BTA)- or benzo[1,2-*c*: 4,5-*c'*]-dithiophene-4,8-dione (BDD)-based polymers, and would enrich the reservoir of high-performance light-harvesting conjugated polymers.

Chemistry of Materials, 2017, **29**(16): 6766

Co_3O_4-Al_2O_3 mesoporous hollow spheres as efficient catalyst for Fischer-Tropsch synthesis

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Wang Xu Si Rui Song Qi-Sheng
Jia Chun-Jiang Yan Chun-Hua

Key words Mesoporous hollow spheres, Mixed metal oxide, Interfacial structure, Aerosol-assisted self-assembly, Fischer-Tropsch synthesis

Nanostructured mixed metal oxides with porous hollow-interior structure hold great promise in environmental-related catalysis, owing to their excellent catalytic properties. However, facile fabrication of such mesoporous architecture is still challenging. Here, by using a transient aerosol-assisted self-assembly (AASA) method, we synthesized the Co_3O_4-Al_2O_3 mesoporous

hollow spheres (MHS) composed of thermally stable Co_3O_4 nanoparticles partially anchored to amorphous interfacial Al_2O_3. The as-prepared Co_3O_4-Al_2O_3 nanocomposites displayed distinct features of large pore volume and stable assembled morphology, and thus showed significant advantages in mass transfer and redox behavior. For Fischer-Tropsch synthesis, a very important reaction in fuel production, the Co_3O_4-Al_2O_3 MHS exhibited significant catalytic performance in conversion, selectivity and stability for the desired gasoline products. Therefore, we provide a facile and controlled approach towards the preparation of mesoporous hollow materials to achieve novel mixed metal oxide nanocatalysts those are good candidates in energy-production application.

Applied Catalysis B: Environmental, 2017, **211**: 176

Manifestation of the structural stability of Mg-doped Zn_4Sb_3 via atomic fine structure investigation

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Ji GW Li J Jiang Song F

Key words Zn_4Sb_3, Structural stability, XAFS, SEM

The structural stability is crucially important for thermoelectric material from the point view of energy harvesting applications. Herein, p-type Zn-Sb semiconductor doped with magnesium ($Mg_{0.04}Zn_{3.96}Sb_3$) was experimentally investigated after thermal cycles to verify its structure stability, via a combination of synchrotron-based X-ray absorption spectroscopy (XAFS), grazing-incidence X-ray diffraction (GI-XRD), scanning electron microscopy (SEM), and energy dispersive spectrometer (EDS). While no visible structure change was discovered from XRD measurement after annealed to 573 K in air, well-preserved atomic structure of Mg-doped Zn-Sb was also demonstrated by XAFS. Interestingly, SEM indicated significantly improved surface morphology whilst EDS clearly showed the relative steadiness of each element's spatial distribution on surface. On basis of these findings, it was concluded in the end that the doping of magnesium substantially improves the thermal stability of zinc-antimonite compounds, and the possible mechanism underneath was also demonstrated.

Solid State Communications, 2017, **261**: 26

Investigation of the fine structure around the copper site in copper/zinc superoxide dismutase by XANES combined with ab initio calculations

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Wang Jianqiang Zhang Shuo Wei Xiangjun Jiang Zheng
Huang Yuying Cui Peixin Zhao Haifeng Chu Wangsheng

Key words Copper/zinc superoxide dismutase, BioXAS, Metalloprotein, MXAN

Copper/zinc superoxide dismutase (CuZnSOD) is an important enzyme that plays a crucial role in protecting oxygen-metabolizing cells against harmful effects of superoxide free-radicals. In this work, the three-dimensional local structure around the copper-binding site in pH 7.0 buffer solution was determined using X-ray absorption near-edge spectroscopy (XANES) combined with *ab initio* calculations in the framework of the multiple-scattering theory performed by MXAN. Extremely accurate bond distances and bond angle information between ligands were returned. The result confirmed that the copper ion binds four conserved His residues and a water molecule in CuZnSOD and prefers a five-coordinated in a distorted square pyramidal geometry.

Radiation Physics and Chemistry, 2017, **137**: 88

Disorder effects on EXAFS modeling for catalysts working at elevated temperatures

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Du Xianlong Wang Jianqiang Jiang Zheng Huang Yuying

Key words Disorder effects, Extended X-ray absorption fine structure spectroscopy (EXAFS), Gaussian fitting mode, Expansion of cumulants, Einstein method

In-situ X-ray absorption fine structure spectroscopy (XAFS) has been widely used to study the structure around active site of catalysts at elevated pressures and temperatures for decades. However, methods of XAFS data analysis can vary significantly, depending on the disorder degree of the material system investigated. In this work, in-situ XAFS was explored to investigate the structural evolutions of the industry $CuO/ZnO/Al_2O_3$ catalyst for methanol synthesis at elevated temperatures in nitrogen (N_2) atmosphere. Due to the large Debye–Waller factor, data analysis using the conventional Gaussian mode resulted in erroneously contracted Cu–Cu bond distances which made the conventional Gaussian mode invalid in this system. To account for the deviation

from harmonic behavior, the cumulant expansion technique was used to correct the error in the bond contraction, and the frequency pattern could be fully reproduced by considering cumulants up to C_3. In order to elucidate the contributions of the structure and thermal components to the Debye–Waller factors, the Einstein method was also used to analyze the data that provides a straightforward proof regarding the effect of the temperature on the in-situ XAFS experiment.

Radiation Physics and Chemistry, 2017, **137**: 93

Zn Single Atom Catalyst for Highly Efficient Oxygen Reduction Reaction

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Key words carbon black, oxygen reduction reaction, single atom catalysts, zinc

The authors report first a new type of nitrogen-triggered Zn single atom catalyst, demonstrating high catalytic activity and remarkable durability for the oxygen reduction reaction process. Both X-ray absorption fine structure spectra and theoretical calculations suggest that the atomically dispersed Zn-N_4 site is the main, as well as the most active, component with O adsorption as the rate-limiting step at a low overpotential of 1.70 V. This work opens a new field for the exploration of high-performance Pt-free electrochemical oxygen reduction catalysts for fuel cells.

Advanced Functional Materials, 2017, **27**(28): 1700802

High performance platinum single atom electrocatalyst for oxygen reduction reaction

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For the large-scale sustainable implementation of polymer electrolyte membrane fuel cells in vehicles, high-performance electrocatalysts with low platinum consumption are desirable for use as cathode material during the oxygen reduction reaction in fuel cells. Here we report a carbon black-supported cost-effective, efficient and durable platinum single-atom electrocatalyst with

carbon monoxide/methanol tolerance for the cathodic oxygen reduction reaction. The acidic single-cell with such a catalyst as cathode delivers high performance, with power density up to 680 mW cm^{-2} at 80 °C with a low platinum loading of 0.09 mg_{Pt} cm^{-2}, corresponding to a platinum utilization of 0.13 g_{Pt} kW^{-1} in the fuel cell. Good fuel cell durability is also observed. Theoretical calculations reveal that the main effective sites on such platinum single-atom electrocatalysts are single-pyridinic-nitrogen-atom-anchored single-platinum-atom centres, which are tolerant to carbon monoxide/methanol, but highly active for the oxygen reduction reaction.

Nature Communications, 2017, **8**: 15938

Photoelectron spectroscopy study of the electronic structures at CoPc/Bi(111) interface

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Key words Photoemission spectroscopy, Electronic structure, CoPc, Bi(111), Interface

Self-assembly of functional molecules on solid substrate has been recognized as an appealing approach for the fabrication of diverse nanostructures for nanoelectronics. Herein, we investigate the growth of cobalt phthalocyanine (CoPc) on a Bi(111) surface with focus on the interface electronic structures utilizing photoelectron spectroscopy. While charge transfer from bismuth substrate to the molecule results in the emergence of an interface component in the Co 3p core level at lower binding energy, core-levels associated to the molecular ligand (C 1s and N 1s) are less influenced by the adsorption. In addition, density functional theory (DFT) calculations also support the empirical inference that the molecule-substrate interaction mainly involves the out-of-plane empty Co 3d orbital and bismuth states. Finally, valence band spectra demonstrate the molecule-substrate interaction is induced by interface charge transfer, agreeing well with core level measurements. Charge transfer is shown to be mainly from the underlying bismuth substrate to the empty states located at the central Co atom in the CoPc molecules. This report may provide a fundamental basis to the on-surface engineering of interfaces for molecular devices and spintronics.

Surface Science, 2017, **661**: 34

Achieving Remarkable Activity and Durability toward Oxygen Reduction Reaction Based on Ultrathin Rh-Doped Pt Nanowires

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The research of active and sustainable electrocatalysts toward oxygen reduction reaction (ORR) is of great importance for industrial application of fuel cells. Here, we report a remarkable ORR catalyst with both excellent mass activity and durability based on sub 2 nm thick Rh-doped Pt nanowires, which combine the merits of high utilization efficiency of Pt atoms, anisotropic one-dimensional nanostructure, and doping of Rh atoms. Compared with commercial Pt/C catalyst, the Rh-doped Pt nanowires/C catalyst shows a 7.8 and 5.4-fold enhancement in mass activity and specific activity, respectively. The combination of extended X-ray absorption fine structure analysis and density functional theory calculations reveals that the compressive strain and ligand effect in Rh-doped Pt nanowires optimize the adsorption energy of hydroxyl and in turn enhance the specific activity. Moreover, even after 10000 cycles of accelerated durability test in O_2 condition, the Rh-doped Pt nanowires/C catalyst exhibits a drop of 9.2% in mass activity, against a big decrease of 72.3% for commercial Pt/C. The improved durability can be rationalized by the increased vacancy formation energy of Pt atoms for Rh-doped Pt nanowires.

Journal of the American Chemical Society, 2017, **139**(24): 8152

Catalytically active ceria-supported cobalt–manganese oxide nanocatalysts for oxidation of carbon monoxide

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A low-concentration cobalt (~6 at%) and manganese (~3 at%) bimetallic oxide catalyst supported on ceria nanorods ($CoMnO_x/CeO_2$), as well as its related single metal oxide counterparts (CoO_x/CeO_2 and MnO_x/CeO_2) was synthesized *via* a deposition–precipitation approach. The fresh samples after air-calcination at 400 °C were tested under the reaction conditions of CO oxidation, and showed the following order of reactivity: $CoMnO_x/CeO_2 > CoO_x/CeO_2 > MnO_x/CeO_2$. X-ray diffraction (XRD) and transmission electron microscopy (TEM) data identified that the structure of

the CeO_2 support was maintained during deposition of metal (Co, Mn) ions while the corresponding vis-Raman spectra verified that more oxygen vacancies were created after deposition–precipitation than those in pure ceria nanorods. Aberration-corrected, high-angle, annular dark-field scanning transmission electron microscopy (HAADF-STEM) images with the help of electron energy loss spectroscopy (EELS) analyses determined two types of cobalt species, *i.e.* ultra-fine clusters (<2 nm) and smaller nanocrystals (up to 5 nm) in CoO_x/CeO_2 while only bigger nanostructures (~10 nm) of cobalt–manganese oxides in $CoMnO_x/CeO_2$. X-ray absorption fine structure (XAFS) measurements demonstrated the presence of a cubic Co_3O_4 phase in all the cobalt-based catalysts. The fitting results of the extended X-ray absorption fine structure (EXAFS) indicated that the introduction of the secondary metal (Mn) oxide significantly enhanced the two-dimensional growth of cobalt oxide nanostructures on the surface of CeO_2. Therefore, the enhanced activity of CO oxidation reaction over the bimetallic cobalt–manganese oxide nanocatalyst can be attributed to the higher crystallinity of the Co_3O_4 phase in this work.

Physical Chemistry Chemical Physics, 2017, **19**(22): 14533

Probing intermediates of the induction period prior to nucleation and growth of semiconductor quantum dots

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Renoud Romain Bian Fenggang Zeng Jianrong Yu Kui

Little is known about the induction period before the nucleation and growth of colloidal semiconductor quantum dots. Here, we introduce an approach that allows us to probe intermediates present in the induction period. We show that this induction period itself exhibits distinct stages with the evolution of the intermediates, first without and then with the formation of covalent bonds between metal cations and chalcogenide anions. The intermediates are optically invisible in toluene, while the covalent-bonded intermediates become visible as magic-size clusters when a primary amine is added. Such evolution of magic-size clusters provides indirect but compelling evidence for the presence of the intermediates in the induction period and supports the multi-step nucleation model. Our study reveals that magic-size clusters could be readily engineered in a single-size form, and suggests that the existence of the intermediates during the growth of conventional quantum dots results in low product yield.

Nature Communications, 2017, **8**: 15467

Enhanced electrochemical sensing arsenic(III) with excellent anti-interference using amino-functionalized graphene oxide decorated gold microelectrode: XPS and XANES evidence

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Key words Electrochemical sensing, Arsenic(III), NH2-GO, Anti-interference, XPS and XANES

To date, the electrochemical method for efficient and accurate determination of As(III) in groundwater with interference-free is still a difficultly but significantly task. Herein, a reliable, high sensitive and excellent anti-interference electrochemical sensing As(III) with amino-functionalized graphene oxide (NH_2-GO) decorated gold (Au) microelectrode was developed in mild media with square wave anodic stripping voltammeter (SWASV). Taking advantage of the synergy between the strong absorption capability of NH_2-GO and the excellent electrocatalytic ability of Au microwire, the NH_2-GO modified Au microelectrode exhibits the enhanced electrochemical performance toward As(III). No obvious interference from other commonly coexisting ions on the determination of As(III) was observed. Furthermore, the robust stability and reproducibility of the electrodes were obtained. Under the optimized conditions, the limit of detection (3σ method) toward As(III) was 0.162 ppb with a sensitivity of 130.631 μA ppb^{-1} cm^{-2}. Notably, the possible mechanism of the enhanced stripping signal was preliminarily explored by using X-ray photoelectron spectroscopy (XPS) and X-ray absorption near edge structure (XANES) techniques. Finally, the analytical application of the raised means on the detection of As(III) in Xingwangzhuang Village groundwater, Inner Mongolia, has been successfully verified.

Sensors and Actuators B: Chemical, 2017, **245**: 230

Poly(3-hexylthiophene) coated graphene oxide for improved performance of bulk heterojunction polymer solar cells

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Key words Graphene oxide, Poly(3-hexylthiophene), Coating, Phase separation, Organic solar cells

An effective method for preparing poly(3-hexylthiophene) (P3HT) coated graphene oxide (GO), (P-GO), based on an ethanol mediated mixing and solvent evaporation method is described. P-GO exhibits good dispersibility in the non-polar solvent o-dichlorobenzene (DCB) allowing the preparation of polymer blend composites. P-GO was doped into P3HT: PCBM blends by solution mixing and shown to facilitate phase separation of P3HT and PCBM in P3HT: PCBM blend films to achieve a more optimum morphology for polymer photovoltaic cells. Bulk heterojunction P3HT: PCBM solar cells exhibit ~18% power conversion efficiency enhancement in the presence of P-GO.

Organic Electronics, 2017, **44**: 149

Supported Rhodium Catalysts for Ammonia–Borane Hydrolysis: Dependence of the Catalytic Activity on the Highest Occupied State of the Single Rhodium Atoms

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Key words hydrolysis, metal-support interactions, rhodium, single-atom catalysts, vanadium dioxide

Supported metal nanocrystals have exhibited remarkable catalytic performance in hydrogen generation reactions, which is influenced and even determined by their supports. Accordingly, it is of fundamental importance to determine the direct relationship between catalytic performance and metal–support interactions. Herein, we provide a quantitative profile for exploring metal–support interactions by considering the highest occupied state in single-atom catalysts. The catalyst studied consisted of isolated Rh atoms dispersed on the surface of VO_2 nanorods. It was observed that the activation energy of ammonia–borane hydrolysis changed when the substrate underwent a phase transition. Mechanistic studies indicate that the catalytic performance depended directly on the highest occupied state of the single Rh atoms, which was determined by the band structure of the substrates. Other metal catalysts, even with non-noble metals, that exhibited significant catalytic activity towards NH_3BH_3 hydrolysis were rationally designed by adjusting their highest occupied states.

Angewandte Chemie International Edition, 2017, **56**(17): 4712

Synthesis and Self-Assembly of Shape Amphiphiles Based on POSS-Dendron Conjugates

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Key words shape amphiphiles, dendrimer, polyhedral oligomeric silsesquioxane, hierarchical structure

Shape has been increasingly recognized as an important factor for self-assembly. In this paper, a series of shape amphiphiles have been built by linking polyhedral oligomeric silsesquioxane (POSS) and a dendron via linkers of different lengths. Three conjugates of octahedral silsesquioxanes (T_8-POSS) and dendron are designed and synthesized and are referred to as isobutyl T_8-POSS gallic acid derivatives (BPOSS-GAD-1, BPOSS-GAD-2, BPOSS-GAD-3). These samples have been fully characterized by ^{1}H-NMR, ^{13}C-NMR, Fourier transform infrared (FT-IR) spectroscopy and matrix-assisted laser desorption/ionization time of flight (MALDI-TOF) mass spectrometry to establish their chemical identity and purity. Driven by different interactions between POSS and dendron, ordered superstructure can be found upon self-assembly. The stabilities and structures of these samples are further studied by using differential scanning calorimetry (DSC), small-angle X-ray scattering (SAXS), wide-angle X-ray diffraction (WAXD), and molecular simulations. The results show that their melting points range from 74 °C to 143 °C and the molecular packing schemes in the assemblies can form lamellar structure of BPOSS-GAD-3 as determined by the different linkers.

Molecules, 2017, **22**(4): 622

WAXD/SAXS study and 2D fitting (SAXS) of the microstructural evolution of PAN-based carbon fibers during the pre-oxidation and carbonization process

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Key words Wid-angle X-ray scattering, Small-angle X-ray scattering, Carbon fiber, Microvoids, Direct model fitting

Microstructural evolution in polyacrylonitrile (PAN) fibers at different temperatures during pre-oxidation and carbonization under stretching was studied by synchrotron wide-angle X-ray

diffraction (WAXD) and small-angle X-ray scattering (SAXS). Microvoids were characterized by the classical SAXS method, and were compared with simulation results obtained by fitting 2D SAXS patterns to a model based on a dilute system of cylindrical microvoids randomly distributed and preferentially orientated along the fiber axis and having a log-normal size distribution. The WAXD results showed that the crystal size, *d*-spacing and preferred orientation decreased during pre-oxidation, and increased during carbonization. A diffraction peak for PAN fibers at 2θ=13.6° disappeared during the final stage of pre-oxidation, meanwhile a new peak at 2θ=23.6° appeared, whose intensity increased during carbonization, indicating the formation of the graphite structure. The average length of the microvoids increased, and new microvoids were formed, which became oriented along the fiber axis as the fiber manufacturing process proceeded. The length of microvoids from simulation results is consistent with that from the classical method, indicating that the model is valid to describe the microvoid structure of fibers.

New Carbon Materials, 2017, **32**(2): 130

The Influence of Epitaxial Crystallization on the Mechanical Properties of Polyamide 66/Reduced Graphene Oxide Nanocomposite Injection Bar

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Tian Feng　Wang Zongbao

Key words　polyamide 66, reduced graphene oxide, nanocomposite, epitaxial crystal

Polyamide 66 (PA66) was chosen as the representative of hydrophilic polymers, to investigate the influence of epitaxial crystals in semi-crystalline polymers/reduced graphene oxide nanocomposite injection-molding bars. A differential scanning calorimeter was used, and the two-dimensional wide-angle X-ray diffraction technique, as well as the two-dimensional small angle X-ray scattering technique, were used to research the crystallization behavior in PA66/RGO nanocomposites. The results indicated that RGO was an effective nucleation agent for PA66. The presence of RGO could enhance the orientation degree of the PA66 crystals and did not influence the crystal structure of the PA66. The non-epitaxial crystals and the epitaxial crystals existed in PA66/RGO nanocomposites. The size of epitaxial crystals was much greater than that of the non-epitaxial crystals. Tensile test results showed that the presence of fewer epitaxial crystals can improve the mechanical properties of a polymer.

Crystals, 2017, **7**(12): 384

Microfocus small-angle X-ray scattering at SSRF BL16B1

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Key words small-angle X-ray scattering, KB mirror, smearing effects, image blind restoration

Offering high-brilliance X-ray beams on micrometer length scales, the μSAXS at SSRF BL16B1 has been established with a KB mirror system for studying small sample volumes, or probing microscopic morphologies. The SAXS minimum q value is 0.1 nm^{-1} with a flux of 1.5×10^{10} photons/s. Two position-resolved scanning experimental methods, STXM and CT, are combined with μSAXS. To improve the significant smearing effect in the horizontal direction, an effective and easy-to-use desmearing procedure for two-dimensional SAXS patterns based on blind deconvolution was developed, and the deblurring results demonstrate the good restoration effect for the defocused image. Finally, a bamboo sample was used in the SAXS-CT experiment to illustrate the performance of the μSAXS method.

Chinese Physics C, 2017, **41**(4): 048001

Synthesis and metal-support interaction of subnanometer copper-palladium bimetallic oxide clusters for catalytic oxidation of carbon monoxide

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Zeng Jie Jia Chun-Jiang Huang Yu-Ying Si Rui

Subnanometer oxide clusters with distinct metal–support interactions have attracted great interest due to their possible superiority in catalytic performance compared to that of conventional metal–oxide nanoparticles. In this paper, we report the solution-based chemical synthesis of a new type of copper–palladium bimetallic oxide clusters anchored to the surface of ceria nanorods. Revealed by aberration-corrected high-angle annular dark-field scanning transmission electron microscopy (HAADF-STEM) and X-ray absorption fine structure (XAFS) techniques, we have identified that both copper and palladium species are fully oxidized with dominant metal–support interaction contributions by a strongly bound M–O_x–Ce (M = Cu or Pd) structure. However, no direct bond between copper oxide and palladium oxide clusters, *i.e.* Cu–O_x–Pd, has been verified by experimental evidences, and thus no synergistic effect on the catalytic activity of bimetallic

copper–palladium oxide clusters, compared to that of single metal (palladium) oxide clusters, has been demonstrated for the CO oxidation reaction.

Inorganic Chemistry Frontiers, 2017, **4**(4): 668

Facile synthesis and hierarchical assembly of polystyrene-block- poly (perfluorooctylethyl acrylates)

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Xu YuJie Zhang WenBin Miao XiaRan Li Hui

Key words Fluoropolymers, Block copolymer, Phase separation, Hierarchical structure, Self-assembly

Hierarchical assembly of macromolecules has been central in creating complex nanostructures. In this work, polystyrene-*block*-poly (perfluorooctylethyl acrylates) (PS-*b*-PFOA) diblock copolymers were synthesized by reversible addition-fragmentation chain transfer (RAFT) polymerization and shown to assemble into hierarchical structures in bulk with the interplay of nanophase separation and crystallization. The molecular weights were determined by gel permeation chromatography (GPC) and ^{1}H NMR spectra. The phase-separated nanostructures of these block copolymers were investigated via small-angle X-ray scattering (SAXS) and wide-angle X-ray diffraction (WAXD) in reciprocal space and by transmission electron microscopy (TEM) in real space. The results showed that well-ordered lamellar morphologies were formed in the bulk of samples with volume fraction of PFOA (f_{PFOA}) around 0.390–0.538. Within the PFOA layers, the side chains were found to further crystallize, forming crystalline layers with thicknesses about twice that of the length of fluorinated side-chains. The SAXS patterns from sheared samples further show that the orientation of crystalline layers was perpendicular to the lamellar layers formed by micro-phase separation.

Polymer, 2017, **113**: 46

Performance on absolute scattering intensity calibration and protein molecular weight determination at BL16B1, a dedicated SAXS beamline at SSRF

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Wang Yuzhu Tian Feng Zhou Ping

Key words beamline, SAXS, absolute intensity, calibration, molecular weight

The optical system and end-station of bending-magnet beamline BL16B1, dedicated to small-angle X-ray scattering (SAXS) at the Shanghai Synchrotron Radiation Facility, is described. Constructed in 2009 and upgraded in 2013, this beamline has been open to users since May 2009 and supports methodologies including SAXS, wide-angle X-ray scattering (WAXS), simultaneous SAXS/WAXS, grazing-incidence small-angle X-ray scattering (GISAXS) and anomalous small-angle X-ray scattering (ASAXS). Considering that an increasing necessity for absolute calibration of SAXS intensity has been recognized in in-depth investigations, SAXS intensity is re-stated according to the extent of data processing, and the absolute intensity is suggested to be a unified presentation of SAXS data in this article. Theory with a practical procedure for absolute intensity calibration is established based on BL16B1, using glass carbon and water as primary and secondary standards, respectively. The calibration procedure can be completed in minutes and shows good reliability under different conditions. An empirical line of scale factor estimation is also established for any specific SAXS setup at the beamline. Beamline performance on molecular weight (MW) determination is provided as a straightforward application and verification of the absolute intensity calibration. Results show good accuracy with a deviation of less than 10% compared with the known value, which is also the best attainable accuracy in recent studies using SAXS to measure protein MW. Fast MW measurement following the demonstrated method also enables an instant check or pre-diagnosis of the SAXS performance to improve the data acquisition.

Journal of Synchrotron Radiation, 2017, **24**: 509

Local structural evolutions of $CuO/ZnO/Al_2O_3$ catalyst for methanol synthesis under operando conditions studied by in situ quick X-ray absorption spectroscopy

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Du XianLong Wang JianQiang
Huang YuYing Jiang Zheng

Key words In situ, Quick X-ray absorption spectroscopy, $CuO/ZnO/Al_2O_3$ catalyst, Operando condition

In situ quick X-ray absorption spectroscopy (QXAFS) at the Cu and Zn K-edge under operando conditions has been used to unravel the Cu/Zn interaction and identify possible active site of $CuO/ZnO/Al_2O_3$ catalyst for methanol synthesis. In this work, the catalyst, whose activity increases with the reaction temperature and pressure, was studied at calcined, reduced, and reacted conditions. TEM and EDX images for the calcined and reduced catalysts showed that copper was

distributed uniformly at both conditions. TPR profile revealed two reduction peaks at 165 and 195 °C for copper species in the calcined catalyst. QXAFS results demonstrated that the calcined form consisted mainly of a mixed CuO and ZnO, and it was progressively transformed into Cu metal particles and dispersed ZnO species as the reduction treatment. It was demonstrated that activation of the catalyst precursor occurred via a Cu^+ intermediate, and the active catalyst predominantly consisted of metallic Cu and ZnO even under higher pressures. Structure of the active catalyst did not change with the temperature or pressure, indicating that the role of the Zn was mainly to improve Cu dispersion. This indicates the potential of QXAFS method in studying the structure evolutions of catalysts in methanol synthesis.

Nuclear Science and Techniques, 2017, **28**(2): 21

Crystal Plane Effect of Ceria on Supported Copper Oxide Cluster Catalyst for CO Oxidation: Importance of Metal–Support Interaction

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Si Rui Ma Chao Shi Shuo Jia ChunJiang Yan ChunHua

Key words copper-ceria catalyst, subnanometer clusters, crystal plane effect, metal-support interaction, redox properties

Copper–ceria as one of the very active catalysts for oxidation reactions has been widely investigated in heterogeneous catalysis. In this work, copper oxide (1 wt % Cu loading) deposited on both ceria nanospheres with a {111}/{100}-terminated surface (**1CuCe-NS**) and with nanorod exposed {110}/{100} faces (**1CuCe-NR**) have been prepared for the investigation of crystal plane effects on CO oxidation. Various structural characterizations, especially including aberration-corrected scanning transmission electron microscopy (Cs-STEM), X-ray absorption fine structure (XAFS) technique, and in situ diffuse reflectance infrared Fourier transform spectroscopy (in situ DRIFTS), were used to precisely determine the structure and status of the catalysts. It is found that the copper oxides were formed as subnanometer clusters and were uniformly dispersed on the surface of the ceria support. The results from XAFS combined with the temperature-programmed reduction technique (H_2-TPR) reveal that more reducible CuO_x clusters with only Cu–O coordination structure exclusively dominated in the surface of **1CuCe-NS**, while the Cu species in **1CuCe-NR** existed in both CuO_x clusters and strongly interacting Cu-[O_x]-Ce. In situ DRIFTS results demonstrate that the CeO_2-{110} face induced a strongly bound Cu-[O_x]-Ce structure in **1CuCe-NR** which was adverse to the formation of reduced Cu(I) active sites, resulting

in low reactivity in CO oxidation (r_{CO} = 1.8 × 10^{-6} mol_{CO} g_{cat}^{-1} s^{-1} at 118 °C); in contrast, CuO_x clusters on the CeO_2-{111} face were easily reduced to Cu(I) species when they were subjected to interaction with CO, which greatly enhanced the catalytic reactivity (r_{CO} = 5.7 × 10^{-6} mol_{CO} g_{cat}^{-1} s^{-1} at 104 °C). Thus, for copper–ceria catalyst, in comparison with the well-known reactive $\{110\}_{CeO2}$ plane, $\{111\}_{CeO2}$, the most inert plane, exhibits great superiority to induce more catalytically active sites of CuO_x clusters. The difference in strength of the interaction between copper oxides and different exposed faces of ceria is intrinsically relevant to the different redox and catalytic properties.

ACS Catalysis, 2017, **7**(2): 1313

Unveiling orbital coupling at the CoPc/Bi(111) surface by ab initio calculations and photoemission spectroscopy

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The interfacial electronic structures of cobalt phthalocyanine adsorbed on a semimetal Bi(111) surface have been systematically investigated herein. Our study first indicates that the CoPc molecule is quite sensitive to the adsorption site on the relatively inert Bi(111) surface. Secondly, apparent change of the electronic structures of CoPc has been revealed upon adsorption as compared to that in the gas phase, due to the orbital coupling between the cobalt partial empty state and the surface state from the bismuth substrate and interfacial charge transfer. Interestingly, the local magnetic moment is still retained for the adsorbed CoPc molecule on the diamagnetic Bi(111) surface, which is different to that on other noble metal substrates. Analysis of the charge density difference and the Bader charge provides evident insight on the mechanism of interfacial charge transfer which is chiefly mediated by the central Co atom and the weak vdW dispersion between the π-conjugated macrocyclic ligand and the bismuth substrate, as further confirmed by experimental XPS results. In the end, our report may provide an appealing route towards the fundamental understanding and reliable engineering of interfacial interactions between magnetic and semimetal nanostructures.

RSC Advances, 2017, **7**(82): 52143

Recent Progress in the Fabrication of Low Dimensional Nanostructures via Surface-Assisted Transforming and Coupling

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Polymerization of functional organics into covalently cross-linked nanostructures via bottom-up approach on solid surfaces has attracted tremendous interest recently, due to its appealing potentials in fabricating novel and artificial low dimensional nanomaterials. While there are various synthetic approaches being proposed and explored, this paper reviews the recent progress of on-surface coupling strategies towards the synthesis of low dimensional nanostructures ranging from 1D nanowire to 2D network and describes their advantages and drawbacks during on-surface process and phase transformations, for example, from molecular self-assembly to on-surface polymerization. Specifically, Ullmann reaction is discussed in detail and the mechanism governing nanostructures' transforming effect by surface treatment is exploited. In the end, it is summarized that the hierarchical polymerization combined with Ullmann coupling makes it possible to realize the selection of different synthetic pathways and phase transformations and obtain novel organometallic nanowire with metalorganic bonding.

Journal of Nanomaterials, 2017: 4796538

On-surface manipulation of atom substitution between cobalt phthalocyanine and the Cu(111) substrate

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Hu Jinbang Liang Zhaofeng Gao Xingyu Li Haiyang
Li Zheshen Song Bo Jiang Zheng Huang Han
Wells Justin W. Song Fei

On-surface fabrication of controllable nanostructures is an appealing topic in the field of molecular electronics. Herein, the adsorption of cobalt phthalocyanine (CoPc) on a Cu(111) surface is investigated utilizing a combination of photoelectron spectroscopy (PES) and density functional theory (DFT). Interestingly, the scenario of atom exchange is discovered at the interface at room temperature (RT), namely the substitution of the cobalt atom in CoPc by a surface Cu adatom. Moreover, thermal annealing enhances the substitution process considerably which is demonstrated to be complete at about 573 K. As revealed by DFT calculations, the driving force for the observed

interface transmetalation is most probably provided by the initial strong molecular-substrate interaction between Co atoms and the Cu(111) surface, the external thermodynamic energy gained from thermal sublimation and thermal annealing, and the tendency to form Co–Cu alloy at the interface. While CoPc has been successfully utilized in electrocatalysts for fuel cell applications and CuPc is commonly used as a leading material in organic solar cells, this report of interface transmetalation from CoPc to CuPc in a solid state environment may offer an encouraging approach towards the artificial engineering of organometallic nanostructures and related properties for surface catalysts, molecular electronics and so on.

RSC Advances, 2017, **7**(23): 13827

In-situ high-energy-resolution X-ray absorption spectroscopy for UO_2 oxidation at SSRF

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Key words X-ray absorption spectroscopy (XAS), In-situ cell, UO_2 oxidation

Based on the high-energy-resolution fluorescence spectrometer on the BL14W1 beamline at Shanghai Synchrotron Radiation Facility, an in-situ high-energy-resolution X-ray absorption spectroscopy technique, with an in-situ heating cell, was developed. The high-energy-resolution fluorescence detection for X-ray absorption near-edge spectroscopy (HERFD-XANES) was tested in a UO_2 oxidation experiment to measure the U L_3-edge, with higher signal-to-noise ratio and higher-energy-resolution than conventional XANES. The technique has potential application for in-situ study of uranium-based materials.

Nuclear Science and Techniques, 2017, **28**(1): 2

A three-crystal spectrometer for high-energy resolution fluorescence-detected X-ray absorption spectroscopy and X-ray emission spectroscopy at SSRF

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Li Jiong Huang Yuying

Key words High resolution X-Ray spectrometer, X-Ray absorption spectroscopy, X-Ray emission spectroscopy

A Johann-type spectrometer for the study of high-energy resolution fluorescence-detected X-ray absorption spectroscopy, X-ray emission spectroscopy and resonant inelastic X-ray scattering

has been developed at BL14W1 X-ray absorption fine structure spectroscopy beamline of Shanghai Synchrotron Radiation Facility. The spectrometer consists of three crystal analyzers mounted on a vertical motion stage. The instrument is scanned vertically and covers the Bragg angle range of 71.5–88°. The energy resolution of the spectrometer ranges from sub-eV to a few eV. The spectrometer has a solid angle of about 1.87×0^{-3} of 4π sr, and the overall photons acquired by the detector could be 10^5 counts per second for the standard sample. The performances of the spectrometer are illustrated by the three experiments that are difficult to perform with the conventional absorption or emission spectroscopy.

X-Ray Spectrometry, 2017, **46**(1): 12

Au_6S_2 monolayer sheets: metallic and semiconducting polymorphs

Wu Qisheng Xu Wen Wu Qu Bingyan Ma Liang
Niu Xianghong Wang Jinlan Zeng Xiao Cheng

Gold–sulfur interfaces, including self-assembled monolayers of thiol molecules on gold surfaces, thiolate-protected gold nanoclusters, and gold sulfide complexes, have attracted intensive interest due to their promising applications in electrochemistry, bioengineering, and nanocatalysis. Herein, we predict two *hitherto* unreported two-dimensional (2D) Au_6S_2 monolayer polymorphs, named as G-Au_6S_2 and T-Au_6S_2. The global-minimum G-Au_6S_2 monolayer can be viewed as a series of $[–S–Au–]_n$ and $[–Au_4–]_n$ chains packed together in parallel. The metastable T-Au_6S_2 monolayer resembles the widely studied T-MoS_2 monolayer structure with each Mo atom substituted with an octahedral Au_6 cluster, while the S atom is bonded with three Au atoms in a μ_3 bridging mode. The G-Au_6S_2 monolayer is predicted to be metallic. The T-Au_6S_2 monolayer is predicted to be a semiconductor with a direct bandgap of 1.48 eV and high carrier mobility of 2721 $cm^2\ V^{-1}\ s^{-1}$, ~10 times higher than that of semiconducting H-MoS_2. Moreover, the T-Au_6S_2 monolayer can absorb sunlight efficiently over almost the entire solar spectrum. These properties render the G- and T-Au_6S_2 monolayers promising materials for advanced applications in microelectronics and optoelectronics.

Materials Horizons, 2017, **4**(6): 1085

J/ψ azimuthal anisotropy in Au+Au collisions at $\sqrt{S_{NN}}$ =200 GeV

Zhou Chensheng STAR Collaboration

The study of J/ψ azimuthal anisotropy allows for a disentanglement of various production mechanisms and possibly an access to charm quark azimuthal anisotropy. *J/ψ* meson produced from direct pQCD processes have little azimuthal anisotropy due to the lack of collectivity or azimuthal preference of initial emitting, while *J/ψ* meson produced from recombination of charm quarks in the medium are expected to inherit the azimuthal anisotropy of the constituent charm quarks. We present measurements of *J/ψ* azimuthal anisotropy, with *J/ψ* reconstructed via the di-electron channel, as a function of transverse momentum in Au+Au collisions at $\sqrt{S_{NN}}$ =200 GeV . This analysis is carried out with data taken by the STAR experiment during RHIC operation in year 2011. Combined with the published results using 2010 data, the updated results provide further support to the conclusion that *J/ψ* production above 2 GeV/*c* is unlikely to be dominated by regeneration of fully thermalized charm quarks.

Journal of Physics: Conference Series, 2017, **832**: 012021

Analysis on partial coherence propagation using the four-dimensional coherence function

Meng Xiangyu Xue Chaofan Yu Huaina Wang Yong
Wu Yanqing Tai Renzhong

Key words Partially coherent radiation, mutual optical intensity, coherence propagation, beamline design

The mutual optical intensity (MOI) is a four-dimensional coherence function and contains the full coherence information of the beam. The propagation of mutual optical intensity through a soft x-ray beamline is analyzed with a new developed model named MOI. The MOI model is based on statistical optics. The wavefront is separated into many elements and every element is assumed to has full coherence and constant complex amplitude, which is reasonable if the dimension of element is much smaller than the coherent length and beam spot size. The propagation of MOI for every element can be analytically solved with Fraunhofer or Fresnel approximations. The total MOI propagation through free space can be obtained by summing the contribution of all elements. Local stationary phase approximation is implemented to simulate MOI propagating through ideal mirrors

and gratings. The MOI model provides not only intensity profile, but also wavefront and coherence information of the beam. These advantages make MOI model a useful tool for beamline design and optimization. The nano-ARPES beamline at SSRF is analyzed using the MOI model. A zone plate is used to focus the beam. The intensity profile and local coherence degree at the zone plate are acquired. The horizontal coherence is much worse than the vertical one. By cutting the horizontal beam with the exit slit the horizontal coherence can be improved but at the flux loss. The quantitative analysis on the coherence improvement and flux loss at different exit slit size are obtained with the MOI model.

Advances in Computational Methods for X-Ray Optics IV, 2017, **10388**: UNSP 103880W

Evaluation on microstructure and mechanical properties of welded joints by GMAW in UNS N10003 alloy

Yu Kun Jiang Zhenguo Shi Xianwu Li Chaowen
Chen Shuangjian Li Zhijun Tao Wang Zhou Xingtai

Key words UNS N10003 alloy, GMAW, Microstructure, Mechanical properties

UNS N10003 alloy is a primary material of the Thorium Molten Salt Reactor (TMSR) in China that is a suitable candidate reactor of the Generation IV nuclear reactors. Gas metal arc welding (GMAW) is more effective than gas tungsten arc welding (GTAW) which is usually used to weld nickel-base alloys. In order to improve welding efficiency, it is necessary to weld nickel-base alloys using GMAW. The purpose of this work is to evaluate effect of GMAW on microstructure evolution and mechanical properties in UNS N10003 alloy. The results of microstructure showed that the sound welded joint without hot cracking can be obtained, although quantities of M_6C-γ eutectic phases with large size were precipitated in fusion zone (FZ) and transformed in heat affected zone (HAZ) because of element segregation. The results of microhardness test indicated that there was no softened zone in the welded joint. The results of tensile test at room temperature and high temperature showed that the short-term time-independent strength was not damaged by the formation of large M_6C-γ eutectic phases.

Proceedings of the ASME Pressure Vessels and Piping Conference, 2017, **6B**: UNSP V06BT06A019

Research of the Rod Drop Time Based on the Control Rod System of TMSR-SF1

Lin Zuokang Zhu Lin Zhao Chunfeng
Cao Yun Wang Xiao

Key words thorium base molten salt reactor, driving mechanism of control rod, scram, control rod drop time

The reactor scram function realized by the rapidly dropping of control rods ensures safety when the reactor accidents (loss of electricity and earthquake, etc.) happen. In the thorium base molten salt reactor (TMSR - SF1), the rod drop time is obviously affected by the resistance which produced in the molten salt as its high density and viscosity. In this paper, the drop time of the control rod is obtained by the theoretical and experimental methods for comparison. Firstly, the drop time is analyzed both in air and water condition with calculation and experiment. And the method used for the resistance calculation of the rod during dropping is verified. Secondly, the similarity criterion is adopted to calculate the drop time in molten salt condition. The study shows that: 1) In air and water condition, the calculation is coincidence with the experimental results within the maximum error less than 2 %. 2) The drop time of the rod in molten salt is 2.8 s with a dropping height 2.4m in reactor, which satisfy the safety requirement of the control system. 3) It is necessary to use another buffer beside the disc spring to protect the driving mechanism of the rod during the rod dropping.

Proceedings of the 25th International Conference on Nuclear Engineering, 2017, **2**: V002T03A073

The feasibility research of thorium breeding using fluoride salt as a fast reactor coolant

Peng Yu Zhu Guifeng Zou Yang Liu Yafen Yu Xiaohan
Cai Xiangzhou Xu Hongjie

Key words Fluoride salts , Coolant selection , Neutron balance , Thorium cycle , Fast reactor

Breeder reactors are considered as a unique tool for fully exploiting natural resources. Fast breeder reactors based on thorium fuel can enhance inherent safety. Fluoride salt has good performance as a coolant in high-temperature nuclear systems. However, there is some doubt about the fuel breeding ability using fluoride salt coolant for fast spectrum due to its moderating ability.

The aim of this study was to choose a proper fluoride salt mixture for Liquid-salt-cooled Solid-fuel Fast Reactor (LSFR) based on thorium-uranium fuel and give parametric studies to provide a design window for flexible self-sustaining core design. Infinite assembly model was used to analyze the salt selection from five candidate fluorides for fast spectrum as coolant. Combining neutron balance analysis with linear least squares fitting method based on 0D model, parametric studies at the neutron balance equation unique solution with burn-up for several parameters such as fuel volume fraction, removing fission gases process, total neutron losses and power density were presented in this paper. It was found that BeF_2-NaF was a promising coolant in the five candidate fluoride salt mixture. This study proved that the design of a self-sustaining core for fluoride-salt-cooled fast breeder based on thorium fuel is achievable. A design window was found in the definition of a self-sustaining core for various fuel volume fractions and neutron loss fractions. Core design and fuel management strategy will be given in future.

Progress in Nuclear Energy, 2017, **101**: 199

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The reactor scram function realized by the rapidly dropping of control rods ensures safety when the reactor accidents (loss of electricity and earthquake, etc.) happen. In the thorium base molten salt reactor (TMSR - SF1), the rod drop time is obviously affected by the resistance which produced in the molten salt as its high density and viscosity. In this paper, the drop time of the control rod is obtained by the theoretical and experimental methods for comparison. Firstly, the drop time is analyzed both in air and water condition with calculation and experiment. And the method used for the resistance calculation of the rod during dropping is verified. Secondly, the similarity criterion is adopted to calculate the drop time in molten salt condition. The study shows that: 1) In air and water condition, the calculation is coincidence with the experimental results within the maximum error less than 2 %. 2) The drop time of the rod in molten salt is 2.8 s with a dropping height 2.4m in reactor, which satisfy the safety requirement of the control system. 3) It is necessary to use another buffer beside the disc spring to protect the driving mechanism of the rod during the rod dropping.

Proceedings of the 25th International Conference on Nuclear Engineering, 2017, **2**: V002T03A073

TMSR fuel cycle evaluation under a screening and decision-making framework

Wu Jianhui Chen Jingen Cai Xiangzhou Yu Chenggang
Zou Chunyan Jia Guobin Li Xiaoxiao Han Jianlong

MSR (Molten salt reactor) is a reactor with the fission material dissolved in the fluoride salt as the fuel, which continuously circulates through the primary loop. The liquid fuel makes the online refueling and reprocessing be possible, consequently, more fuel cycle options would be presented due to the introduction of various refueling fuel type and reprocessing mode (continuous / batch reprocessing) comparing with that of the solid fuel reactor systems. It is important to evaluate all the possible fuel cycle options and screen out the promising ones to narrow the R&D activities of TMSR (Thorium-based Molten-Salt Reactor nuclear energy system) program. In this study, we firstly established a screening and decision-making framework, then conducted an initial evaluation work and identified the potential promising fuel cycle options. Synthesizing the goal of TMSR program and technology readiness, we proposed a "Three-steps" fuel cycle development strategy with the aim for gradually increasing the thorium resource utilization while considering the challenges of the reprocessing technology.

Proceedings of the 25th International Conference on Nuclear Engineering, 2017, **7**: V007T10A024

Analysis of Sustainable Thorium Fuel Utilization in Molten Salt Reactors Starting from Enriched Uranium

Cui Deyang Cai Xiangzhou Chen Jingen Yu Chenggang

Molten salt reactor (MSR), as one of the six systems selected by the Generation IV International Forum (GIF) for future advantaged reactors research and development (R&D), has excellent performances such as high inherent safety, desirable breeding capacity, low radioactive waste production, flexible fuel cycle and non-proliferation. Meanwhile, thorium, as an appealing alternative nuclear fuel to uranium, is more abundant than uranium in the earth's crust. Realization of thorium fuel cycle in MSRs will greatly contribute to sustainable energy supply for global development. The objective of this paper is to analyze and evaluate thorium fuel utilization in a program in which MSRs are expected to be developed step by step. The program can be described as follows:

1 The first stage is a converter reactor fueled with low enriched uranium. With limited

processing based on current chemical partitioning technology and fuel-feeding techniques in the generation-I MSR;

2 The second stage is a ^{233}U production reactor. By using the enriched uranium, it can produce ^{233}U which does not exist in nature;

3 The third stage is a thorium breeding reactor. It is a breeder reactor with Th/^{233}U fuel cycle, and sustainable thorium utilization for energy production is expected to be eventually realized.

By employing an in-house developed tool based on SCALE6.1, the performance of MSR fueled with low enriched uranium is firstly assessed. It is found that MSR is attractive regarding conversion ratio when compared with light water reactors. Then we illustrate the feasibility of ^{233}U production in MSR. Enriched uranium with two enrichments are used as driver fuels to start MSR and produce ^{233}U. The results show that ^{233}U production can be achieved and the double time is about 79.1 years for 20% enriched uranium and 28.3 years for 60% enriched uranium. Finally, the performance of MSR based on pure Th/^{233}U fuel cycle is evaluated. It is found that breeding fissile material is possible in MSR and the breeding ratio is desirable (1.049). Comparison of the three-stage MSRs is also conducted and the results indicate that the resource utilization efficiency is much higher in stage-III than that in the first two stages and much less minor actinides is produced in MSR operating on Th/^{233}U fuel cycle than that in traditional light water reactor.

Proceedings of the 25th International Conference on Nuclear Engineering, 2017, **5**: V005T05A033

An Innovative Spherical Fuel Element to Inhibit the Infiltration of Liquid Fluoride Salt in Molten Salt Reactor

Zhong Yajuan Lin Jun Xu Liujun Jiang Haitao Zhiyong Zhu

To inhibit the infiltration of liquid fluoride salt and easy to load and unload, fuel element in molten salt reactor (MSR) was isostatically pressed with an innovative design: A fuel-free low density graphite core of ≤ 30 mm diameter embedded in fuel-zone shell of ≥ 2.5 mm thickness, and then enveloped in a high density graphite shell of ≥ 5 mm thickness. Bulk density of the spherical fuel element can be designed from the range of 1.65–1.80 g/cm^3, which is lower than the density of the liquid fluoride salt to make sure the fuel element can float in the MSR to load and unload. Characteristics of mercury infiltration and molten salt infiltration in graphite shell were investigated and compared with A3-3 graphite to identify the infiltration behaviors. The results indicated that the graphite shell has a low porosity about 9%, and an average pore diameter of 100 nm. The fluoride salt occupation of A3-3 was 10 wt% under 6.5 atm, whereas the salt gain did not infiltrate in graphite shell even up to 6.5 atm. It demonstrated that the outside graphite shell could inhibit the

infiltration of liquid fluoride salt effectively. At the operating temperature of MSR (700 °C), thermal conductivity of graphite shell was 13.61 W/m K. The coefficient of thermal expansion (CTE) of outside graphite shell lied in 6.01×10^{-6} K^{-1} ($\alpha_{/\!/}$) and 6.15×10^{-6} K^{-1} ($\alpha_{\perp}$) at the temperature range of 25–700 °C. The anisotropies factor of graphite shell calculated by CTE maintained below 1.12, which could meet the requirement of the spherical fuel element (below 1.30). The constant isotropic properties of graphite shell are beneficial for the integrity and safety of the spherical fuel element for a MSR.

Proceedings of the 25th International Conference on Nuclear Engineering, 2017, **3**: UNSP V003T02A0023-1

Thermal Hydraulics Analysis of the Fluoride-Salt-Cooled, High Temperature Reactor

Fu Yao Sun Qiang Zhou Chong Zou Yang

Fluoride-salt-cooled, high-temperature reactor (FHR) technology combines the robust coated particle fuel of high-temperature, gas-cooled reactors with the single phase, high volumetric heat capacity coolant of molten salt reactors and the low-pressure pool-type reactor configuration of sodium fast reactors. This paper discusses one key technology area required to further define and develop the FHR: the thermal hydraulic performance of the core, primary system and second loop. Shanghai Institute of Applied Physics (SINAP) is leading the China Academy of Science (CAS) FHR program. A TMSR-SF1 reactor with a fluoride cooled pebble bed design has been suggested by SINAP, and the design is currently in progress. For this preliminary thermal hydraulic assessment, a TMSR-SF1 system model was developed using RELAP5. The RELAP5 model was used to help define and size systems such as the intermediate coolant salt selecting. A loss of flow transient was also simulated to evaluate the performance of the reactor during an anticipated transient event. A steady-state calculation was carried out and the calculated initial conditions show the influence of different salt. The loss of forced flow (LOFF) transient simulation results show that the passive residual heat removal system can effectively remove all decay heat from the primary loop under this extreme accident scenario. Some initial recommendations for modifying system component designs, such as heat exchanger with different salt and install place of pump, are also discussed.

Proceedings of the 25th International Conference on Nuclear Engineering, 2017, **5**: V005T05A020

Breeding Properties Study on High Power Thorium Molten Salt Reactor

Liu Yafen Guo Rui Cai Xiangzhou Yan Rui
Zou Yang Zhou Bo

The Molten Salt Reactor (MSR), the only one using liquid fuel in the six types 'Generation IV' reactors, is very different from reactors in operation now and has initiated very extensive interests all over the world. This paper is primarily aimed at investigating the breeding characteristics of high power (1000 MWe) Thorium Molten Salt Reactor (TMSR) based on the two-fluid Molten Salt Breeder Reactor (MSBR) with superior breeding performance. We explored the optimized structure to be a thorium based molten salt breeder reactor with different core conditions and different post-processing programs, and finally got the breeding ratio of 1.065 in our TMSR model. At last we analyzed the transient security of our optimized model with results show that the temperature coefficient of core is −3 pcm/K and a 2000 pcm reactivity insertion can be successfully absorbed by the core if the insertion time is more than or equal to 5 seconds and the core behaves safely.

Proceedings of the 25th International Conference on Nuclear Engineering, 2017, **5**: V005T05A026

Control Scheme Research of 10MW Fluoride Salt Cooled High Temperature Experiment Reactor

Ruan Jian Zou Yang Li Minghai Xu Hongjie

Fluoride salt cooled High temperature Reactor (FHR) is a kind of Gen-IV reactor which possesses many attractive features, such as high temperature, low pressure etc. Thermal-hydraulic features of molten salt are different from coolants of traditional reactors, which dominate operation transient behavior of FHR. However, as a new type reactor with sphere fuel element and fluoride salt coolant, FHR has inadequate operating experience and data used for reactor control and the design of power regulating system. Therefore, research of power regulation strategy is very important for FHR in automatic control operation and commercial application.

A code programmed in Fortran platform is used for investigating the system transient behavior, control logic and strategy. Based on the transient analysis code OCFHR for FHR, power control logic strategy is studied on a model of 10 MW Fluoride salt cooled High Temperature Experiment Reactor. OCFHR is a specialized code in FHR transient analysis, which contains point reactor model, simplified core thermal-hydraulic model, molten salt-salt exchanger and molten salt-air

exchanger with a tube-shell type, control rod system and power regulation and control model. The control module of OCFHR uses the incremental PID controller to regulate control parameters and adopts the compound mode of control rod adjustment, load adjustment and molten salt flow adjustment, so that it can adjust the control rod position, primary and secondary molten salt flow rate and air flow rate of load at different operating power levels.

Two kinds of steady operation strategies are studied in this paper, which are a) constant outlet coolant temperature and b) constant average coolant temperature. The power level is regulated by control rod while the working temperatures are adjusted by shifting the load with weight coefficients of power and temperature deviations.

The results show that the incremental PID controller with optimized parameters can achieve the control requirement. Both of temperature control strategies gain great performances under 10%FPand 50%FP power regulation. The target power is reached quickly and accurately by using the incremental PID controller while the temperature control is very time-consuming. Compared with b), strategy a) has less temperature overshoot but larger power overshoot and longer adjusting time. The step wise power regulation for FHER is doable when a wide power adjustment range is needed and the simulation 10%FP treated as a step works well. Besides, the preliminary study of varying secondary coolant flow rate also indicates that the secondary loop plays an important part in restraining the deviation of secondary coolant temperatures during the process of balancing the power and load, so it is better to adjust the secondary coolant flow in terms of the power regulation range.

Proceedings of the 25th International Conference on Nuclear Engineering, 2017, **5**: V005T05A009

Application of the Probability-Based Safety Analysis for the Reliability Evaluation of a Special Fuel Salt Release System Design in the Molten Salt Reactor

Yang Qun Li Minghai Hou Jie
He Zhaozhong Chen Kun

In the molten salt reactor (MSR), the fuel salt can be discharged out of the core to avoid a more serious consequence in the accident. In this paper, a special core fuel salt release system (CFSRS) is described. Its equipment reliability and human reliability are evaluated subsequently to identify the key failure factors and provide suggestions for the design, by means of the fault tree analysis and the human reliability analysis (HRA) respectively. Results show that the human error

is a dominant factor of CFSRS failure in the accident scenario. A good operator training or a sufficient diagnosis time can greatly improve the CFSRS human reliability. Regardless of the human error, to obtain a balanced design and a low equipment failure probability of less than 2E−5, the redundant design of CFSRS including the pipe heating subsystem is necessary.

Proceedings of the 25th International Conference on Nuclear Engineering, 2017, **5**: V005T05A027

Development and Use of an Open-Source, User-Friendly Package To Simulate Voltammetry Experiments

Wang, Shuo Wang, Jing Gao, Yanjing

Key words Upper-Division Undergraduate, Graduate Education/Research, Chemical Engineering, Computer-Based Learning, Electrochemistry, Kinetic

An open-source electrochemistry simulation package has been developed that simulates the electrode processes of four reaction mechanisms and two typical electroanalysis techniques: cyclic voltammetry and chronoamperometry. Unlike other open-source simulation software, this package balances the features with ease of learning and implementation and can run on mainstream operating systems. In an elctroanalysis lecture for graduate students, we have simulated the cyclic voltammetry of an electron transfer reaction with varied scan rates. The dynamical concentration profiles were demonstrated in an animation to help students understand the relation between currents and evolving concentration profiles, and the relations between peak currents and scan rates were also discussed.

Journal of Chemical Education, 2017, **94(**10): 1567

Elliptic flow of electrons from heavy-flavor hadron decays in Au + Au collisions at$\sqrt{S_{NN}}$ =200, 62.4, and 39 GeV

STAR Collaboration

Key words relativistic nuclear collisions, quark-gluon plasma, ion collisions, pb collisions, qcd matter, star, collaboration, fluctuations, perspective, tomography

We present measurements of elliptic flow (v_2) of electrons from the decays of heavy-flavor hadrons (e_{HF}) by the STAR experiment. For Au+Au collisions at $\sqrt{S_{NN}}$ = 200 GeV we report v_2, for transverse momentum (pT) between 0.2 and 7 GeV/c, using three methods: the event plane method (v_2{EP}), two-particle correlations (v_2{2}), and four-particle correlations (v_2{4}). For

Au+Au collisions at $\sqrt{S_{NN}}$ = 62.4 and 39 GeV we report $v_2\{2\}$ for pT < 2 GeV/c. $v_2\{2\}$ and $v_2\{4\}$ are nonzero at low and intermediate pT at 200 GeV, and $v_2\{2\}$ is consistent with zero at low pT at other energies. The $v_2\{2\}$ at the two lower beam energies is systematically lower than at $\sqrt{S_{NN}}$ = 200 GeV for pT < 1 GeV/c. This difference may suggest that charm quarks interact less strongly with the surrounding nuclear matter at those two lower energies compared to $\sqrt{S_{NN}}$ = 200 GeV.

Physical Review C, 2017, **95**(3): 034907

Compact beam transport system for free-electron lasers driven by a laser plasma accelerator

Liu Tao Zhang Tong Wang Dong Huang Zhirong

Key words Extreme-Ultraviolet, Operation, Atoms

Utilizing laser-driven plasma accelerators (LPAs) as a high-quality electron beam source is a promising approach to significantly downsize the x-ray free-electron laser (XFEL) facility. Amulti-GeVLPA beam can be generated in several-centimeter acceleration distance, with a high peak current and a low transverse emittance, which will considerably benefit a compact FEL design. However, the large initial angular divergence and energy spread make it challenging to transport the beam and realize FEL radiation. In this paper, a novel design of beam transport system is proposed to maintain the superior features of the LPA beam and a transverse gradient undulator (TGU) is also adopted as an effective energy spread compensator to generate high-brilliance FEL radiation. Theoretical analysis and numerical simulations are presented based on a demonstration experiment with an electron energy of 380 MeV and a radiation wavelength of 30 nm.

Physical Review Accelerators and Beams, 2017, **20** (2): 020701

Parameter optimization and start-to-end simulation for the phase-merging enhanced harmonic generation free electron laser

Qi Zheng Feng Chao Deng Haixiao
Liu Bo Zhao Zhentang

Key words Seeded FEL, Harmonic generation, Transverse gradient, PEHG

Recently, a novel scheme called the phase-merging enhanced harmonic generation (PEHG) free-electron laser (FEL) has been developed to achieve higher harmonic bunching in a single stage

set up. However, previous studies of the PEHG mechanism ignored the practical lattice configuration, leaving out the impact of the intrinsic beam divergence on the phase-merging effect. In this paper, a new method based on the beam transport matrix is proposed to comprehensively study the optimization conditions of the harmonic generation FELs. On the basis of this method, the new optimization conditions of the PEHG are obtained by taking into account both the intrinsic horizontal beam size and the intrinsic horizontal beam divergence. The parameter optimization and three dimensional start-to-end simulations are carried out using the typical beam parameters of the Shanghai Soft X-ray Free Electron Laser user facility. The simulation results are in agreement with the theoretical analysis and demonstrate the validity of the PEHG-FEL.

Nuclear Instruments and Methods in Physics Research Section A: Accelerators, Spectrometers, Detectors and Associated Equipment, 2017, **875**: 119

Precise magnetic field control of the scanning magnets for the APTRON beam delivery system

Miao Chun-Hui Liu Ming Yin ChongXian
Zhao ZhenTang

Key words Proton therapy, Scanning magnet, Hysteresis, Feedforward control

A design for precise scanning magnetic field control for the beam delivery system of the Shanghai Advanced Proton Therapy Facility (APTRON) is presented in this paper. With a novel feedforward algorithm to compensate for magnet hysteresis, the scanning magnetic field can be controlled to within a precision of +/- 2.5 G. The main advantage of the proposed feedforward algorithm is that the average settling time is shorter compared with that of a conventional feedback algorithm with acceptable tolerance.

Nuclear Science and Techniques, 2017, **28**(12): 172

Gain cascading scheme of a free-electron-laser oscillator

Li Kai Deng Haixiao

Key words X-Ray Pulses, Stimulated-Emission, Extreme-Ultraviolet, Magnetic-Field, Storage-Ring, Fel, Generation, Radiation, Coherent, Operation

The low-gain free-electron laser (FEL) oscillators are cuttingedge tools to produce fully coherent radiation in the spectral region from terahertz to vacuum ultraviolet, and potentially in hard x ray. In this paper, it is proposed to utilize an FEL oscillator with multistage undulators to enable gain cascading in a single pass, making it possible to achieve shorter single pulse lengths,

higher peak power, and even higher pulse energy than the normal FEL oscillator. Theoretical analysis and numerical simulations in the infrared and hard x-ray regions show that our proposal is effective.

Physical Review Accelerators and Beams, 2017, **20**(11): 110703

Design of a nondestructive two-in-one instrument for measuring the polarization and energy spectrum at an X-ray FEL facility

Zhang Qingmin Deng Bangjie Chen Yuanmiaoliang
Liu Bochao Chen Shaofei Fan Jinquan Feng Lie
Deng Haixiao Liu Bo Wang Dong

Key words Gaseous detectors, Inspection with x-rays, Instrumentation for FEL, Polarimeters

The free electron laser (FEL), as a next-generation light source, is an attractive tool in scientific frontier research because of its advantages of full coherence, ultra-short pulse duration, and controllable polarization. Owing to the demand of real-time bunch diagnosis during FEL experiments, precise nondestructive measurements of the polarization and X-ray energy spectrum using one instrument are preferred. In this paper, such an instrument based on the electron time-of-flight technique is proposed. By considering the complexity and nonlinearity, a numerical model in the framework of Geant4 has been developed for optimization. Taking the Shanghai Soft X-ray FEL user facility as an example, its measurement performances' dependence on the critical parameters was studied systematically, and, finally, an optimal design was obtained, achieving resolutions of 0.5% for the polarization degree and 0.3 eV for the X-ray energy spectrum.

Journal of Instrumentation, 2017, **12** : T1003

Ultrabroad and Angle Tunable THz Filter Based on Multiplexed Metallic Bar Resonators

Liu Weiwei Dai Zijie Yang Jing Sun Quan Gong Cheng
Zhang Nan Ueno Kosei Misawa Hiroaki

Key words Terahertz filter, metamaterial, broadband, angle tunable

An ultrabroad and angle tunable terahertz filter based on multiplexed metallic bar resonators is designed, fabricated, and characterized in this letter. We found that the bandwidth of the filter could

be greatly extended by the multiplexed configurations. When the number of gold bars in a unit cell increases from 1 to 5, the bandwidth will be broadened from 0.13 to 1.20 THz. Besides, the modulation depth of the filter can be tuned by rotating the sample to change the angle between the long axis of the metallic bars and THz polarization. When the deflection angle decreases from 90 degrees to 0 degrees, the transmission of the filter decreases from 1 to 0.26. Therefore, the multiplexed metallic bar structure provides a feasible method to pursue a tunable broadband terahertz metamaterial filter.

IEEE Photonics Technology Letters, 2018, **30**(24): 2103

A novel input power control strategy for high-power dynamic dipole power supply for proton therapy

Tan Songqing Li Rui Guo Chunlong Shi Tao
Zhao Yongqun Li Xiaopeng

Key words Input power control, Dynamic power supply, Proton therapy

This paper proposes a novel input power control strategy for high-power dynamic power supply for proton therapy. A buck chopper is staged in series between the input rectifier and the output chopper of the power supply to buffer the input power fluctuation, which can reduce the reactive power exchange between the power supply and power grid and reduce the power distribution requirements. The validity of this proposed control principle has been verified on a high-power dynamic dipole power supply for proton therapy.

Nuclear Instruments & Methods in Physics Research Section A-Accelerators Spectrometers Detectors and Associated Equipment, 2018, **911**: 25

First-principle atomistic thermodynamic study on the early-stage corrosion of NiCr alloy under fluoride salt environment

Yin Ya-Ru Ren Cui-Lan Han Han Dai Jian-Xing
Wang Hao Huai Ping Zhu Zhi-Yuan

Key words Surface Segregation, Adsorption, Chlorine, Energy, Moisture, Cu(111), Points

The atomic morphology change in the NiCr alloy surface induced by fluorine-chemisorption was investigated by the ab initio atomistic thermodynamic method to elucidate early-stage

corrosion processes of nickel-based alloys in strong oxidizing environment. The surface phase diagrams of Cr-doped Ni(111) surface as a function of fluorine chemical potential were obtained to track the surface structures that are most likely to be fostered in various temperature and pressure conditions. The adsorption of fluorine on the top site of Cr in the alloy surface was the most energetically favorable one. With increasing fluorine chemical potential, more fluorine atoms started to agglomerate in the trapping sink of Cr. Fluorine-fluorine repulsion interaction coupled with strong F-Cr bonding could facilitate a decided morphology modification of the metal substrate. Moreover, an insight into the desorption pathways for potential species revealed that in the presence of fluorine, the dissociation of Cr predominantly stems from the relatively easy desorption in the form of CrF_2/CrF_3 molecules from the non-passivated Ni-based alloy surface.

Physical Chemistry Chemical Physics, 2018, **20**(45): 28832

Influence of alpha-clustering nuclear structure on the rotating collision system

Xu Zhiwan Zhang Song Ma Yugang
Chen Jinhui Zhong Chen

Key words Chiral magnetic effect, Chiral vortical effect, Initial geometrical effect, Quark-gluon plasma, Relativistic heavy-ion collisions

In recent years, the collective motion properties of global rotation of the symmetric colliding system in relativistic energies have been investigated. In addition, the initial geometrical shape effects on the collective flows have been explored using a hydrodynamical model, a transport model, etc. In this work, we study the asymmetric $^{12}C+ ^{197}Au$ collision at 200 GeV/c and the effect of the exotic nuclear structure on the global rotation using a multi-phase transport model. The global angular momentum and averaged angular speed were calculated and discussed for the collision system at different evolution stages.

Nuclear Science and Techniques, 2018, **29**(12): 186

Formation and Characterization of Zr4+ Stabilized by Neutral Tridentate Ligands in the Gas Phase

Chen Xiuting Li Qingnuan Gong Yu

Key words Multiply charged cation, Zirconium, Pyridinedicarboxamide, Diglycolamide, Gas phase

Ligated tetrapositive metal ions are rare gas-phase species which tend to form complexes with lower charges due to the high 4th ionization energies of metals. We report the observation of tetrapositive $Zr(TMPDA)_3^{4+}$ and $Zr(TMOGA)_3^{4+}$ complexes in the gas phase by electrospray ionization of $Zr(ClO_4)_4$/TMPDA and $Zr(ClO_4)_4$/TMOGA mixtures. The Zr^{4+} center in both complexes is coordinated by nine atoms from three neutral diamide ligands forming nine-coordinate twisted tricapped trigonal prismatic geometry on the basis of DFT calculations. Collision-induced dissociation of both complexes resulted in the loss of protonated ligands to form tripositive $Zr(TMPDA)(TMPDA\text{-}H)^{3+}$ and $Zr(TMOGA)(TMOGA\text{-}H)^{3+}$ products which retain the IV oxidation state of zirconium at the cost of charge reduction from 4+ to 3+ of the whole complexes. The very high 4th ionization energy of zirconium (34.34 eV) makes tetrapositive zirconium complex the most challenging tetracation to be stabilized against charge reduction in the gas phase to date.

Journal of the American Society for Mass Spectrometry, 2018, **29**(12): 2327

Nonlinear energy chirp compensation with corrugated structures

Wang Zhen Feng Chao Huang Dazhang
Gu Qiang Zhang Meng

Key words Corrugated structure, Nonlinear energy chirp, High-repetition-rate FEL

Herein, a feasible method is proposed to compensate the high-order effect during bunch length compression, thereby enhancing the peak current of a high-repetition-rate X-ray free-electron laser source. In the proposed method, the corrugated structure is inserted downstream of the high-order harmonic cavities to function as a passive linearizer and enhance the longitudinal profile of the electron beam. Three-dimensional simulations are performed to analyze the evolution of the longitudinal phase space, and the results demonstrate that the profile of the electron beam is improved and the peak current can be easily optimized to over 2 kA with a bunch charge of 100 pC.

Nuclear Science and Techniques, 2018, **29**(12): 175

Stress analysis of the TMSR graphite component under irradiation conditions

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Ding Dong Tsang Derek-Kwong-Lai

Key words Nuclear graphite, Stress analysis, Irradiation, Permeation zone

TMSR uses nuclear graphite as a neutron moderator, a reflector, and the structural material, and utilizes molten salt as a coolant. When running normally, the graphite components are immersed in the molten salt. Thus, the nuclear graphite comes into direct contact with the molten salt, which infiltrates the open pores of the nuclear graphite. This infiltration may influence the stress analysis of the graphite component. In this study, a User Material subroutine was used to analyze the stress distribution of the graphite component, both with and without molten salt infiltration. Many influence factors were taken into consideration, such as the dose gradient, the shape of the permeation zone, and the permeation area. The results show that the dose gradient, shape, and area of the permeation zone all significantly influence the stress distribution. Furthermore, the results of the stress analysis indicate that for a regular graphite component with a square cross section, the peak maximum principal stress value occurs at the center of the cross section, and the symmetry of the maximum principal stress distributions was modified by quarter circle and half ellipse permeation zones.

Nuclear Science and Techniques, 2018, **29**(12): 173

Crystal structure of the periplasmic domain of TssL, a key membrane component of Type VI secretion system

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Xu Dongqing Ran Tingting He Jianhua Wang Weiwu

Key words TssL, Type VI secretion system, Crystal structure, Peptidoglycan binding site

Type VI secretion system (T6SS), as a macromolecular system, is commonly found in Gram-negative bacteria and responsible for exporting effectors. T6SS consists of 13 core proteins. TssL is a component of the membrane complex and plays a pivotal role in T6SS. Here, we report the crystal structure of the C-terminal periplasmic domain of TssL ($TssL_{Cter}$) from Serratia marcescens FS14. The $TssL_{Cter}$ (310-503) contain a five-stranded anti-parallel beta-sheet flanked by five alpha-helices and a short N-terminal helix. Structural comparisons revealed that it belongs to the OmpA-like family with a remarked difference in the conformation of the loop3-5. In

OmpA-like family, the corresponding loop is located close to loop2-3, forming a cavity with a small opening together with the longest alpha 5, whereas in $TssL_{Cter}$, loop3-5 flipped away from this cavity region. In addition, significant differences in the peptidoglycan (PG) binding site suggest that big conformational change must take place to accomplish the PG binding for $TssL_{Cter}$. Furthermore, a long flexible loop between helices alpha 1 and alpha 2 is unique in TssL. TssL would have a big conformational change during the delivery of the Hcp needle and effectors. So we speculate that the long flexible endows TssL the adaptation of its evolutionary new function.

International Journal of Biological Macromolecules, 2018, **120**: 1474

Molecular dynamics investigation on the local structures and transport properties of uranium ion in LiCl-KCl molten salt

Dai Jianxing Zhang Wei Ren Cuilan Han Han Guo Xiaojing Li Qingnuan

Key words UCl_3-LiCl-KCl molten salt, Local structures, Diffusion coefficient, Viscosity, Molecular dynamics method

The effects of temperature and composition on the structures and transport properties of UCl_3-LiCl-KCl salts were systematically investigated by using molecular dynamics simulation with a polarizable force field. In the molten salt of pure UCl_3, there exist networks of $[UCl_n]$ (n = 6, 7, 8, ...) clusters, dominated by corner-sharing, Cl-linked $[UCl_8]^{5-}$. The networks became sparser with the UCl_3 concentration decreasing. The local structures of U^{3+} complexes in LiCl-KCl salts were also compared with that of typical fission products such as Sc^{3+}, Y3+, La^{3+} and Tb^{3+}. It is found that the local structures of the U^{3+} complexes in LiCl-KCl were very similar to that of La^{3+}, while the U-Cl coordination bonds were less stable than that of Y-Cl, Sc-Cl, and Tb-Cl complexes. Finally, two basic transport properties, diffusion coefficient and viscosity of UCl_3-LiCl-KCl were predicted to a broader range than the previous reported data. These results help to understand the underlying mechanisms related to the pyrochemical processing for separation of trivalent uranium ions from other fission product ions in LiCl-KCl salts.

Journal of Nuclear Materials, 2018, **511**: 75

Th-U breeding performance in a Channel-type molten salt Fast reactor with different starting fuels

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Key words Channel-type Molten Salt Fast Reactor, Th-U breeding, Starting fuel scenario, Effective delayed neutron fraction

A Channel-type Molten Salt Fast Reactor (CMSFR) concept is studied to improve the Th-U breeding performance and to reduce the loss ratio of effective delayed neutron fraction (β_{eff}). In the CMSFR, fuel salt is filled in the active zone of the cylindrical core for fission heat generation, while fertile salt is contained in SiC tubes distributed regularly in the core for ^{233}U breeding and for transferring fission heat from the fuel salt to the secondary loop. To enhance the neutron capture reaction rate of ^{232}Th, both radial and axial Th fertile blankets are adopted. Only a small part of fuel salt in the reprocessing system is adopted for fission products removing and refueling, which reduces significantly the required initial loading of fuel salt compared with a conventional Molten Salt Reactor (MSR). Based on an in-house developed analysis code for reprocessing system of MSR, the Th-U breeding capability of CMSFR with different molten salt reprocessing rates (from 101 per day to 501 per day) is simulated for a 50-year operation. The simulated results show that the doubling time of ^{233}U with ^{233}U as starting fuel shortens significantly to about 37 years compared with the Molten Salt Fast Reactor (MSFR). Furthermore, the Th-U breeding capability with Pu, TRU and Low Enriched Uranium (LEU) as starting fuels is also analyzed. The simulated results indicate that the doubling time of ^{233}U with Pu and TRU as starting fuels is shortened to 22 years and 17 years, respectively. It indicates that both Pu and TRU can be employed for a transition approach to Th-U fuel cycle. The largest molar proportion of Pu with TRU as starting fuel during operation is about 7.1 mol% which is under the Pu solubility limit. Although the Th-^{233}U breeding with LEU as starting fuel can also be achieved at the end of life of operation, it needs external ^{233}U supply (about 0.6 tons) during the first 20 years operation. Both Temperature Reactivity feedback Coefficient (TRC) and β_{eff} for all the starting scenarios are also investigated. The TRC for all the starting scenarios is always negative enough during 50-year operation. The total loss ratio of β_{eff} with ^{233}U, LEU and Pu/TRU as starting fuels is only 13.76%, 13.47% and 13.56%, respectively, which is much smaller than that of the MSFR. Considering the limitation of reactor period T > 15s, the largest introduced reactivity for ^{233}U, LEU or Pu/TRU as starting fuel shall not be greater than 110 pcm, 202 pcm and 103 pcm, respectively.

Annals of Nuclear Energy, 2018, **122**: 91

The packing factor of the pebble bed in molten salt reactor

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Zhang Jie Mei Mudan Cai Xiangzhou

Key words Molten salt, Pebble bed reactor, Packing factor

Many concepts of molten salt cooled pebble bed reactor have been developed in recent decades. The packing factor (PF) of the pebble bed in the molten salt reactor should be investigated because it is of great importance for reactor design. Model experiments based on the solid fuel thorium-based molten salt reactor (TMSR-SF) were performed. Experimental results show that the PF of the pebble bed in TMSR-SF (D=21d, H=18d, d is pebble diameter) is about 0.57±0.02. The pebble bed in liquid environment is looser than that in dry condition. The PF increases with the diameter of the reactor core and the height of the pebble bed. The geometry of the lower cone reflector may induce large variety of packing factor if the angle of reflector is smaller than the angle of repose of the pebble bed. The loading rate and flow velocity in TMSR-SF are considered to be of little influence on PF. Results from the experiments will be of reference value for the design of reactors.

Annals of Nuclear Energy, 2018, **122**: 118

Preliminary study on TRUs utilization in a small modular Th-based molten salt reactor (smTMSR)

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Zou Yang Chen Jingen

Key words Small modular reactors, Molten salt reactors, Thorium fuel cycle, TRUs

Small modular reactors (SMRs) can provide an energy option with low carbon emission, enhanced safety conviction, convenient construction and operation. Meanwhile, molten salt reactors (MSRs) have been recognized as one of the reference reactors of the Generation IV International Forum (GIF) with the unique potential (inherent safety, no fuel fabrication, online fuel reprocessing, etc). Combining advantages of SMRs and MSRs, the small modular Th-based molten salt reactor (smTMSR) has excellent performances such as inherent safety, economics, sustainability, and proliferation resistance. Moreover, thorium is still an attractive fuel in a smTMSR with characteristics of online refueling and reprocessing. In this paper, we attempt to study the capability of the transition to thorium fuel cycle in a thermal smTMSR by analyzing the neutronic characteristics using TRUs as starting fuel. Optimizations are conducted to produce the required

amount of ^{233}U for starting a new smTMSR based on various fuel fractions in thermal energy region. It is concluded that the ^{233}U production is superior with higher fuel fraction in the core, which indicates that a thermal smTMSR with a proper fuel fraction can achieve the transition to thorium fuel cycle. The HM and Pu mole proportions which may have a negative influence on the molten salt stability are analyzed. Moreover, the temperature feedback coefficient as a key safety parameter is also discussed. With a suitable fuel fraction in thermal region, the smTMSR can well satisfy the restrictions of HM and Pu mole proportions and safety demands.

Nuclear Engineering and Design, 2018, **339**: 75

Studies of particle size distribution of Non-Exchangeable Organically Bound Tritium activities in the soil around Qinshan Nuclear Power Plant

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Qin Lai-lai Deng Ke Ma Zhao-wei Yang Guo
Liu Jia-yu Liu Wei

Key words Non-exchangeable organically bound tritium, Soil particle size, Vertical profile, Spatial distribution

The NE-OBT (Non-Exchangeable Organically Bound Tritium) in the soil plays a significant role in tritium migration and transformation. In order to further understand the NE-OBT activity in the soil, the particle size, vertical profile and spatial distribution of the NE-OBT activities in the soil were determined around the Qinshan Nuclear Power Plant (NPP) in China. The experimental results indicated that the NE-OBT preferred to concentrate in the soil particle sizes of 53-250μm within the soil depth of 5cm-25cm. The NE-OBT activity showed significantly vertical variations, however, its largest activity did not appear at the surface soil (0-5 cm). Meanwhile, the NE-OBT had a significant spatial distribution, its activity decreased with the increasing distance from the NPP, especially from the HWRs. In this study, the NE-OBT activities have no significant relationship to the organic matter content in the soil. But the vertical profile distribution of the NE-OBT activity has a strong correlation with the NE-OBT/HTO ratio in the soil, which reflect the capability of living organisms converting HTO into NE-OBT. According to these analyses, we supposed that the NE-OBT in the soil may be derived from the microbial transformation of HTO.

Journal of Environmental Radioactivity, 2018, **192**: 362

Uniform Pt quantum dots-decorated porous g-C_3N_4 nanosheets for efficient separation of electron-hole and enhanced solar-driven photocatalytic performance

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Key words g-C_3N_4, Pt quantum dot, Porous structure, Solar-driven photocatalysis

Uniform Pt quantum dots-decorated porous g-C_3N_4 nanosheets (Pt/CN) are fabricated by a facile impregnation-ultrasonic-calcination method, using melamine as precursor. The as-prepared samples are evidently investigated by X-ray diffraction, UV-vis diffuse reflection spectra, N_2 adsorption, transmission electron microscope, surface photovoltage spectroscopy and photoluminescence. The deposited Pt quantum dots with particle size of ~5nm are decorated on the surface of porous g-C_3N_4 nanosheets uniformly. The Pt/CN nanosheets show conspicuous solar-driven photocatalytic activity for splitting water to produce H_2. The solar-driven photocatalytic hydrogen production rate of Pt/CN is up to similar to 107 μmol $h^{-1}g^{-1}$, which is about 5 times higher than that of pristine g-C_3N_4. The enhancement can be attributed to the porous structure offering adequate surface active sites and the efficient decoration of uniform Pt quantum dots on g-C_3N_4 nanosheets facilitating the separation of photogenerated electron-hole pairs, which is confirmed by surface photovoltage spectroscopy and photoluminescence. The strategy for fabricating Pt quantum dots-decorated g-C_3N_4 nanosheets offers new insights for constructing other high-performance quantum dot-semiconductor photocatalytic materials.

Journal of Colloid and Interface Science, 2018, **531**: 119

Unexpectedly High Salt Accumulation inside Carbon Nanotubes Soaked in Dilute Salt Solutions

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Li Deyuan Fang Gang Liu Renduo
Yan Long Fang Haiping

Key words Fast Water Transport, Molecular-Dynamics, Cation, Ion, Membranes, Liquid, Energy, Phase, Flow, Selectivity

We experimentally demonstrate the formation of salt aggregations with unexpectedly high concentration inside multiwalled carbon nanotubes (CNTs) soaked only in dilute salt solution sand

even in solutions containing only traces of salts. This finding suggests the blocking of fluid across CNTs by the salt aggregations when CNTs are soaked in a dilute salt solution with the concentration of seawater or even lower, which may open new avenues for the development of novel CNT-based desalination techniques. The high salt accumulation of CNTs also provides a new CNT-based strategy for the collection or extraction of noble metal salts in solutions containing traces of noble metal salts. Theoretical analyses reveal that this high salt accumulation inside CNTs can be mainly attributed to the strong hydrated cation-pi interactions of hydrated cations and pi electrons in the aromatic rings of CNTs.

Physical Review Letters, 2018, **121**(22): 226102

Controlling crystal polymorphism of isotactic poly(1-butene) by incorporating long chain branches

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Key words Crystallization Behavior, Phase-Transformation, Mechanical-Properties, Form-III, Transition, Polypropylene, Morphology, Poly-1-Butene, Copolymers, Kinetics

Isotactic poly(1-butene) (iPB-1) is a high performance plastic with outstanding properties, such as flexibility, superior creep, environmental stress cracking and abrasive resistance. However, it exhibits a complex crystal polymorphism and polymorphic transformation behavior, which has limited its commercial development. In this paper, the incorporation of long chain branches (LCBs) causes coil contraction in the melt, which favors the direct melt-crystallization of form III that was generally crystallized from solutions and made of unconventional highly twined lamellae. Consequently, low-to-moderately branched iPB-1 samples as-crystallize from the melt into mixtures of form II and form III by compression-molding and fast cooling of the melt to room temperature, and the fraction of crystals of form III (f_{III}) increases with increasing concentration of LCBs, whereas highly branched samples can as-crystallize into pure form III with uniform crystal size distribution. The corresponding thermomechanical properties can be modified by controlling f_{III}.

Soft Matter, 2018, **14**(44): 8872

Better scCO$_2$ Foaming of Polypropylene via Earlier Crystallization with the Addition of Composite Nucleating Agent

Yang Chenguang Xing Zhe Wang Mouhua Zhao Quan
Wang Minglei Zhang Maojiang Wu Guozhong

Key words Pressure-Induced-Flow, Facile Preparation, Particle-Size, Behavior, Density, Nanocomposites, Strength, Morphology, Nanofibers, Radiation

A method of earlier crystallization was applied to prepare high-performance polypropylene (PP) foam using supercritical CO_2 (scCO$_2$) with the addition of a composite nucleating agent (CNA). Increased crystallization point and decreased crystal size of PP were obtained in the presence of CNA. Earlier crystallization induced cell formation in an early stage of foaming, this, combined with enhanced heterogeneous nucleation caused by microcrystal growth, resulted in well-defined cellular structure. The cell size of PP/CNA foam decreased from 87 to 30 μm, and the cell density was more than 20 times that of the neat PP foam. Moreover, the first compression stress of PP/CNA foam increased from 125 to 180 kPa compared to neat PP foam. We proposed that earlier crystallization promoted the emergence of a large number of microcrystals at the beginning of the foaming process, which effectively suppressed cell growth and prevented cell rupture and collapse.

Industrial & Engineering Chemistry Research, 2018, **57**(46): 15916

Reexamining the isospin-relaxation time in intermediate-energy heavy-ion collisions

Wang Hansheng Xu Jun Li Baoan Shen Wenqing

Key words Effective-Mass, Mean-Field, Dynamics, Constraints, Dependence, Asymmetry, Physics, Nuclei, Matter

Isospin-relaxation times characterizing isospin transport processes between the projectile and the target with different N/Z ratios and that between the neck and the spectator with different isospin asymmetries and densities in intermediate-energy heavy-ion collisions are studied within an isospin-dependent Boltzmann-Uehling-Uhlenbeck transport model using the lattice Hamiltonian approach. The respective roles and timescales of the isospin diffusion and drift as the major mechanisms of isospin transport in intermediate-energy heavy-ion collisions are discussed. Effects

of nuclear symmetry energy and neutron-proton effective mass splitting on the isospin relaxation times are examined.

Physical Review C, 2018, **98**(5): 054608

Synchrotron Big Data Science

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Key words Big Data, Computation, Large Facility, Machine Learning, Synchrotron

The rapid development of synchrotrons has massively increased the speed at which experiments can be performed, while new techniques have increased the amount of raw data collected during each experiment. While this has created enormous new opportunities, it has also created tremendous challenges for national facilities and users. With the huge increase in data volume, the manual analysis of data is no longer possible. As a result, only a fraction of the data collected during the time- and money-expensive synchrotron beam-time is analyzed and used to deliver new science. Additionally, the lack of an appropriate data analysis environment limits the realization of experiments that generate a large amount of data in a very short period of time. The current lack of automated data analysis pipelines prevents the fine-tuning of beam-time experiments, further reducing their potential usage. These effects, collectively known as the "data deluge," affect synchrotrons in several different ways including fast data collection, available local storage, data management systems, and curation of the data. This review highlights the Big Data strategies adopted nowadays at synchrotrons, documenting this novel and promising hybridization between science and technology, which promise a dramatic increase in the number of scientific discoveries.

Small, 2018, **14**(46): 1802291

Effects of nanobubbles on peptide self-assembly

Wang Yujiao Shen Zhiwei Guo Zhen Hu Jun Zhang Yi

Key words Air-Water-Interface, Neurodegenerative Diseases, Protein Aggregation, Amyloid Fibrils, Mechanism, Surfaces, Biology, Fibers, Growth

It is believed that the aggregation of amyloid proteins or peptides is promoted by the presence of an air-water interface, and substantial evidence suggests that the characteristics of the air-water interface play critical roles in foam-induced protein aggregation during foam fractionation. However, the effects of the air-water interface on the self-assembly of amyloid-like peptides have

not yet been elucidated clearly at the nanometer scale. In this work, air nanobubbles produced in water solution were employed for studying interfacial effects on the self-assembly of a model amyloid peptide termed P11. An atomic force microscopy study showed that the air nanobubbles induced the formation of peptide fibrils with a 9-13 nm helix structure in the P11 solution. Thioflavin T fluorescence and circular dichroism spectroscopic analysis indicated that the nanobubbles induced the change of the peptide conformation to a beta-sheet structure. Based on these observations, we have proposed a mechanism to explain how the nanobubbles affect the self-assembly of the P11 peptide at the nanometer scale. Since air nanobubbles are present in water solutions in addition to an air-water interface in normal experiments in vitro, our results indicate that nanobubbles must be taken into account to achieve a complete understanding of protein aggregation events.

Nanoscale, 2018, **10**(42): 20007

Anionic uranyl oxyfluorides as a bifunctional platform for highly selective ion-exchange and photocatalytic degradation of organic dyes

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Zhou Jing Guo Xiaojing Bao Hongliang
Huang Yuying Wang Jianqiang

Key words Variable Dimensionality, Cationic Dyes, Crystal Transformation, Hydrothermal Synthesis, Layered Material, High-Capacity, Uranium, Framework, Topology, System

Uranium is unique owing not only to its intriguing physiochemical properties, but also to the diverse coordination chemistry that uranyl adopts and bonding that enables rich and unpredictable topologies of uranium-bearing materials. Six anionic uranium oxyfluorides with various dimensionalities, including a 3D framework (MeUF), four 2D lamellar structures (EtUF-1, PrUF, BuUF-1, and BuUF-2), and a 1D chained topology (EtUF-2), have been rationally constructed by employing tetra-alkyl ammonium ions as structure-directing agents. By combining the tunable interlayer distance of the lamellar structures with the photooxygenation properties of uranyl ions, a bifunctional platform for highly selective ion-exchange and photocatalytic degradation over organic dyes has been developed. Specifically, BuUF-2 can efficiently capture 94.5% methylene blue (MB^+) within 24 h from solution with remarkable selectivity related to both the size and the charge of organic dyes. Such size- and charge-dependent selectivity toward organic dyes has been documented for MOFs, but is rare for 2D lamellar materials. Furthermore, the removal of MB+ can

be largely accelerated under UV radiation (*e.g.* 84.7% for BuUF-2 within 1h) due to the photocatalytic activities of EtUF-1, EtUF-2, PrUF, and BuUF-2.

Dalton Transactions, 2018, **47**(42)

Electrochemical and Spectroscopic Study of Homo- and Hetero-Dimetallic Phthalocyanines as Catalysts for the Oxygen Reduction Reaction in Acidic Media

Wang Xiaojiang Liu Yang Wang Ying Ren Rong
Chen Hengquan Jiang Zheng He Qinggang

Key words Density Functional Calculations, Electrochemistry, Heterodimetallic Phthalocyanines, Oxygen Reduction Reaction, X-Ray Absorption Spectroscopy

Metallophthalocyanines (MPc, M=Fe or Co) have been investigated extensively as a typical type of transition metal macrocyclic catalysts for the oxygen reduction reaction (ORR). However, the understanding about ORR catalyzed by binuclear even heterodimetallic phthalocyanines in acidic condition is still not sufficient. Herein we synthesized two homodimetallicphthalocyanine (FePc-PcFe and CoPc-PcCo) and a heterodimetallic phthalocyanine (FePc-PcCo). The electrocatalytic activity of as-synthesized compounds were characterized by cyclic voltammetry (CV) and rotating disk electrode (RDE). Generally, the binuclear metallophthalocyanines show higher activity than their monomeric analogues including FePc and CoPc. Also, the Fe compounds exhibit better catalytic performance than the Co phthalocyanines. However, interestingly the heterodimetallic phthalocyanine FePc-PcCo shows similar half-wave potential and ORR activity with FePc-PcFe, rather than CoPc-PcCo. This may be explained by XPS and XAS, which reveal a similar square-planar structure existed in FePc-PcCo and FePc-PcFe and a non-planar structure in CoPc-PcCo. Furthermore, the increasing of the ORR activity among those five catalysts is well in agreement with the descending LUMO energies in DFT calculations. A lower LUMO energy indicates a favorable adsorption of O_2, which in turn affects the ORR performance.

ChemElectroChem, 2018, **5**(22): 3478

Design of a 7-MeV APF DTL with robust considerations

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Li Deming Zhao Minghua Zhao Zhentang

Key words Alternating phase focused, Drift tube linac, Nonlinear correlated stacking optimization method, Error analysis, Robust consideration

A design principle with robust considerations has been applied to design a new alternating phase focused (APF) drift tube linear accelerator (linac) for particle beam therapy. By assuming a sinusoidal synchronous phase formula and a linearly increasing electrode voltage scheme, the structure of the APF linac is automatically optimized with a cost function including robustness using the nonlinear correlated stacking optimization method (CSM). The design procedure includes the radio frequency quadrupole (RFQ) to drift tube linac (DTL) matching, and an end-to-end simulation of the APF acceleration beam dynamics. Moreover, the stability of the solution obtained is analyzed with respect to various independent errors as well as a number of joint errors. The designed APF DTL linac together with an already established RFQ is planned to replace the existing Alvarez-type permanent magnet focused DTL linac aiming at easier manufacturing and cost reduction.

Nuclear Instruments & Methods in Physics Research Section A-Accelerators Spectrometers Detectors and Associated Equipment, 2018, **908**: 49

The high level application architecture of the control system for SHINE

Lv Huihui Leng Yongbin Yan Yingbing Wang Heyun

Key words SHINE, Control system, EPICS, High level application

Shanghai HIgh repetition rate XFEL aNd Extreme light facility(SHINE) is a quasi-continuous wave hard X-ray free electron laser facility, which is currently under construction. Such kind of accelerators typically comprise more than hundreds of devices, and control systems are required to manage all the devices in a uniform manner. The control system of SHINE will be based on Experimental Physics and Industrial Control System (EPICS) with a dedicated high-speed data channel and an integrated information system to fulfill the requirement of high repetition rate. Then the high level control applications are designed to hold the information base as well as a set of cooperating services for data access. Modular design is utilized to simplify development and deployment. Modules of parameter and lattice/model are introduced as examples.

Nuclear Instruments & Methods in Physics Research Section A-Accelerators Spectrometers Detectors and Associated Equipment, 2018, **908**: 167

Investigating different Λ and $\bar{\Lambda}$ over-bar polarizations in relativistic heavy-ion collisions

Han Zhangzhu Xu Jun

Key words Nuclear Collisions

Based on the chiral kinetic equations of motion, spin polarizations of various quarks, due to the magnetic field induced by spectator protons as well as the quark-antiquark vector interaction, are studied within a partonic transport approach. Although the magnetic field in QGP enhances the splitting of the spin polarizations of partons compared to the results under the magnetic field in vacuum, the spin polarizations of s and $\bar{s}$ quarks are also sensitive to the quark-antiquark vector interaction, challenging that the different Λ and $\bar{\Lambda}$ spin polarization is a good measure of the magnetic field in relativistic heavyion collisions. It is also found that there is no way to obtain the large splitting of the spin polarization between Λ and $\bar{\Lambda}$ at $\sqrt{s_{NN}}$ = 7.7 GeV with partonic dynamics.

Physics Letters B, 2018, **786**: 255

Nanoplatelet modulation in 2D/3D perovskite targeting efficient light-emitting diodes

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Han Yujie Song Tao Zhang Qiao Gao Xingyu Sun Baoquan

Key words Halide Perovskite, Hybrid Perovskite, Energy, Emitters, Voltage, Cspbx3, Cells, Films

Light-emitting diodes (LEDs) based on two-dimensional (2D) perovskite nanoplatelets exhibit high electroluminescence (EL) efficiency because of the quantum confinement effect, which increases electron-hole recombination to promote radiative emission. It is well-known that a 2D nanoplatelet structure (〈n〉 = 1) is detrimental for luminescence efficiency due to possible thermal quenching of excitons at room temperature. Here, a simple strategy is developed to suppress growth of NMA_2PbBr_4(〈n〉 = 1) nanoplatelets by carefully tuning the precursor ratio of cesium bromide (CsBr), formamidinium bromide (FABr) and 1-naphthylmethylammonium bromide (NMABr). The sub-domain size of the perovskite crystal decreases as the long-chain ligand NMABr ratio increases, leading to enhanced photoluminescence quantum yields (PLQY) due to size confinement effect when the NMABr ratio is below 60%. Unfortunately, the NMA_2PbBr_4 component in 2D/3D perovskites also grows with increasing NMABr ratio, which results in poor EL efficiency. FABr

incorporation can provide additional control over suppression of NMA_2PbBr_4 growth in 2D/3D perovskites. A compact and uniform perovskite film with reduced NMA_2PbBr_4 content achieves PLQY of approximate to 61%. Benefiting from these features, a green perovskite LED yields current efficiency of 46.8 cd A^{-1} with an external quantum efficiency of 14.9%. This study paves a new way to modulate the crystal structure in perovskites via a simple and effective method for high-performance LEDs.

Nanoscale, 2018, **10**(41): 19322

Graphene oxide-silver nanocomposites modulate biofilm formation and extracellular polymeric substance (EPS) production

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Lin Chenglie Shi Jiye Fan Chunhai Lv Min Wang Lihua

Key words Antibacterial Activity, Nanoparticle, Bacteria, Mechanisms, Resistance, Nanomaterials, Composites, Nanosheets, Evolution, Toxicity

Biofilms with positive and negative actions ubiquitously affect medical infections, environmental remediation and industrial processes. However, it remains challenging to control the growth of harmful biofilms as well as to exploit the use of beneficial biofilms. Here we investigated the effect of an antibacterial graphene oxide-silver nanoparticles (GO-AgNPs) composite on Pseudomonas aeruginosa biofilm formation. We found that GO-AgNPs prevented biofilm formation in a dose-dependent manner, with a threshold of 15 μg mL^{-1}. Interestingly, the bacterial biomass significantly decreased, but extracellular polymeric substance (EPS) production remarkably increased in mature biofilms treated with GO-AgNPs of an appropriate concentration, suggesting that GO-AgNPs effectively modulate biofilm development and structure. Moreover, we established that GO-AgNPs caused bacterial death via both physical damage and oxidative stress, showing the synergic action of GO and AgNPs. These findings facilitate the use of graphene-based nanocomposites for greener antibiotic applications.

Nanoscale, 2018, **10**(41): 19603

The effects of aerogen-bonding on the geometries and spectral properties of several small molecular clusters containing XeO_3

Miao Junjian Xiong Zhenhai Gao Yi

Key words Aerogen Bonding, Molecular Cluster, IR Spectrum, Raman Spectrum, Density Functional Theory, Noncovalent Interaction

Aerogen bonding, as a specific noncovalent interaction, has attracted wide attention recently. A number of theoretical studies have proposed this effect based on the analysis of electronic structures of aerogen-containing systems though, the spectral characteristics have not been identified, which becomes the obstacle for the experimental confirmation of this interaction. In this paper, we employed the density functional theory to explore the energetic and geometric properties, infrared, Raman spectra of five small molecular clusters $XeO_3 \cdot H_2O$, $XeO_3 \cdot NH_3$, XeO_3 dimer, XeO_3 trimer, and $XeO_3 \cdot 2H_2O$. Our results show the binding energies of the most favorable conformations for the dimers are larger than -10.00 kcal mol^{-1} and those for trimers are larger than -20.00 kcal mol^{-1}, which indicates the strong aerogen bonding is favorable for the stabilities of these clusters. More importantly, some new IR and Raman vibrations at fingerprint region (< 1000 cm^{-1}) are identified, which corresponds to the formation of aerogen bonds. This study provides a viable way for the experimentalists to characterize the aerogen bonding in future. ·

Journal of Physics-Condensed Matter, 2018, **30**(44): 444001

Application of Electronic Counting Rules for Ligand-Protected Gold Nanoclusters

Xu Wen Wu Zeng Xiao Cheng Gao Yi

Key words Structural-Characterization, Structure Prediction, Crystal-Structure, Clusters, Metal, Nanoparticles, Evolution, Size, Nanomolecules

Understanding special stability of numerous ligand-protected gold nanoclusters has always been an active area of research. In the past few decades, several theoretical models, including the polyhedral skeletal electron pair theory (PSEPT), superatom complex (SAC), and superatom network (SAN), among others, have been developed for better understanding the stabilities and structures of selected ligand-protected gold nanoclusters. This Account overviews the recently proposed grand unified model (GUM) to offer some new insights into the structures and growth mechanism of nearly all crystallized and predicted ligand-protected gold nanoclusters.

The main conceptual advancement of the GUM is identification of the duet and octet rules on the basis of the "big data" of 70+ reported ligand-protected gold nanoclusters. According to the two empirical rules, the cores of the gold nanoclusters can be regarded as being composed of two kinds of elementary blocks (namely, triangle Au_3 and tetrahedron Au_4), each having 2e closed-shell valence electrons (referred as $Au_3(2e)$ and $Au_4(2e)$), as well as the secondary block (icosahedron Au_{13}) with Se closed-shell valence electrons (referred as Au_{13} (8e)). The two elementary blocks ($Au_3(2e)$ and $Au_4(2e)$) and the secondary block (Au_{13} (8e)), from electron counting point of view, can be regarded as an analogy of the highly stable noble-gas atoms of He and Ne, respectively. In each elementary block, the Au atoms exhibit three different valence-electron states (i.e., 1e, 0.5e, and 0e), depending on the type of ligands bonded with these Au atoms. Such three valence-electron states are coined as three "flavors" of gold (namely, bottom, middle, and top "flavor"), a term borrowed from the quark model in the particle physics. Upon application of the duet and octet rules with accounting the three valence states of gold atoms, the $Au_3(2e)$, $Au_4(2e)$, and $Au_{13}(8e)$ blocks can exhibit 10 (denoted as Δ_1-Δ_{10}), 15 (denoted as T_1-T_{15}), and 91 (denoted as I_1-I_{91}) variants of valence states, respectively. When packing these blocks (with distinct electronic states) together, it forms the gold core of ligand-protected gold nanocluster. As such, the special stabilities of the ligand-protected gold nanoclusters are explained based on the local stability of each block. With GUM, rich and complex structures of ligand-protected gold nanoclusters have been analyzed through structure anatomy. Moreover, the growth of these clusters can be simply viewed as sequential addition of the blocks, rather than as addition of the gold atoms. Another useful application of the GUM is to analyze the structural isomerism. The three types of isomerism for the gold nanoclusters, i.e., core, staple, and complex isomerism, can be considered as an analogy of chain, point, and functional isomerism (known in organic chemistry), respectively. GUM can be applied to predict new clusters, thereby guiding experimental synthesis. Indeed, a number of ligand-protected gold nanoclusters with high stabilities were rationally designed based on the GUM.

Accounts of Chemical Research, 2018, **51**(11): 2739

Formation and stability of ultrasonic generated bulk nanobubbles

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Key words　Bulk Nanobubble, Ultrasonic, Nanoparticle Tracking Analysis, Dissolved Oxygen

Although various and unique properties of bulk nanobubbles have drawn researchers' attention over the last few years, their formation and stabilization mechanism has remained unsolved. In this

paper, we use ultrasonic methods to produce bulk nanobubbles in the pure water and give a comprehensive study on the bulk nanobubbles properties and generation. The ultrasonic wave gives rise to constant oscillation in water where positive and negative pressure appears alternately. With the induced cavitation and presence of dissolved air, the bulk nanobubbles formed. "Nanosight" (which is a special instrument that combines dynamic light scattering with nanoparticle tracking analysis) was used to analyze the track and concentration of nanobubbles. Our results show that in our experiment, sufficient bulk nanobubbles were generated and we have proven they are not contaminations. We also found nanobubbles in the ultrasonic water change in both size and concentration with ultrasonic time.

Chinese Physics B, 2018, **27**(11)

Neutronics modeling and analysis of the TMSR-SF1 fuel lattice and full core with explicit fuel particle distribution and random pebble loadings

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Dave Akshay J. Zou Yang Hu Lin-wen

Key words TMSR-SF1, Monte Carlo, Flibe, Particle distribution, Pebble loading

The first Solid Fueled Thorium Molten Salt Reactor (TMSR-SF1), a Fluoride-salt-cooled High Temperature Reactor (FHR) designed by the TMSR group of Chinese Academy of Science (CAS), is expected to be constructed in the near years. The combination of TRistructural-ISOtropic (TRISO) coated-fuel particles, pebble bed core, and FLIBE coolant leads to various neutronics challenges, such as the double heterogeneity, distribution of TRISO particles, high density packed pebble bed, neutronics characteristics of FLIBE salt, and *etc*. For the purpose of evaluating candidate neutronics codes, benchmark study will be conducted for the infinite fuel pebble lattice with explicitly described fuel particle distribution. For investigating key physics phenomena of the randomly packed pebble bed core, two coordinate generation methods will be explored in this study: Discrete Element Method (DEM) that accounts for inter-particle forces and a mathematical model (MM) that fills arbitrary do- mains through simple geometric rules on the addition of particles. While the former generates packing distributions closer to real-world scenarios, the latter is more computationally effective. The pebble loading effect on eigenvalues and fission power distribution will be studied. Emphasis is placed on the FLIBE salt density reactivity effect - the most unique feature of the FHR comparing to the conventional High Temperature Gas-cooled Reactors (HTGRs). Neutron balance based reactivity decomposition method will be employed for describing the underlying physics.

Progress in Nuclear Energy, 2018, **109**: 171

The wave optical whole process design of the soft X-ray interference lithography beamline at SSRF

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Wang Liansheng Yang Shumin Zhao Jun Tai Renzhong

Key words Synchrotron Radiation, Soft X-Ray Interference Lithography Beamline, Spatial Coherence, Wave Optics, Mutual Optical Intensity

A new spatially coherent beamline has been designed and constructed at the Shanghai Synchrotron Radiation Facility. Here, the design of the beamline is introduced and the spatial coherence is analyzed throughout the whole process by wave optics. The simulation results show good spatial coherence at the endstation and have been proven by experiment results.

Journal of Synchrotron Radiation, 2018, **25**: 1869

Effect of SO_4^{2-} on the corrosion of 316L stainless steel in molten FLiNaK salt

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Angjian Jia Yanyan Xue Wandong Yu Guojun Zhou Xingtai

Key words Molten salt, FLiNaK, Corrosion, Sulphate, 316L stainless steel, MnS

The effect of SO_4^{2-} on the corrosion behavior of 316 L stainless steel (SS) in molten FLiNaK (LiF-NaF-KF: 46.5-11.5-42 mol.%) salt was studied. Results reveal that the SO_4^{2-} in the salt remarkably accelerates the corrosion of 316 L SS by promoting the dissolution of Cr, leading to increasing intergranular corrosion of the alloy. On the other hand, the results of structural characterization indicate that the SO_4^{2-} can react with Mn to form MnS at the grain boundaries of the alloy. The galvanic couple between MnS and steel matrix could further accelerate the intergranular corrosion of 316 L SS in molten fluoride salt environments.

Corrosion Science, 2018, **144**: 224

The effect of moisture on the desorption behavior of UF_6 from NaF adsorbent

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Wang Chenyang Zhang Linjuan Dou Qiang Li Qingnuan

Key words Fluoride volatility method, UF_6 purification, NaF adsorbent, orption-desorption, X-ray absorption fine structure spectroscopy

NaF is one of the most important sorption materials used in the UF_6 purification, the stability of the complex formed after NaF absorbed UF_6 was investigated by in situ Raman spectroscopy. The desorption behavior of UF_6 from NaF adsorbent was examined by FT-IR, which show that UF_6 did not desorb significantly from the NaF adsorbent until the temperature was above 200℃, and the maximum desorption rate was reached at approximately 330℃. Na_2UF_8 was hydrolyzed to form $UO_2F_2 \cdot nH_2O$ when it exposed to air containing moisture, there existed two desorption peaks for the air-exposed Na_2UF_8 complex in a fluorine atmosphere, one appeared at approximately 325℃, attributed to the decomposition of UF_6 from Na_2UF_8, and another was located at approximately 401℃, attributed to the conversion of UO2F2 to UF_6 by fluorine and the subsequent release of UF_6.

Journal of Radioanalytical and Nuclear Chemistry, 2018, **318**(2): 1325

Chemical and electrochemical studies on the solubility of UO_2 in molten FLINAK with ZrF_4 additive

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Key words Molten fluorides, UO_2 solubility, ZrF_4 additive, CV, SWV

The solubility of UO_2 in molten FLINAK with ZrF_4 additive was studied by using chemical and electro-chemical methods. The chemical results showed that the solubility of UO_2 was lower by 0.247 wt% in molten FLINAK. When more than 2.91 wt% of ZrF_4 was added into the FLINAK-UO_2 melts, the maximum solubility of UO_2 at 1.422 wt% can be achieved. Moreover, compared with the FLINAK- UO_2 melts, a new cathodic peak at approximately 0.21 V (*vs.* alkalis$^+$/alkalis) was detected in FLINAK-ZrF_4-UO_2 melts by using cyclic voltammetry (CV) and square wave voltammetry (SWV). This cathodic peak was attributed to the higher electroactive species $ZrOF_2$ confirmed by CV and potentiostatic electrolysis. Thus, it can be concluded that the dissolution of UO_2 is caused by the reaction of $UO_2 + ZrF_4 = UOF_2 + ZrOF_2$. The SWVs of FLINAK-$ZrF_4$-$UO_2$ system further showed that the concentration of ZrOF2 species in the bath gradually increased with the addition of ZrF_4, which further proves that the dissolution of UO_2 is facilitated by ZrF_4 additive.

Journal of Nuclear Materials, 2018, **510**: 256

Improving the ceramic yield of polycarbosilane by radiation cross-linking in the presence of multifunctional monomers

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Key words Ceramic Yield, Cross-Linking, Polycarbosilane, Radiation

An interesting method for radiation cross-linking polycarbosilane (PCS) at high efficiency and low cost was developed by adding multifunctional monomers (trimethylolpropane trimethacrylate (TMPTMA) or divinylbenzene (DVB)). The effect of multifunctional monomers on the radiation cross-linking and ceramic yield of PCS was investigated. The results revealed that the addition of a small amount of multifunctional monomer can substantially improve the ceramic yield and reduce the absorbed dose by promoting cross-linking. The ceramic yields of radiation cross-linked PCS/2%DVB (300 kGy) and PCS/2%TMPTMA (300 kGy) were 74 wt% and 78 wt%, respectively, while that of the radiation cross-linked PCS (300 kGy) was only 64 wt%. The presence of double bonds in multifunctional monomers stimulated the combination reactions of free radicals in PCS induced by-ray irradiation and subsequently enhanced the efficiency of cross-linking. Furthermore, it was found that the incorporation of a small amount of multifunctional monomer hardly affected the chemical composition and crystallization behavior of the final SiC ceramics.

International Journal of Applied Ceramic Technology, 2018, **15**(6): 1510

Review of fully coherent free-electron lasers

Feng Chao Deng Haixiao

Key words Free-electron laser, Fully coherent, Seeded FEL, FEL oscillator

Generation of intense, fully coherent radiation with wide spectral coverage has been a long-standing challenge for laser technologies. Several techniques have been developed in recent years to extend the spectral coverage in optical physics, but none of them hold the potential to produce X-ray laser pulses with very high-peak power. Urgent demands for intense X-ray light sources have prompted the development of free-electron lasers (FELs), which have been proved to be very useful tools in many scientific areas. In this paper, we give an overview of the basic principle of FELs, techniques for realizing fully coherent FELs, and the development of fully coherent FEL facilities in China.

Nuclear Science and Techniques, 2018, **29**(11)

The morphology and structure of crystals in Qing Dynasty purple-gold glaze excavated from the Forbidden City

Liu Zhen Jia Cui Li Li Li Xiaolong Ji Luoyuan Wang Lihua
Lei Yong Wei Xiangjun

Key words ε-Fe_2O_3, Crystal Structure, Morphology, Purple-Gold Glaze, The Forbidden City

Ancient Chinese purple-gold glaze (zijinyou) is popular for its beautiful figuration, unique allure and fine craftsmanship. To understand the crystalline nature in the purple-gold glaze, the morphology and structure of crystals precipitated in the glaze layer of purple-gold glaze porcelain fired during the Qing Dynasty were characterized by a variety of methods combining X-ray and electron-based techniques. A large quantity of single-phase twinning ε-Fe_2O_3 crystals with lengths of 1-3μm, widths of less than 1μm, and thickness of approximately 150nm are found dispersed across the glaze surface to a depth of approximately tens of micrometers. These crystals show stratification across the cross-section of the purple glaze consisting of 4 sublayers according to the crystal size. The formation of ε-Fe_2O_3 crystals primarily contributed to the reddish-brown tones of the purple-gold glaze. The presence of anorthite, a strong reducing atmosphere during the firing process and the vitreous nature of the glaze influenced the growth of ε- Fe_2O_3 crystals. These results suggest the controllability of single-phase ε-Fe_2O_3 crystals by identifying and understanding the underlying chemical processes in ancient Chinese crystalline glaze porcelain, and the findings will provide insights for modern material scientists in preparing ε-Fe_2O_3 crystals with large sizes and high purities.

Journal of the American Ceramic Society, 2018, **101**(11): 5229

DNA Nanostructure-Based Systems for Intelligent Delivery of Therapeutic Oligonucleotides

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Gu Hongzhou Fan Chunhai

Key words DNA nanostructures, Intelligent Delivery, Therapeutic Oligonucleotides

In the beginning of the 21st century, therapeutic oligonucleotides have shown great potential for the treatment of many life-threatening diseases. However, effective delivery of therapeutic oligonucleotides to the targeted location *in vivo* remains a major issue. As an emerging field, DNA

nanotechnology is applied in many aspects including bioimaging, biosensing, and drug delivery. With sequence programming and optimization, a series of DNA nanostructures can be precisely engineered with defined size, shape, surface chemistry, and function. Simply with hybridization, therapeutic oligonucleotides including unmethylated cytosine-phosphate-guanine dinucleotide oligos, small interfering RNA (siRNA) or antisense RNA, single guide RNA of the regularly interspaced short palindromic repeat-Cas9 system, and aptamers, are successfully loaded on DNA nanostructures for delivery. In this progress report, the development history of DNA nanotechnology is first introduced, and then the mechanisms and means for cellular uptake of DNA nanostructures are discussed. Next, current approaches to deliver therapeutic oligonucleotides with DNA nanovehicles are summarized. In the end, the challenges and opportunities for DNA nanostructure-based systems for the delivery of therapeutic oligonucleotides are discussed.

Advanced Healthcare Materials, 2018, **7**(20): 1701153

Combustion Fabrication of Nanoporous Graphene for Ionic Separation Membranes

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Ali Mohammad Chand Zhang Haijuan Chen Jia Hu Peizhuo
Fan Chunhai Qiu Hongdeng

Key words Combustion Fabrication, Ionic Separation, Membrane Separation, Nanoporous Graphene

Porous graphene membranes hold great promise for high-selectivity separation. Moreover, their practical application is limited by the lack of a simple and efficient method for the synthesis of porous graphene. Here, a rapid and scalable method is developed for the synthesis of porous graphene via partial combustion of graphene oxide imperfectly covered by hydrotalcite. This method is not only less energy- and time-intensive than existing ones, but also allows precise control of pore size. Remarkably, the resulting membrane of porous graphene exhibits high selectivity for K^+ and Na^+ (α= 3.84) separation. Hence, this facile route for preparing membranes of porous graphene oxide might direct application membranes in environmental, energy, desalination, and biomedical fields.

Advanced Functional Materials, 2018, **28**(43): 1805026

DNA Nanostructure-Programmed Like-Charge Attraction at the Cell-Membrane Interface

Ding Hongming Li Jiang Chen Nan Hu Xingjie Yang Xiafeng
Guo Linjie Li Qian Zuo Xiaolei Wang Lihua Ma Yuqiang
Fan Chunhai

Key words Mammalian-Cells, Drug-Delivery, Cancer-Cells, Tumor-Cells, Ph Changes, Nanoparticles, Origami, Nanocarriers, Molecules, Pathways

Cell entry of anionic nano-objects has been observed in various types of viruses and self-assembled DNA nanostructures. Nevertheless, the physical mechanism underlying the internalization of these anionic particles across the negatively charged cell membrane remains poorly understood. Here, we report the use of virus-mimicking designer DNA nanostructures with near-atomic resolution to program "like-charge attraction" at the interface of cytoplasmic membranes. Single-particle tracking shows that cellular internalization of tetrahedral DNA nanostructures (TDNs) depends primarily on the lipid-raft-mediated pathway, where caveolin plays a key role in providing the short-range attraction at the membrane interface. Both simulation and experimental data establish that TDNs approach the membrane primarily with their corners to minimize electrostatic repulsion, and that they induce uneven charge redistribution in the membrane under the short-distance confinement by caveolin. We expect that the nanoscale like-charge attraction mechanism provides new clues for viral entry and general rules for rational design of anionic carriers for therapeutics.

ACS Central Science, 2018, **4**(10): 1344

Effect of confinement on water rotation *via* quantum tunnelling

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Gao Yi Wang Zhigang

Key words Hydrogen-Bond, Carbon Nanotubes, Dimer

Water exhibits different behaviors in confined space compared to free space, which is critical for desalination, biosensing, and many potential applications. Recent studies indicated that quantum tunnelling plays an important role in the orientation of H_2O molecules and the H-bond network of water clusters, but whether this effect is important in confined space remains elusive. Here, we

studied the quantum tunnelling effect of water dimers in carbon nanotubes with different sizes by first-principles calculations. Our results show that though this effect may be negligible at room temperature, it becomes dominant at low temperatures up to similar to 100 Kelvin. In particular, with the injection of a small amount of energy to excite a specific vibrational mode, the tunnelling rotation effect can be significantly enhanced, which provides a new strategy to tune the H-bond network of confined water.

Nanoscale, 2018, **10**(39): 18622

Antinuclei in heavy-ion collisions

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Tang Aihong Xu Zhangbu

Key words Heavy ions, Antinuclei, Antihypernuclei, Hypernuclei, Muonic antiatoms, CPT symmetry, Baryogenesis, Coalescence

We review progress in the study of antinuclei, starting from Dirac's equation and the discovery of the positron in cosmic-ray events. The development of proton accelerators led to the discovery of antiprotons, followed by the first antideuterons, demonstrating that antinucleons bind into antinuclei. With the development of heavy-ion programs at the Brookhaven AGS and CERN SPS, it was demonstrated that central collisions of heavy nuclei offer a fertile ground for research and discoveries in the area of antinuclei. In this review, we emphasize recent observations at Brookhaven's Relativistic Heavy Ion Collider and at CERN's Large Hadron Collider, namely, the antihypertriton and the antihelium-4, as well as measurements of the mass difference between light nuclei and antinuclei, and the interaction between antiprotons. Physics implications of the new observations and different production mechanisms are discussed. We also consider implications for related fields, such as hypernuclear physics and space-based cosmic-ray experiments.

Physics Reports-Review Section of Physics Letters, 2018, **760**: 1

Nanodiamond autophagy inhibitor allosterically improves the arsenical-based therapy of solid tumors

Cui Zhifen Zhang Yu Xia Kai Yan Qinglong Kong Huating
Zhang Jichao Zuo Xiaolei Shi Jiye Wang Lihua Zhu Ying
Fan Chunhai

Key words Acute Promyelocytic Leukemia, Cell-Death, Cancer, Trioxide, Apoptosis, Hydroxychloroquine, Chloroquine, Carcinoma, Drugs, Model

Arsenic trioxide (ATO) is a successful chemotherapeutic drug for blood cancers via selective induction of apoptosis, however its efficacy in solid tumors is limited. Here we repurpose nanodiamonds (NDs) as a safe and potent autophagic inhibitor to allosterically improve the therapeutic efficacy of ATO-based treatment in solid tumors. We find that NDs and ATO are physically separate and functionally target different cellular pathways (autophagy vs. apoptosis), whereas their metabolic coupling in human liver carcinoma cells remarkably enhances programmed cell death. Combination therapy in liver tumor mice model results in similar to 91% carcinoma decrease as compared with similar to 28% without NDs. Treated mice show 100% survival rate in 150 days with greatly reduced advanced liver carcinoma-associated symptoms, and similar to 80% of post-therapy mice survive for over 20 weeks. Our work presents a novel strategy to harness the power of nanoparticles to broaden the scope of ATO-based therapy and more generally to fight solid tumors.

Nature Communications, 2018, **9**: 4347

Simulating the chiral magnetic wave in a box system

Zhou Wenhao Xu Jun

Key words Heavy-Ion Collisions

The chiral magnetic wave from the interplay between the chiral magnetic effect and the chiral separation effect is simulated in a box system with the periodic boundary condition based on the chiral kinetic equations of motion. Simulation results are compared with available limits from theoretical derivations, and effects of the temperature, the magnetic field, and the specific shear viscosity on the key properties of the chiral magnetic wave are discussed. Our study serves as a baseline for further simulations of chiral anomalies in relativistic heavy-ion collisions.

Physical Review C, 2018, **98**(4): 044904

The beam-based alignment for soft X-ray free-electron lasers via genetic algorithm

Zeng Li Feng Chao Gu Duan Li Juan Zhao Zhentang

Key words Beam-based alignment, Modified genetic algorithm, Soft X-ray

The overlap between the electron beam and the radiation field is one of the most important characteristics during the free-electron laser (FEL) amplification processes, which will dramatically influence the quality of the FEL radiation. The beam-based alignment (BBA), first proposed in

1980s, has achieved great success in both theoretical and experimental studies on hard X-ray FELs. This paper gives a brief analysis on the undulator misalignment, which has been ignored in the original BBA algorithm. These misalignments, as revealed by the calculation and simulation, tend to have significant impacts on the soft X-ray FELs which are driven by the low energy accelerators. Furthermore, we demonstrate a method that can probably solve this dilemma using a searching algorithm - genetic algorithm.

Nuclear Instruments & Methods in Physics Research Section A-Accelerators Spectrometers Detectors and Associated Equipment, 2018, **905**: 104

Serum protein corona-responsive autophagy tuning in cells

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Li Qingnuan Lv Min Shi Jiye Yan Qinglong Cui Zhifen
Fan Chunhai Zhu Ying Wang Lihua

Key words Carbon Nanotubes, Silver Nanoparticles, Quantum Dots, Cytotoxicity, Oxide, Dependence, Chemistry, Peptides, Disease, Impact

Autophagy represents an important cellular response to nanoparticles (NPs), whose modulation holds great promise for developing nanomedicine. Here, we systematically studied cell autophagy responses elicited by the NP-protein corona with diverse protein corona types surrounding NPs with different sizes, shapes, and compositions. We demonstrated that these physicochemical properties of NP-protein coronas exerted a remarkable influence on cell autophagy responses. Particularly, for surface protein type-associated modulation of cell autophagy, we correlated the autophagy level to adsorbed protein type on Fe_3O_4 NPs. Accordingly, we could modulate cell autophagy in response to various levels of protein adsorption. Our work provides new clues to modulate cell autophagy by rational designing NP-protein complexes, which could aid in further biological and therapeutic applications.

Nanoscale, 2018, **10**(37): 18055

Theoretical study of fluorine-induced surface segregation of Cr in non-passivated Ni-based alloys

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Zhang Xun Huai Ping Zhu Zhiyuan

Key words FLINAK Salt Environments, Augmented-Wave Method, Corrosion, Energy, Adsorption, Oxidation, Moisture, Behavior, Metals, System

The effects of fluorine adsorption on the surface segregation behaviors of chromium in nickel-based alloys are systematically investigated by selecting three typical low-index Cr-doped Ni (111), (100), and (110) surfaces based on the first-principles calculations. The Cr doped in the nickel substrate is identified to possess a local trapping effect for fluorine in the full space and contributes to the more exothermic adsorption of fluorine. In turn, the chemisorption of fluorine on the Cr-doped Ni surfaces can dramatically incur the preferential top-surface segregation for Cr from nickel bulk. The increased adsorption energy of fluorine on Cr-doped Ni surfaces compensates for the larger surface energy of Cr relative to Ni. The strong F-Cr bonding from the deeper hybrid state of F 2p-Cr *3d* helps to release strain energy caused by atomic size mismatch. At higher fluorine coverage, the driving force for Cr to segregate at nickel surfaces is significantly increased, as the fluorine starts to agglomerate in the vicinity of Cr. Such chemisorption-induced surface abnormal segregation of Cr to the topmost surface plays a critical role in the preferential dealloying of Cr at the early-stage corrosion of non-passivated nickel-based alloys in molten fluoride salts.

Journal of Applied Physics, 2018, **124**(13): 135302

Formation and Stability of Surface/Bulk Nanobubbles Produced by Decompression at Lower Gas Concentration

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Zou Zhenglei Tai Renzhong Zhang Lijuan Hu Jun

Key words Atomic-Force Microscopy, Hydrophobic Surfaces, Mica/Water Interface, Water, Bubbles, Temperature

Nanobubbles have many fascinating properties and the mechanism of their formation and stability still needs further exploration. According to the conventional theory and experiences, it was suggested that surface/bulk nanobubbles would only be produced at conditions of high gas concentration and stabilized in a gas oversaturated state. However, we showed here that both surface and bulk nanobubbles could be formed at conditions of low gas concentration and exist in an unsaturated gas environment in water for a long time. In our experiments, the surface/bulk nanobubbles were produced by a new method of water decompression started from the normal pressure. Sufficient surface/bulk nanobubbles could be generated during the decompression within a certain time and were quite stable even after the pressure was recovered to the normal pressure. The evolution process of the bulk nanobubbles with the time of decompression was studied and it was found that the concentration of the bulk nanobubbles was firstly increased and then decreased. In addition, the size of the bulk nanobubbles was increased during this decompression process. Our

results revealed new information on the unique behavior of nanobubbles and should be helpful to understand their formation and stability mechanism as well as their applications.

Journal of Physical Chemistry C, 2018, **122**(39): 22418

Achieving a Record-High Yield Rate of 120.9 μg_{NH3} mg_{cat}^{-1} h^{-1} for N_2 Electrochemical Reduction over Ru Single-Atom Catalysts

Geng Zhigang Liu Yan Kong Xiangdong Li Pai Li Kan Liu Zhongyu Du Junjie Shu Miao Si Rui Zeng Jie

Key words N-2 Electrochemical Reduction, NH_3 Production, Ru Single Atoms, Single-Atom Catalysts

The electrochemical reduction of N_2 into NH_3 production under ambient conditions represents an attractive prospect for the fixation of N_2. However, this process suffers from low yield rate of NH_3 over reported electrocatalysts. In this work, a record-high activity for N_2 electrochemical reduction over Ru single atoms distributed on nitrogen-doped carbon (Ru SAs/N-C) is reported. At -0.2 V versus reversible hydrogen electrode, Ru SAs/N-C achieves a Faradaic efficiency of 29.6% for NH_3 production with partial current density of -0.13 mA cm^{-2}. Notably, the yield rate of Ru SAs/N-C reaches 120.9 μg_{NH3} mg_{cat}^{-1} h^{-1}, which is one order of magnitude higher than the highest value ever reported. This work not only develops a superior electrocatalyst for NH_3 production, but also provides a guideline for the rational design of highly active and robust single-atom catalysts.

Advanced Materials, 2018, **30**(40): 1803498

Operando X-ray spectroscopic tracking of self-reconstruction for anchored nanoparticles as high-performance electrocatalysts towards oxygen evolution

Song Sanzhao Zhou Jing Su Xiaozhi Wang Yu Li Jiong Zhang Linjuan Xiao Guoping Guan Chengzhi Liu Renduo Chen Shuguang Lin Hongji Zhang Shuo Wang Jianqiang

Key words Water Oxidation Catalysts, Absorption Spectroscopy, Perovskite, Surface, Transition, Oxides, Fe, Challenges, Nanosheets, Stability

Exploring high-performance electrocatalysts for the oxygen evolution reaction (OER) is pivotal for renewable energy storage and conversion. The surface self-reconstruction during the OER is considered as the key of highly active catalysts, whereas identifying the local electronic and geometric structure of the reconstruction-derived components is challenging. Herein, an *in situ* exsolution method towards the typical $LaCo_{0.8}Fe_{0.2}O_{3-\delta}$ perovskite is developed to obtain a new type of lanthana-anchored CoFe catalyst. The optimized catalyst exhibits a low overpotential of 293 mV to reach the current density of 10 mA cm^{-2} in 0.1 M KOH. Most importantly, operando X-ray absorption spectroscopy (XAS) measurements demonstrate that the CoFe species in the catalyst are nearly transformed into unique (Co/Fe)O(OH) with a definite coordination-unsaturated structure under electrochemical conditions, which actually contributes to this superior performance. Moreover, the presence of the lanthana support promotes this transformation. Our work not only suggests a facile reconstructive strategy to dramatically enhance the OER activity of perovskite oxides in alkaline media, but also unravels the fine structure of true active sites through operando X-ray spectroscopic tracking.

Energy & Environmental Science, 2018, **11**(10): 2945

Assessment of Catalytic Activities of Gold Nanoclusters with Simple Structure Descriptors

Xu Haoxiang Cheng Daojian Gao Yi Zeng Xiaocheng

Key words Au Nanoparticles, CO Oxidation, Geometry Descriptor, Density Functional Theory, Activity Prediction, Catalyst Design

The de novo design of nanocatalysts with high activity is a challenging task, since prediction of catalytic activities of nanoclusters on the basis of simple descriptors is still a frontier of research. Herein, we present a simple model to build a geometry-adsorption-activity relationship for gold nanoclusters using CO oxidation as the benchmark probe. On the basis of extensive density functional theory calculations, the geometry indices (generalized local coordination number and curvature angle of the surface Au atoms) of numerous Au nanoclusters are found to be well correlated with the binding strength of CO and O_2, as well as the activation barriers of CO oxidation by using the Bronsted-Evans-Polanyi (BEP) relationship and Sabatier analysis. In particular, this predictive model with simple structure descriptors can be extended to Au nanoparticles (NPs) with larger sizes and various shapes. Such a predictive model can provide a useful rule of thumb for experimentalists to quickly assess catalytic activity from only gathering the structural characteristics of Au NPs before performing more involved catalytic measurements. This

model may also offer a cost-effective way for the rational design of nanocatalysts: for example, to assist experimentalists in making Au nanoclusters with the maximum number of active sites.

ACS Catalysis, 2018, **8**(10): 9702

Effects of silicon carbide on the corrosion of metallic materials in molten LiF-NaF-KF salt

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Key words Nickel, Stainless steel, Molten salts, Ceramic, High temperature corrosion

The effects of silicon carbide (SiC) on the corrosion behavior of metallic materials in molten LiF-NaF-KF (FLiNaK) salt were investigated. Results reveal that the corrosion products of SiC in molten FLiNaK salt can react with nickel-based alloy GH3535, Ni metal, 316L stainless steel, and Cr metal to form $Ni_{31}Si_{12}$, Ni_3Si, $CrFe_8Si$, and Cr_3Si, respectively. The formation of silicide enhances the corrosion of GH3535 alloy in molten FLiNaK salt. The depletion of Cr along grain boundaries in alloys can promote the diffusion of silicon into the alloys and increase the corrosion depth.

Corrosion Science, 2018, **143**: 157

Effects of alloying elements on the corrosion behavior of Ni-based alloys in molten NaCl-KCl-$MgCl_2$ salt at different temperatures

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Key words Ni-Based Alloy, Molten Chloride Salt, Corrosion, Alloying Element

The effects of alloying elements on corrosion of Ni-based alloys in NaCl-KCl-$MgCl_2$ under Ar in the temperature range of 600 ~ 800 ℃ were investigated by immersion test, SEM/EDS, EPMA and XRD techniques. A thermodynamic potential-pO^{2-} diagram for Cr, Ni at 700 ℃ was constructed. The alloy corrosion is attributed to the dissolution of Cr to form Cr chlorides into salt. The elements Cr, Mo and W can affect the alloy corrosion. The corrosion is accelerated and the intergranular corrosion becomes more pronounced with temperature. Furthermore, the effects of the alloying elements on corrosion have a strong temperature dependence. The related mechanisms are discussed.

Corrosion Science, 2018, **143**: 187

Corrosion performance of Ni-16%wt.Mo-X%wt.SiC alloys in FLiNaK molten salt

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Holmes Rohan Avdeev Maxim Jia Yanyan
Huang Hefei Zhou Xingtai

Key words Molten Salt Corrosion, Corrosion Resistance, FLiNaK, MSR, Nuclear Reactor

The corrosion performance of Ni-16%wt.Mo-X%wt.SiC (X = 0.5, 1.5, 2.0, 2.5 and 3.0) alloys prepared via mechanical alloying followed by consolidation using spark plasma sintering (SPS) from pure Ni, Mo and SiC powders is investigated. Corrosion testing at 650 ℃/200 h in FLiNaK molten salt showed that increasing the volume fraction of SiC in the initial Ni-Mo-SiC powder mixture leads to formation of large amount of Mo_2C precipitates, which readily dissolve into FLiNaK molten salt. Hence, only the corrosion resistance of NiMo-SiC alloys with a low SiC content (< 2 wt.%) is comparable to that of Hastelloy-N alloy.

Corrosion Science, 2018, **143**: 240

Oscillator Strengths and Integral Cross Sections of the Valence-shell Excitations of the Oxygen Molecule Studied by Fast Electron and Inelastic X-Ray Scattering

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Key words Astronomical Databases: Miscellaneous, Methods: Laboratory: Molecular, Molecular Data

The oscillator strengths and integral cross sections (ICSs) of the Schumann-Runge continuum, and the longest band and second band of the oxygen molecule have wide applications in studies of the Earth's atmosphere and the stellar atmospheres, but there still exist apparent discrepancies among the available data. In this work, the generalized oscillator strengths of the valence-shell excitations of oxygen have been determined independently by the high-energy electron scattering and high-resolution inelastic X-ray scattering. Based on the cross-checked generalized oscillator strengths, the optical oscillator strengths and ICSs of these excitations have been obtained, which give an independent cross-check to the previous experimental and theoretical results. The present data can be used as the basic input parameters in the theoretical models for the astronomical

observations, and will be helpful for deepening our understanding of the atmospheres of Earth, Venus, Saturn, Pluto, Europa, and other oxygen-rich planets and satellites.

The Astrophysical Journal Supplement Series, 2018, **238**(2): 26

Contact Angle Measurement in Lattice Boltzmann Method

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Wang Chunlei Zhang Chaoying

Key words Contact Angle Measurement, Contact Angle Hysteresis, Lattice Boltzmann Method

Contact angle is an essential characteristic in wetting, capillarity and moving contact line, however, although contact angle phenomena are effectively simulated, an accurate and real-time measurement for contact angle has not been well studied in computational fluid dynamics, especially in dynamic environments. Here, we design a geometry-based mesoscopic scheme for on-the-spot measurement of the contact angle in the lattice Boltzmann method. The measuring results without gravity effect are in good agreement with the benchmarks from the spherical cap method. The performances of the scheme are further verified in gravitational environments by simulating sessile and pendent droplets on smooth solid surfaces and dynamic contact angle hysteresis on chemically heterogeneous surfaces. This scheme is simple and computationally efficient. It requires only the local data and is independent of multiphase models.

Computers & Mathematics with Applications, 2018, **76**(7): 1686

Preparation and Investigation of Multicomponent Alkali Nitrate/Nitrite Salts for Low Temperature Thermal Energy Storage

Li Xiang Wang Yang Wu Shuang Xie Leidong

Key words Thermal Energy Storage, Low Temperature, Molten Salts, Thermal-Physical Properties

A novel eutectic salt of alkali nitrate/nitrite mixture with low melting point was investigated using thermal analysis methods for thermal energy storage. The eutectic salt mixture system $LiNO_3$-$NaNO_3$-KNO_3-$NaNO_2$-KNO_2 was prepared based on eutectic composition X_{LiNO3}=33.5, X_{NaNO3} =1.2, X_{KNO3} =1.2, X_{NaNO2}=17.4 and X_{KNO2} = 46.7 (in mole fraction). Using Differential Scanning

Calormetry (DSC) apparatus, the melting point, enthalpy of fusion and specific heat capacity of the eutectic salt mixture were experimentally determined under an argon atmosphere. The density of eutectic salt mixture based on Archimedean principle was measured as a function of temperature. By means of the Thermogravimetric Analyzer (TGA) equipment, the decomposition temperature and the upper limit of operating temperature of eutectic salt mixture were determined. Viscosity of eutectic salt was also measured experimentally using a rotational coaxial cylinder viscometer constructed. Meanwhile, the empirical estimation method based on additive principle was used to predict thermal-physical properties (density and viscosity) of eutectic salt mixture. Results indicate that the predicted values were in good agreement with experiment values. Based on the thermal-physical properties of eutectic salt mixture, this novel five-component eutectic system can be used as excellent heat transfer and storage materials for low temperature thermal energy storage (TES) applications.

Energy, 2018, **160**: 1021

Real-time label-free analysis of the thermostability of DNA structures using GelRed

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Li Jiang Xu Jia-Qiang Wang Li-Hua

Key words GelRed, Secondary structure, GC content, Conformational transformation

In biological systems, conformational transformations of nucleic acids play critical roles in genetic regulation. However, it remains a tricky task to design and optimize specific labeling strategies to track these changes. In this study, we exploited an intercalating fluorescent dye, GelRed, to characterize different DNA structures. We studied the correlation between fluorescence intensity and DNA structural properties. We showed that single-stranded DNAs with predicted self-folded secondary structures show much stronger fluorescence than those without such structures. For double-stranded DNAs, we observed that fluorescence intensity is positively correlated to their GC content. We also demonstrated that GelRed can be used to monitor DNA conformational changes upon temperature variations in real time. Based on these findings, we concluded that the fluorescence intensity of a GelRed-stained DNA structure has a good correlation with its thermostability in the form of a change in Gibbs free energy.

Nuclear Science and Techniques, 2018, **29**(10): 138

Numerical study of the dynamic characteristics of a single-layer graphite core in a thorium molten salt reactor

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Zou Yang Tsang D. K. L.

Key words Graphite core, Dynamic behavior, ABAQUS

A reactor core in a thorium molten salt reactor uses graphite as a moderator and reflector. The graphite core is a multi-layered arrangement of graphite bricks that are loosely connected to each other using a system of keys and dowels. Consequently, the graphite core is a type of discrete stack structure with highly nonlinear dynamic behavior. Hence, it is important to investigate the dynamic characteristics of the graphite core. In this study, a three-dimensional single-layer graphite core model, which is a part of the thorium molten salt reactor side reflector structure, was analyzed using the explicit method in ABAQUS 2016 to study the core dynamic behavior when subjected to different excitations. The design parameters, such as the diameter of the dowel, the gap between key and keyway and the bypass flow gap between two adjacent bricks, were also considered in this model. To reduce excessive demands on available computational resources considering the effect of molten salt, the spring-dashpot model was applied to model the interaction forces between the molten salt and graphite bricks. Numerical simulation results show that the effect of molten salt is a reduction in the peak maximal principal stress, and a larger gap between two bricks is beneficial to maintain the integrity of the graphite core under earthquake loading. The results obtained by the simulation can be used as a reference for future designs of a molten salt graphite core.

Nuclear Science and Techniques, 2018, **29**(10): 141

ESR study of free radicals in polysilazane irradiated by gamma rays

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Key words ESR, gamma-Rays irradiation, Free radicals, Polysilazane

Free radicals trapped in polysilazane (PSZ) induced by gamma-ray irradiation in an Ar atmosphere at room temperature and their decay behaviors were investigated via electron spin resonance (ESR). The G value of the whole initial free radicals was calculated to be 1.8 radicals/100 eV. The free radicals trapped in PSZ were rather stable in Ar at room temperature, and their half-life was estimated to be 470 h according to the decay line. However, they decayed rapidly

via reactions with oxygen when exposed to air, and their half-life decreased to 4 h. Interestingly, the free radicals could not be eliminated completely even though the temperature was increased up to 200 ℃ in an Ar atmosphere. Combing with ESR parameters calculation using DFT method, we found that Si-centered radicals were the main products of PSZ after irradiation in Ar at room temperature. Additionally, we proposed the probable conversion reactions of these radicals under different post-treatment conditions.

Radiation Physics and Chemistry 2018, **151**: 108

Theoretical investigation of Ti and Ni co-doping on the anti-disproportionation ability of ZrCo alloy

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Cheng Hongwei Gao Jie Zeng Youshi Liu Wei Li Yan

Key words $ZrCoH_3$, ZrCo, Ti, Ni, Hydrogen-Induced Disproportionation, First-Principles Calculation

First-principles calculations are utilized to investigate the effect of Ti and Ni co-doping on the anti-disproportionation ability of ZrCo alloy. In Ti and Ni co-doped $ZrCoH_3$, the Ti-H(8e) bond shows a strong ionic feature and the Ni-H(8e) bond exhibits covalent bonding characteristic. Judged by the Zr-H(8e) bond length, the size of the 8e site and H diffusion barrier out of the 8e site in $ZrCoH_3$, it can be concluded that the Ti + Ni co-doping can impair the anti-disproportionation ability of Ti doping in ZrCo alloy, which uncovers the mechanism of the negative effect of Ni on the Ti-doped ZrCo alloy found in the previous experimental results.

Materials Research Express, 2018, **5**(10): 105501

Effect of concentration of Cr^{3+} in LiF-NaF-KF salt on the corrosion of SiC

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Han Ling Zhang Xiaonan Wang Jianqiang

Key words Molten Fluoride Salts, High Temperature Corrosion, X-Ray Photoelectron Spectroscopy, Raman Spectroscopy, Silicon Carbide

Effect of the concentration of Cr^{3+} in molten LiF-NaF-KF salt on the corrosion of SiC was investigated. Results reveal that increasing initial concentrations of Cr^{3+} in salt can enhance both the loss of Si and the deposition of Cr on SiC, which results in the weight change of SiC from loss

to gain. The corrosion of SiC in molten LiF-NaF-KF salt with Cr^{3+} should be attributed to the oxides in SiC, the oxygen-containing impurities and Cr^{3+} in salt. The oxygen-containing impurities in salt react with SiC to form oxides that can be corroded by fluoride salt. The Cr^{3+} in salt can react with SiC and the oxides (SiOx)

Journal of Nuclear Materials, 2018, **509**: 527

^{149}Sm evolution behavior in a small modular molten salt reactor

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Key words Small Modular Molten Salt Reactor, Core burnup, Flow effect

Compared with the well-studied neutron poison ^{135}Xe, ^{149}Sm received much less attention in the conventional reactors because of the comparatively smaller neutron absorption cross section. But in Molten Salt Reactor (MSR), gaseous fission products such as xenon and krypton are largely removed by the gas removal system, the behavior of ^{149}Sm, which exists in molten salt, therefore becomes important. During MSR's operation, the liquid fuel continuously circulates through the core (with neutron flux functioning) and outer-loop (the part of primary loop at external core, with negligible neutron flux), the nuclide evolution law is much different from that in the solid fueled reactors, thereby accurately evaluating the time behavior of ^{149}Sm is much needed. In this work, the control equations precisely describing the nuclide evolution of ^{149}Sm as well as its precursor ^{149}Pm entrained in the flowing salt are deduced, and a time behavior during different power cycles is then investigated for a small modular molten salt reactor based on the deduced equations. To fundamentally understand the flow effect on ^{149}Sm time behavior, the corresponding results are compared with those calculated by using the existent method, in which the flowing fuel is treated as the static fuel. Because the disappeared ^{149}Pm regardless at the core and outer-loop is all converted to ^{149}Sm, the flow state has a same equilibrium atomic density with that at the static state. But the time for achieving the equilibrium at the flow state is prolonged due to the time for ^{149}Pm decayed to ^{149}Sm being extended at a same ^{149}Pm production rate. This effect also leads to a lower "samarium peaking (overshoot)" for power up/down, as well as a lower ^{149}Sm concentration after scram which subsequently decreases the neutron poison (around 210 pcm) as the core start-up again. This work provides a precise description for the evolution of ^{149}Sm for circulating fuel, which should be included in the core design and source term analysis of safety study of a MSR.

Annals of Nuclear Energy, 2018, **120**: 100

Infrared Spectra of the $SO_2F_2^-$ Anion in Solid Argon and Neon

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Key words Ion-Molecule Reactions, Matrix-Isolation, Theoretical Investigations, Vibrational Frequencies, Sulfur-Fluoride, Thermochemistry, Spectroscopy, Complexes, Oxidation, Affinity

Sulfonyl fluoride anion ($SO_2F_2^-$) was produced during codeposition of laser-ablated metal atoms, ions, and electrons with SO_2F_2 in argon and neon matrixes at 4 K. The structure of $SO_2F_2^-$ was determined by infrared spectroscopy and density functional theory calculations. On the basis of the experiments using $^{34}SO_2F_2$ and $S^{18}O_2F_2$ samples, the three absorptions at 1284.9, 1109.3, and 567.0 cm^{-1} in argon and 1289.0, 1116.2, and 576.8 cm^{-1} in neon were assigned to the antisymmetric and symmetric O-S-O stretching and SO_2 wagging modes of $SO_2F_2^-$, respectively. These assignments were further supported by frequency and isotopic frequency ratio calculations. The $SO_2F_2^-$ anion possesses a $^2A_1$ ground state with nonplanar C_2v symmetry. Compared with the neutral SO_2F_2 molecule, dramatic increases in the S-F bond length (0.295 Å) and F-S-F bond angle (41.0°) were found for the anion, which result from the S-F antibonding character of the singly occupied molecular orbital. The $SO_2F_2^-$ anion was formed via electron capture by SO_2F_2 in the gas phase before being deposited into the cryogenic matrix. The matrix environment stabilized this anion, but it was destroyed by UV-vis irradiation and presumably converted to the neutral SO_2F_2 molecule.

Journal of Physical Chemistry A, 2018, **122**(38): 7723

Fabricating Quasi-Free-Standing Graphene on a SiC(0001) Surface by Steerable Intercalation of Iron

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Liang Zhaofeng Li Haiyang Zhu Zhiyuan Huang Yaobo
Kong Lingyuan Wang Yu Jiang Zheng Huang Han
Wells Justin W. Song Fei

Key words Epitaxial-Graphene, Electronic-Properties, Silicon-Carbide, High-Quality, Growth, Semiconductor, Transistors, Graphite, Single, Layers

Graphene has been granted with appealing attributes for new-generation electronics due to its unique electronic properties. However, the interaction between graphene and the supporting

substrate substantially limits its technological application. Here, we demonstrate the transformation of epitaxial monolayer graphene on SiC(0001) into decoupled bilayer graphene using steerable iron intercalation manipulated by thermal annealing. By means of Raman scattering and photoemission measurements, we have performed an in-depth investigation of the intercalation procedure and shown the quasi-free-standing nature of the decoupled bilayer graphene afterward, as characterized by its unique structural and electronic properties. The intercalation of Fe atoms can be manipulated through temperature-driven processes after adsorption on top of the graphene layer, and this substantially modifies the interfacial interaction between the buffer layer and SiC substrate and, correspondingly, the doping level of the pristine graphene, ultimately resulting in the decoupling of buffer layer from the substrate. Although the decoupling of epitaxial graphene grown on silicon carbide has previously been a critical issue, our study highlights a feasible approach for producing high-quality quasi-free-standing graphene on SiC in a well-controlled manner, and for tuning the intrinsic electronic properties of lateral graphene/SiC lateral structure by ferromagnetic element intercalation.

Journal of Physical Chemistry C, 2018, **122**(37): 21484

Anomalous behavior of membrane fluidity caused by copper-copper bond coupled phospholipids

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Key words Particle Mesh Ewald, Force-Field, Dynamics, Ions, Phosphatidylcholine, Lipids, Shell, Cu^{2+}, Phosphatidylethanolamine, Conformation

Membrane fluidity, essential for cell functions, is obviously affected by copper, but the molecular mechanism is poorly understood. Here, we unexpectedly observed that a decrease in phospholipid (PL) bilayer fluidity caused by Cu^{2+} was more significant than those by Zn^{2+} and Ca^{2+}, while a comparable reduction occurred in the last two ions. This finding disagrees with the placement in the periodic table of Cu just next to Zn and far from Ca. The physical nature was revealed to be an anomalous attraction between Cu^{+} cations, as well as the induced motif of two phospholipids coupled by Cu-Cu bond (PL-diCu-PL). Namely, upon Cu^{2+} ion binding to a negatively charged phosphate group of lipid, Cu^{2+} was reduced to Cu^{+}. The attraction of the cations then caused one Cu^{+} ion simultaneously binding to two lipids and another Cu^{+}, resulting in the formation of PL-diCu-PL structure. In contrast, this attraction cannot occur in the cases of Zn and Ca ions. Remarkably, besides lipids, the phosphate group also widely exists in other biological molecules, including DNA, RNA, ADP and ATP. Our findings thus provide a new view for

understanding the biological functions of copper and the mechanism underlying copper-related diseases, as well as lipid assembly.

Scientific Reports, 2018, **8**: 14093

Uranium-Induced Changes in Crystal-Field and Covalency Effects of Th^{4+} in $Th_{1-x}U_xO_2$ Mixed Oxides Probed by High-Resolution X-ray Absorption Spectroscopy

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Li Jiong Yu Haisheng Jiang Zheng Liu Hongtao
Zhang Linjuan Lin Jian Chen Ning Lin Xiao
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Key words Local-Structure, Electronic-Structure, Charge-Distribution, Thorium, Spectrometer, Dissolution, Scattering, Behavior, Density, XAS

Knowledge of the local Th structure is a prerequisite for a better understanding of the physicochemical properties of the thorium-based mixed oxides (Th-MOX) involved in the Th-based nuclear fuel cycle. The crystalline electric field (CEF) splitting of the 6d shell in $Th_{1-x}U_xO_2$ (x=0.25, 0.5, 0.75) solid solution was probed by the Th L_3 edge high-energy-resolution fluorescence-detected (HERFD) X-ray absorption near-edge spectroscopy (XANES) collected at the $L_{\beta5}$ emission line, which cannot be obtained by conventional X-ray absorption methods. The detected CEF split between the 6d e_g and t_{2g} orbitals in ThO_2 consisting of ordered Th-O_8 cubes with cubic symmetry is ~3.5 eV for the Th^{4+} ion. Because the split peaks of the white line corresponding to the crystal-field splitting of the unoccupied 6d states were resolved in the HERFD-XANES spectra, the analysis of these split peaks combined with first-principles calculations revealed that an increase of the U content involves the distortion of the Th-O_8 cubes in the $Th_{1-x}U_xO_2$ mixed oxides. The lower symmetry of the Th-O_8 cube induced by the incorporated U tends to reduce the local crystal-field around Th^{4+} as well as the hybridization of Th $6t_{2g}$-O 2p which is mainly responsible for the covalent property of the Th-O bond. The phenomenon is noticeable in $Th_{0.25}U_{0.75}O_2$, whose CEF splitting is decreased by approximately 10%, and covalent mixing between Th 6d t_{2g} and O 2p orbitals is substantially reduced compared to that of pure ThO_2.

Inorganic Chemistry, 2018, **57**(18): 11404

Highly Efficient CO_2 Electroreduction on ZnN_4-based Single-Atom Catalyst

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Jiang Zheng Gu Lin Xu Weilin

Key words Carbon Dioxide, Electroreduction, Single-Atom Catalysts, Zinc

The electrochemical reduction reaction of carbon dioxide (CO2RR) to carbon monoxide (CO) is the basis for the further synthesis of more complex carbon-based fuels or attractive feedstock. Single-atom catalysts have unique electronic and geometric structures with respect to their bulk counterparts, thus exhibiting unexpected catalytic activities. A nitrogen-anchored Zn single-atom catalyst is presented for CO formation from CO2RR with high catalytic activity (onset overpotential down to 24 mV), high selectivity (Faradaic efficiency for CO (FE_{CO}) up to 95% at -0.43V), remarkable durability (> 75h without decay of FE_{CO}), and large turnover frequency (TOF, up to 9969 h^{-1}). Further experimental and DFT results indicate that the four-nitrogen-anchored Zn single atom (Zn-N_4) is the main active site for CO2RR with low free energy barrier for the formation of *COOH as the rate-limiting step.

Angewandte Chemie International Edition, 2018, **57**(38): 12303

System-level performance optimization of molten-salt packed-bed thermal energy storage for concentrating solar power

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Key words Concentrating solar power, Thermal energy storage, Packed-bed, Cut-off temperature, Cost optimization

Molten-salt packed-bed thermal energy storage using thermocline technology is more cost-competitive than the conventional two-tank thermal energy storage, due to its integrated design and the employment of a low-cost packed-bed. However, such a storage configuration suffers the main drawback of a low capacity factor when applied to concentrating solar power because of the adoption of conservative cut-off temperatures. The present work evaluates the feasibility of taking less conservative cut-off temperatures to improve the utilization of the packed-bed thermal energy storage from the perspectives of a system-level operation and storage economy. The investigations are carried out on two levels. The first-level investigation reveals the effects of both the charging

and discharging cut-off temperature on the thermal performance of the packed-bed thermal energy storage under ideal operating conditions. Three typical packed-bed configurations are involved. The results show that the capacity factor of the packed-bed thermal energy storage increases as the charging cut-off temperature increases and the discharging cut-off temperature decreases, especially for the configurations using latent-heat when the adopted cut-off temperatures jump over the phase change points of the encapsulated phase change materials. The second-level investigation discusses the impacts of different levels of deep charges (using high charging cut-off temperatures) on the scale design of the packed-bed thermal energy storage, the daily operation of the low temperature molten-salt pump (LT-pump) and the central receiver of a 100 MWe conventional concentrating solar power tower plant. The results indicate that a deeper charge operation is always accompanied with a smaller required packed-bed size as well as a higher required delivery capacity and higher pressure head of the LT-pump and that it always results in a larger daily pumping consumption, a higher peak inlet temperature ramping rate and a higher receiver pressure drop. The maximum allowable charging cut-off temperature is identified to be 500 ℃ for each packed-bed configuration, according to the operating limitations on the pump and receiver. Moreover, a cost analysis is carried out to obtain the optimum charging cut-off temperature for each packed-bed configuration. The obtained results show that performing deep charges with the cost-optimized charging cut-off temperatures can effectively improve the cost competitiveness of the molten-salt packed-bed TES integrated into concentrating solar power plants.

Applied Energy, 2018, **226**: 225

Hindered Gas Transport through an Aqueous Salt Solution Interface

Fang Gang Chen Jige

Key words Water-Solubility, Carbon-Dioxide, Hydrogen, Ions, Diffusion, Mechanism, Hydration, Oxide

Gas transport through water plays an important role in various natural processes and applications as the most common form in liquid-gas transport. Conventionally, it is expected that the flux of gas through water would be determined by the gas solubility and diffusion in water. However, it is still unclear whether such behavior holds in aqueous salt solutions. In this paper, we find that the methane transport is heavily hindered through the Pure water aqueous salt solutions by molecular dynamics simulations. Surprisingly, the hindrance to methane is not caused by the methane solubility or the diffusion change in aqueous salt solutions, but by the gas concentration

barrier at the liquid-gas interface. Our simulation results show that the gas concentration barrier originates from the variance of the mass density profile in aqueous salt solutions. Furthermore, it is found that the flux of methane is negatively linearly dependent upon the gas concentration barrier at the liquid-gas interface by investigating various salt solutions with different cations and anions, for example, Na^+, K^+, Mg^{2+}, Ca^{2+}, Cl^-, Br^-, and in different concentrations and at different temperatures. Our work implies the gas accumulation at the liquid-gas interface as the deciding factor for gas transport through liquid and would be helpful in liquid-gas transport applications like shale gas and flammable ice exploitation.

Journal of Physical Chemistry C, 2018, **122**(36): 20774

Operando Spectroscopic Identification of Active Sites in NiFe Prussian Blue Analogues as Electrocatalysts: Activation of Oxygen Atoms for Oxygen Evolution Reaction

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Li Jiong Zhang Shuo

Key words Water Oxidation, Perovskite, Oxide, Nanosheets, Generation, Hydroxide, Catalyst, Hybrid, Arrays

Developing highly efficient oxygen evolution reaction (OER) catalysts and understanding their activity are pivotal for electrochemical conversion technologies. Here, we report NiFe Prussian blue analogue (PBA) as a promising electrocatalyst for OER in alkaline conditions. This material has an impressively low overpotential of 258 mV that reaches a current density of 10 mA cm^{-2}. Post-mortem characterization showed that the as-prepared catalyst is entirely transformed into amorphous nickel hydroxide after the electrochemical treatment, and $Ni(OH)_2$ acts as the active species. Operando X-ray spectroscopic studies further found that this in situ generated $Ni(OH)_2$ displays an unique feature that allows deprotonation under applied potential creating $NiOOH_{2-x}$ that contains Ni^{4+} ions. The deprotonation reaction is reversible and potential-dependent, i.e., the amount of Ni^{4+} increases with increasing applied potential. Theoretical calculations were used to show that the role of Ni^{4+} is to trigger oxidized oxygen ions as electrophilic centers with the subsequent activation of anion redox reactions for OER.

Journal of the American Chemical Society, 2018, **140**(36): 11286

A numerical comparison between internal cooling and side cooling of the reflection mirror for Spatial and Spin (S^2) beam-line at SSRF

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Cao Jiefeng Xu Zhongmin

Key words Synchrotron Radiation, Heat Load, Internal Cooling, Side Cooling, Finite Element Analysis (FEA)

To select a more appropriate cooling method for a reflection mirror of Spatial and Spin (S^2) beam-line at SSRF (Shanghai Synchrotron Radiation Facility), both of the internal cooling method and side cooling method were proposed and compared at various selected energy points (the most important 50 eV, 80 eV, 100 eV and 867 eV) based on finite element analysis (FEA). For the internal cooling mode, several internal rectangular channels were drilled under the irradiation surface of mirror. For the side cooling mode, two pieces of perforated copper blocks in contact with two side surfaces of mirror were employed. Moreover, a series of side cooling modes with different tube lengths (145 mm, 200 mm, 225 mm, 248 mm and 250 mm) were analyzed. It was found that the side cooling mode with tube length of 248 mm indicated the best slope error results in all of the side cooling methods. By comparing the temperature, thermal stress distribution and slope error between the internal cooling mode and side cooling mode with tube length of 248 mm, it showed that all of the above mentioned indicators for both cooling modes were consistent with the design standards. However, the internal cooling mode presented the better results than this specific side cooling mode. In particular, by comparing some critical important influencing factors, such as the commercial cost, manufacturing process difficulty, manufacturing period and micro vibration issues, the side cooling mode with tube length of 248 mm presented better engineering operability, thus it was selected as the final cooling method for the reflection mirror of Spatial and Spin (S^2) beam-line at SSRF.

Nuclear Instruments & Methods in Physics Research Section A-Accelerators Spectrometers Detectors and Associated Equipment, 2018, **902**: 190

Observation of β-delayed ^{2}He emission from the proton-rich nucleus ^{22}Al

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Bai Z. Cao X. G. Dai Z. T. Ding B. He W. B. Huang M. R. Jin S. L.
Lin C. J. Lv M. Liu L. X. Li Y. Ma R. Ma J. B. Wang J. S.
Wang S. T. Wang J. G. Wang H. W. Ye S. Q. Yang Y. Y. Zhou C. L.
Zhao M. H. Zhang H. Q. Ma Y. G. Shen W. Q.

Key words Magic Number, 2-Proton, Decay

The β-delayed two-proton emission from ^{22}Al was investigated experimentally through the implantation-decay method. A β-delayed two-proton decay branch from ^{22}Al were identified based on the coincidence of the charged particles and γ-ray signals. The relative momentum (q_{pp}) and the opening angle (θ_{pp}) distributions of the two beta-delayed protons are measured and a strong peak at q_{pp} ~ 20 MeV/c, as well as a peak at θ_{pp} ~ 30° are observed clearly. The beta-delayed ^{2}He emission from ^{22}Al with a probability of 29 (13)% by fitting the experimental data with the results of Monte Carlo simulations.

Physics Letters B, 2018, **784**: 12

Chemical interaction dictated energy level alignment at the N,N '-dipentyl-3,4,9,10-perylenedicarboximide/$CH_3NH_3PbI_3$ interface

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Xiong Yimin Gao Xingyu Qi Dongchen Cao Liang

Key words Perovskite Solar-Cells, Electronic-Structure, $CH_3NH_3PbI_3$ Perovskite, Photovoltaic Efficiency, Organic Semiconductors, Transport Layer, Degradation, Lead, Transformation

Here, we report the electronic structures at the N, N'-dipentyl-3,4,9,10-perylenedicarboximide (PTCDI-C5)/$CH_3NH_3PbI_3$ interface identified in-situ by X-ray photoemission spectroscopy and ultraviolet photoemission spectroscopy. Strong chemical reactions are found to occur upon the deposition of PTCDI-C5 molecules on $CH_3NH_3PbI_3$. Electron donation from PTCDI-C5 molecules to $CH_3NH_3PbI_3$ leads to the filling of surface states and the emergence of an interfacial gap state with its onset tailed to the Fermi level. As a consequence, the downward surface band bending resulting from surface states acting as donor states at the pristine perovskite surface is reduced by

0.2 eV. After the energy level alignment at the interface is established, the perovskite conduction band minimum is found to be in line with the lowest unoccupied molecular orbital favoring the electron extraction with a moderate valence band maximum-highest occupied molecular orbital offset of ~ 0.7 eV. The present results demonstrate that interfacial chemical reactions can dictate energetics at organic/perovskite interfaces. Understanding the chemical interaction and resultant electronic structures at those interfaces is crucial for efficient and long-term stable perovskite-based devices when passivation of chemical active sites and matched energy level could be readily reached.

Applied Physics Letters, 2018, **113**(11): 113901

Accelerated active phase transformation of NiO powered by Pt single atoms for enhanced oxygen evolution reaction

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Li Xiaopeng Jiang Zheng Liu Zhipan

Key words Surface Walking Method, Water Oxidation, Nickel-Oxide, Reduction Reaction, Alkaline-Solution, Thin-Films, Catalysts, Electrocatalysts, Performance, Transition

Phase transformation of electrode materials widely occurs in electrocatalytic reactions. Metal oxides are promising electrocatalysts for the oxygen evolution reaction (OER), their phase transformation is a key step for the multi-electron OER, and requires extra overpotential. However, little attention has been paid to accelerating and enhancing the phase transformation. Here, we report for the first time that single-atom Pt incorporated into the bulk crystalline phase of porous NiO nanocubes (0.5wt% Pt/NiO) can greatly promote the active phase (NiOOH) evolution. The Pt doping was achieved by a scalable nanocasting approach using SiO_2 as the hard template. In comparison with Pt/NiO samples with PtO_2 nanoparticles segregated at the NiO surface (1 wt% Pt), as well as atomistic Pt atoms solely bound at the surface by atomic layer deposition, the bulk Pt doping shows the strongest power in facilitating active phase transformation, which leads to improved OER activity with reduced overpotential and Tafel slope. Experiential data revealed that the charge-transfer from Pt to Ni through O leads to a local weaker Ni-O bond. First principles calculations confirmed that rather than acting as an active site for the OER, monatomic Pt effectively increases the phase transformation rate by reducing the migration barrier of nearby Ni atoms. Our discoveries reveal the relationships of the heteroatom doped structure and phase transformation behavior during the electrochemical process and offer a new route for designing high-performance electrocatalysts.

Chemical Science, 2018, **9**(33): 6803

Infrared Spectroscopic and Theoretical Studies of Group 3 Metal Isocyanide Molecules

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Key words Density-Functional Calculations, Pure Rotational Spectrum, Gaussian-Basis Sets, DFT Calculations, Solid Argon, Matrix Preparation, Transition-Metals, Wave-Functions,

A series of group 3 metal isocyanide complexes were prepared via the reactions of laser ablated scandium, yttrium, and lanthanum atoms with $(CN)_2$ in an argon matrix. The product structures were identified on the basis of their characteristic infrared absorptions from isotopically labeled $(CN)_2$ samples as well as the calculated frequencies and isotopic frequency ratios. Group 3 metal atoms reacted with $(CN)_2$ to form $M(NC)_2$ (M = Sc, Y, La) when the samples were subjected to $\lambda > 220$ nm irradiation. Other products such as $M(NC)_3$ and MNC were produced together with $M(NC)_2$ through either the reactions of $M(NC)_2$ and $(CN)_2$ or the loss of one CN ligand from $M(NC)_2$. CCSD(T)// B3LYP calculations reveal that ScNC possesses a $^3\Delta$ ground state, while $^1\Sigma^+$ is most stable for YNC and LaNC. All of the $M(NC)_2$ and $M(NC)_3$ complexes were predicted to have doublet and singlet ground states, respectively. Group 3 metal cyanides are less stable than the isocyanides by at least 4 kcal/mol at the CCSD(T) level, and their C-N stretches are much weaker than the N-C stretches of the isocyanides. No absorption can be assigned to the M(CN)(x) complex, which would appear between 2100 and 2250 cm^{-1}.

Journal of Physical Chemistry A, 2018, **172**(95): 7099

Multiparticle azimuthal cumulants in p+Pb collisions from a multiphase transport model

Nie Maowu Huo Peng Jia Jiangyong Ma Guoliang

Key words Long-Range, Angular-Correlations, Anisotropy, Flow, Escape, Side, PPB

A new subevent cumulant method was recently developed, which can significantly reduce the nonflow contributions in long-range correlations for small systems compared to the standard cumulant method. In this work, we study multiparticle cumulants in p+Pb collisions at $\sqrt{S_{NN}}$ = 5.02 TeV with a multiphase transport model (AMPT), including two- and four-particle cumulants ($c_2\{2\}$ and $c_2\{4\}$) and symmetric cumulants [SC(2, 3) and SC(2, 4)]. Our numerical results show that $v_2\{2\}$ is consistent with the experimental data, while the magnitude of $c_2\{4\}$ is smaller than the experimental data, which may indicate that either the collectivity is underestimated or some

dynamical fluctuations are absent in the AMPT model. For the symmetric cumulants, we find that the results from the standard cumulant method are consistent with the experimental data, but those from the subevent cumulant method show different behaviors. The results indicate that the measurements from the standard cumulant method are contaminated by nonflow effects, especially when the number of produced particles is small. The subevent cumulant method is a better tool to explore the real collectivity in small systems.

Physical Review C, 2018, **98**(3): 034903

Synchrotron Radiation Based Study of the Catalytic Mechanism of Ag^+ to Chalcopyrite Bioleaching by Mesophilic and Thermophilic Cultures

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Zhang Duorui Zheng Lei Ma Chenyan Zhao Yidong Wen Wen

Key words Chalcopyrite, Bioleaching, Ag^+, Mesophilic Culture, Thermophilic Culture, SR-XRD, XANES

The catalytic mechanism of Ag^+ for chalcopyrite bioleaching by mesophilic culture (at 30 ℃) and thermophilic culture (at 48 ℃) was investigated using synchrotron radiation-based X-ray diffraction (SR-XRD) and S K-edge and Fe L-edge X-ray absorption near edge structure (XANES) spectroscopy. Bioleaching experiments showed that copper extraction from chalcopyrite bioleaching by both cultures was promoted significantly by Ag^+, with more serious corrosion occurring on the minerals surface. SR-XRD and XANES analyses showed that the intermediates S^0, jarosite and secondary minerals (bornite, chalcocite and covellite) formed for all bioleaching experiments. For these secondary minerals, the formation of bornite and covellite was promoted significantly in the presence of Ag^+ for both cultures, while Ag^+ has almost no effect on the formation of chalcocite. These results provided insight into the catalytic mechanisms of Ag^+ to chalcopyrite bioleaching by the mesophilic and thermophilic cultures, which are both probably due to the rapid formation of bornite by Ag+ and the conversion of bornite to covellite.

Minerals, 2018, **8**(9): 382

Improvement of Corrosion Resistance of Hastelloy-N Alloy in LiF-NaF-KF Molten Salt by Laser Cladding Pure Metallic Coatings

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Key words laser cladding, Hastelloy-N alloy, metallic coating, corrosion resistance, FLiNaK molten salt

The corrosion protection of Hastelloy-N alloy in LiF-NaF-KF (commonly referred to as FLiNaK) molten salt has been developed by pure Ni and Co coatings using the laser cladding technique. An immersion experiment with samples was performed in molten FLiNaK salt at 900 ℃ for 100 h. It was found that the corrosion rates of the pure Ni-coated specimen and the pure Co-coated specimen are 39.9% and 35.7% of that of Hastelloy-N alloy, respectively. A careful microstructural characterization indicates that a selective dissolution of the elemental Cr occurred in the surface of bare Hastelloy-N alloy, showing a severe intergranular corrosion. For pure metal-coated specimens, in contrast, only metal oxide formed during the laser cladding process dissolved into the molten fluoride salt. The dense pure metal (Ni or Co) coatings exhibit a slightly general corrosion and protect the Hastelloy-N substrate effectively. The possible corrosion mechanism for both coated and uncoated Hastelloy-N under the current experimental condition are discussed in this work.

Coatings, 2018, **8**(9): 322

Formation of chromium carbide coatings on HT250 steel by thermal diffusion processes in fluoride molten salt bath

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Sun Hua Zhang Peng Xie Leidong

Key words Fluoride molten salt, Thermal diffusion processes, Chromium carbide coatings

LiF-NaF-KF (46.5-11.5-42 mol %, FLiNaK) molten salt was used in the thermal diffusion (TD) process to form chromium carbide coatings on gray cast iron HT250 at 900 ℃ for 8 h. The structure and chemical composition of the coating were observed by scanning electron microscopy coupled with energy dispersive X-ray microanalysis (SEM-EDX) and X-ray diffraction (XRD). Both the nanoindentation hardness and Vickers hardness were measured. A 3-5 μm thick chromium

carbides layer and approximately 10 μm thick transition layer were formed on the surface of gray cast iron HT250. The chromium carbides layer was composed of $Cr_{23}C_6$ and Cr_7C_3. The hardness of gray cast iron HT250 was increased 6 times after treatment. The tribological behavior was also improved. These results demonstrate that fluoride salts can be used as base salts to form excellent chromium carbides coatings via the TD process.

Vacuum, 2018, **155**: 219

Optimization of Th-U fuel breeding based on a single-fluid double-zone thorium molten salt reactor

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Chen J. G. Xu H. J.

Key words Molten salt reactor, Neutronics and modeling, Th-U fuel breeding

Molten salt reactor (MSR) shows great promise of high thermal-electric conversion efficiency, inherent safety, and on-line reprocessing. Furthermore, fuel breeding can be realized in both thermal and fast spectrum reactors with Th-U fuel cycle, which can make use of the abundant resource of thorium.

In order to combine the advantages of high breeding ratio (BR) in fast spectrum and low fissile inventory for criticality in thermal spectrum, a single-fluid double-zone thorium-based molten salt reactor (SD-TMSR) core configuration is proposed. First, assemblies in both the inner and the outer zones are optimized by adjusting the ratios of molten salt and graphite with consideration of BR, ^{233}U inventory, double time (DT), and temperature coefficient of reactivity (TCR) at the startup time, aiming to have a minimal DT for fuel breeding and a negative TCR for security. The results show that DT has the optimum value when the ratios of molten salt and graphite in the inner zone and the outer zone are 0.357 and 1.162, respectively. And the TCR can be improved to -2 pcm/K when the side length of the graphite hexagonal prism is 7.5 cm. Then, based on the optimized geometry, the bum-up calculations with a series of on-line reprocessing rates are carried out with a self-developed MSR reprocessing sequence (MSR-RS). The results show that on-line reprocessing is beneficial to the Th-U fuel breeding. When the reprocessing rate is 200 *l/d*, iso-breeding can be achieved. When the reprocessing rate is 5 m^3/d, the performance of Th-U breeding is improved significantly, and only 16 years is needed for the ^{233}U doubling. The results also show that TCR remains negative and inherent safety is satisfied during all the operation time.

Progress in Nuclear Energy, 2018, **108**: 144

Fuel pebble optimization for the thorium-fueled Pebble Bed Fluoride salt-cooled high-temperature reactor (PB-TFHR)

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Key words FHR, Pebble, Thorium, Temperature coefficient of reactivity, Burnup

Thorium-fueled Pebble Bed Fluoride salt-cooled High-temperature Reactor (PB-TFHR) is a newly developed reactor concept featuring the technology of High Temperature gas-cooled Reactor (HTR) and the molten salt cooling for thorium-based fuels. To attain a deep bumup with enough negative temperature coefficient of reactivity (TCR), a systematic study for the graphite-to-heavy metal ratio (C/HM) from 66 to 800 and the ^{233}U-to-HM ratio (^{233}U/HM) from 5.0% to 20.0% are carried out. Neutronics characteristics, including the effective multiplication factor (k_{eff}), the TCR and the conversion ratio (CR) are analyzed in terms of neutron usage, core safety and bumup. The results show that the fuel pebble with a higher ^{233}U/HM owns a wider range of under moderated area, which is favorable to improve TCR. Moreover, a strongly negative TCR is obtained by optimizing the C/HM and ^{233}U/HM ratios. In order to evaluate the ^{233}U saving for thorium based fuel, the bumup per fissile mass (Bu) is introduced. Bu can be improved through reducing C/HM, and it increases firstly and then achieves saturation as ^{233}U/HM increases. A bumup level of 122 GWd/tHM can be achieved for the recommended pebble design with ^{233}U/HM of about 12.5% and C/HM of about 124. With the optimized design, an improved TCR can be obtained with a value of about -2.77 pcm/K, which is much more superior to our previous work.

Progress in Nuclear Energy, 2018, **108**: 179

AlN coatings on Hastelloy-N alloy offering superior corrosion resistance in LiF-KF-NaF molten salt

Zhu Hongmei Li Baichun Chen Minghui Liu Zhili Tang Zhongfeng Qiu Changjun

Key words Hastelloy-N alloy, Laser cladding, AlN coating, Corrosion resistance, LiF-KF-NaF molten salt

High-temperature corrosion resistance is a big issue for structural materials in molten salt reactors. A simple but effective laser cladding technique has been utilized for producing a compact AlN coating on Hastelloy-N alloy. The results show that the laser-cladded AlN coating improves the compatibility of Hastelloy-N alloy in LiF-NaF-KF molten salt at 900℃ significantly. The

uncoated Hastelloy-N alloy is composed of γ-Ni and M_6C phases, showing a typical intergranular corrosion with a precipitation of new $Cr_9Mo_{25}Ni_{20}$ phase after corrosion. In contrast, the AlN coating exhibits a silghtly unifrom corrosion and protects the Hastelloy-N substrate effectively. The laser-cladded specimes are composed of γ-Ni and AlN before and after corrosion. The possible reasons for the discrepancy in the corrosion behavior between uncoated and coated specimens are discussed in this job.

Journal of Fluorine Chemistry, 2018, **213**: 80

Influence of α-Al_2O_3 and AlF_3 on pyrohydrolysis of Li_3AlF_6

Peng Jia Zheng Xiaobei Liu Yuxia Zhang Lan

Key words Pyrohydrolysis, Accelerator, Li_3AlF_6 molten salt, Reaction mechanism

In this study, Li_3AlF_6 was employed to simulate the molten salt LiF-BeF_2 to explore its pyrohydrolysis behavior and that of its components, i.e., LiF and AlF_3, respectively. The influence of the accelerators alpha-Al_2O_3 and AlF_3 on the pyrohydrolysis of LiF and Li_3AlF_6 was investigated. Finally, the solid pyrohydrolytic products were characterized by means of X-ray diffraction, and the corresponding reaction mechanisms were proposed. These experimental results indicated that AlF_3 was completely hydrolyzed to the corresponding oxide α-Al_2O_3 at 650 ℃ in 1h, whereas the complete hydrolysis of LiF and Li_3AlF_6 required the assistance of either α-Al_2O_3 or AlF_3 under the same conditions. The influence of the accelerator α-Al_2O_3 and AlF_3 on the pyrohydrolytic behavior of Li_3AlF_6 provides references for future research studies on the pyrohydrolysis of LiF-BeF_2 and multi-component molten salts.

Nuclear Science and Techniques, 2018, **29**(9): 125

Mechanical-force-promoted peptide assembly: a general method

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Lou Shitao Zhang Yi

Key words Self-assembly, Peptide, Nanomechanical stimulus, Support lipid bilayers, Atomic force microscope

A general method was developed for promoting peptide assembly and protein polymerization to form nanoscale patterns on various surfaces with an atomic force microscope (AFM) operated in a liquid. By scanning solid surfaces with an AFM tip, we showed that peptide monomers assemble

at a higher rate in the tip-scanned area compared to other regions. The promotion is attributed to the mechanical force applied by the scanning tip. This kind of mechanical-force-promoted assembly was also observed with different peptides on various substrates. The force promoting peptide assembly provides a simple and practical solution for preparing and building peptide and protein architectures for future nanodevices.

Nuclear Science and Techniques, 2018, **29**(9): 131

Electronic structure tuning during facile construction of two-phase tungsten based electrocatalyst for hydrogen evolution reaction

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Chen Zhaoyang Sun Fanfei Xu Yinghua

Key words Electrocatalysis, Tungsten phosphide, Tungsten carbide, Hydrogen evolution reaction, X-ray absorption spectroscopy

Fabrication of effective electrocatalysts combining two pure phases including carbide and phosphide with a certain proportion by the clean and simple strategies still remain a challenge. Here we synthesized tungsten carbide/tungsten phosphide-coated N-doped carbon (W_2C/WP@NC) by one-step pyrolysis process without participation of PH_3. In this synthesis process phosphotungstic acid, a heteropolyacid provided P and W atoms while 2,6-diaminopyridine, a heterocyclic compound with strong alkalinity acted as C and N source. 2,6-diaminopyridine was carefully chosen because it made a contribution to the complete decomposition of phosphotungstic acid where WO_4^{2-} and PO_4^{3-} groups were formed which both were essential to formation of WP phases. An overpotential of 83 mV which was required to achieve a current density of 10 mA cm^{-2} in 0.5 M H_2SO_4 exhibited the high electrocatalytic activity of W_2C/ WP@NC catalyst in hydrogen evolution reaction (HER). The weight ratio of W_2C/WP was calculated by Rietveld refinement and near edge X-ray absorption fine structure (XANES). W L_3-edge XANES spectra of different samples confirmed that little amount of WP could tune the electron state on W species. The enhanced HER performance was attributed to the favorable electron distribution on W species in W_2C/ WP@NC which approached to the balance between H-atom adsorption and desorption.

Electrochimica Acta, 2018, **283**: 834

Molten-salt synthesis of porous $La_{0.6}Sr_{0.4}Co_{0.2}Fe_{0.8}O_{2.9}$ perovskite as an efficient electrocataiyst for oxygen evolution

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Wang Yu Han Ling Long Youwen Hu Zhiwei Wang Jianqiang

Key words Iron-Rich, Perovskite, Oxygen Evolution Reaction, Energy Storage And Conversion, Molten Salt

The development of an efficient and low-cost electrocatalyst for the oxygen evolution reaction (OER) *via* an eco-efficient route is a desirable, although challenging, outcome for overall water splitting. Herein, an iron-rich $La_{0.6}Sr_{0.4}Co_{0.2}Fe_{0.8}O_{2.9}$ (LSCF28) perovskite with an open porous topographic structure was developed as an electrocatalyst by a straightforward molten-salt synthesis approach. It was found that porosity correlates with both the iron content and the molten-salt approach. Benefiting from the large surface area, high activity of the porous internal surface, and the optimal electronic configuration of redox sites, this inexpensive material exhibits high performance with a large mass activity of 40.8 $A.g^{-1}$ at a low overpotential of 0.345 V in 0.1 M KOH, surpassing the state-of-the-art precious metal IrO_2 catalyst and other well-known perovskites, such as $Ba_{0.5}Sr_{0.5}Co_{0.8}Fe_{0.2}O_3$ and $SrCoO_{2.7}$. Our work illustrates that the molten-salt method is an effective route to generate porous structures in perovskite oxides, which is important for energy conversion and storage devices.

Nano Research, 2018, **11**(9): 4796

Preliminary in situ teeth study of the narrow-ridged finless porpoises remains using microsynchrotron radiation X-ray fluorescence and laser ablation inductively coupled plasma mass spectrometry

Zheng Yi Zhang Ya Tang Wenqiao Guo Hongyi Zhu Yan
Dong Zhaohui Jiang Hui

Key words Nuclear Microprobe, Marine, PIXE, Enamel, Diet

In recent years, a growing number of the narrow-ridged finless porpoises were found dead near the Yangtze River estuary. In this region lived two sympatric subspecies, respectively, the East

Asian finless porpoise and the Yangtze finless porpoise. So far, it is difficult to distinguish these two subspecies due to their similar shape and unavailable molecular marker. In this work, synchrotron radiation X-ray fluorescence (SRXRF) and laser ablation inductively coupled plasma mass spectrometry (LA-ICP-MS) were applied for in situ teeth trace chemical analysis to study subspecies identification and migration near the Yangtze River estuary. Teeth Sr concentration and $^{87}Sr/^{86}Sr$ ratios, determined by SRXRF and LA-ICP-MS techniques, have potential application in the identification of the finless porpoise subspecies. Only one (Sample S4) of the six samples was concluded as the Yangtze finless porpoise, and the others were the East Asian finless porpoise. This study also proved that the Sr/Ca and Zn/Ca ratios could be used as a useful environmental indicator to detect the migratory history of narrow-ridged finless porpoises.

X-Ray Spectrometry, 2018, **47**(5): 388

First-principles study on structural, mechanical and electronic properties of thorium dichalcogenides under high pressure

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Ke Xuezhi Huai Ping

Key words Phase transition, Phonon dispersion, Elastic constant, Semiconductor-metal transition, First-principles calculations

By merging ab initio calculations and particle-swarm optimization algorithm, we have predicted two new phases of thorium dichalcogenides ThX_2 (X = S, Se and Te) in the $Fm\bar{3}m$ and *I4/mmm* symmetry. The $Fm\bar{3}m$ phase is proved to be the ground-state phase of ThS_2 and ThSe2. The calculated enthalpies indicate that the $Fm\bar{3}m$ to *Pnma* phase transition pressures are about 2.3 GPa and 0.35 GPa for ThS_2 and $ThSe_2$, respectively, and the *Pnma* to *I4/mmm* phase transition pressures are about 37 GPa, 17 GPa and 2 GPa for ThS_2, $ThSe_2$ and $ThTe_2$, respectively. The phonon dispersion curves and elastic constants suggest that all of the $Fm\bar{3}m$, *Pnma* and *I4/mmm* phases are dynamically and mechanically stable. The electronic calculations show that a pressure-induced semiconductor to metal transitions of these three compounds will occur following the *Pnma* to *I4/mmm* phase transition. Our calculated bulk modulus B_0 and elastic constants C_{ij} of the various phases of these compounds show that the materials become softer one after another from ThS_2 to $ThSe_2$ and then to $ThTe_2$.

Journal of Nuclear Materials, 2018, **508**: 147

Research on chemical durability of iron phosphate glass wasteforms vitrifying SrF_2 and CeF_3

Liu Xueyang Qiao Yanbo Qian Zhenghua Ma Hongjun

Key words Iron phosphate glass, Fluoride, Vitrifying, Chemical durability

A part of the radioactive waste produced in the Thorium Molten Salt Reactor (TMSR) will be present as fluorides. Because of some characters of fluoride, it is undesirable for immobilizing the waste as other usual oxide waste in borosilicate glass that often produces immiscibility. However, iron phosphate glasses have been made with up to 30 wt% SrF_2 and 20 wt% CeF_3, and about 20 wt% SrF_2 and CeF_3 combined. The iron phosphate glass matrix mixed with fluoride waste could be melted at temperatures between 1050 ℃ and 1200 ℃ in only 30-60 min, its melting temperature is lower than that of borosilicate glass. Powder X-ray diffraction (XRD) showed that the glassy wasteforms that contains more than 20 wt% SrF_2 and CeF_3 mixture, or more than 20 wt% CeF_3 would start crystallizing. The product consistency test (PCT) was used to identify the chemical durability of the glass. Glass powder (-100 to +200 mesh) after washing was soaked in 10 ml of deionized water at 90 ℃ for 7 days. The normalized elemental mass release of elements Sr, Ce and F were calculated at the level of 10^{-3} g/m^2, through the concentration of element measured after PCT, that was equivalent to or better than that of borosilicate glass wasteforms. Iron phosphate glasses are concluded to be a practical alternative for vitrifying the radioactive waste of TMSR.

Journal of Nuclear Materials, 2018, **508**: 286

Microstructural evolution of amorphous Si_2BC_3N nanopowders upon heating at high temperatures: High pressures reverse the nucleation order of SiC and BN(C)

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Chen Qingqing Yang Zhihua Tian Feng Li Xiaoyun Zhou Yu

Key words amorphous, crystallization, high pressure, mechanical alloying, Si-B-C-N

Amorphous Si_2BC_3N nanopowders (NPs) were heated at 1000-1700 ℃ temperatures for 30minutes in 1atm N_2. The changes in phases, chemical bonds, and microstructures were investigated by XRD, XPS, NMR, TEM, and first-principles calculation. Increases in heating temperatures lead to the nucleation and growth of SiC and BN(C) grains, along with partial transformation of SiC_4 units from amorphous to β/α-SiC, and collapse of B-C-N bonds. SiC

nucleates prior to BN(C) at 1atm, while it goes in the opposite order at high pressures (≥1 GPa). High pressures also shift the initial temperatures of crystallization of amorphous Si_2BC_3N NPs from 1400 ℃ (1atm) to 1150 ℃ (5GPa).

Journal of the American Ceramic, 2018, **101**(9): 4321

A Green and lower-temperature synthesis of two-color fluorescent nitrogen dopedgraphene quantum dots

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Key words N-doped graphene quantum dots, Two-color fluorescent emission, Dye sensitizer, Photocatalytize degradation

Herein, the nitrogen-doped graphene quantum dots (N-GQDs) were produced by a facile thermal treating strategy at low temperature using citric acid (CA) and urea as the precursors. The as-prepared N-GQDs with different ratios of the precursors exhibited blue or green emission with relatively high quantum yield in the ethanol solution. While in the aqueous solution, the quantum dots displayed both blue and green emissions, which indicate two independent luminescent centers coexisted in the N-GQDs. Considering of the excellent absorption ability of the N-GQDs in the visible-light region, the N-GQDs was combined with titanium dioxide (TiO_2) as the dye sensitizer. And, the products showed 16 times catalytic degradation ability than that of pure TiO_2 for rhodamine B (RhB).

Dyes and Pigments, 2018, **156**: 379

Directed flow in an extended multiphase transport model

Guo Chong-Qiang Liu He Xu Jun

Key words Microscopic Models, Matter

We have studied the rapidity-odd directed flow in $^{197}Au+^{197}Au$ collisions in the beam energy range from $\sqrt{S_{NN}}$ = 7.7 to 39 GeV within the framework of an extended multiphase transport model with both partonic and hadronic mean-field potentials incorporated. Effects of the partonic scatterings, mean-field potentials, hadronization, and hadronic evolution on the directed flow are investigated, and it is found that the final directed flow is mostly sensitive to the partonic scatterings and the hadronization mechanism. Our study shows that a negative slope of the proton directed flow does not necessarily need the equation of state with a first-order phase transition.

Physical Review C, 2018, **98**(2)

Hydrogen embrittlement susceptibility of a Ni-16Mo-7Cr base superalloy

Han Fenfen He Suixia Liu Min Zhou Xingtai

Key words Hydrogen embrittlement, Nickel base superalloy, Intergranular cracking, Scanning electron microscopy

This study investigated the hydrogen embrittlement sensitivity of a Ni-16Mo-7Cr base superalloy under different hydrogen pre-charging states. Detailed electromicroscopy characterization has been employed on the hydrogen pre-charged alloy after tensile testing to understand the mechanism of hydrogen-assisted cracking. The results show that the tensile strength of the alloy is remarkably decreased with the increasing of hydrogen pre-charging time, whereas the yield strength remains stable all the time. The fractographic study combined with ECCI analysis by Scanning Electron Microscopy demonstrates that the cracks propagated predominantly along the grain boundary in the presence of hydrogen, and a few can propagate along planar dislocation slip bands (DSBs) especially along the intersections between nonparallel DSBs. The proposed hydrogen embrittlement mechanism for the Ni-16Mo-7Cr base superalloy is that the coalescence and widening of the nano-voids, which are resulted from the interaction between the hydrogen and dislocations, cause the crack initiation and propagation along the grain boundary, and further cause the alloy intergranular fracture.

Materials Science & Engineering A: Structural Materials: Properties, Microstructure and Processing, 2018, **733**: 291

Understanding and prediction of the structures of ligand-protected gold nanoclusters using electron counting rule

Gao Yi Xu Wenwu Zeng Xiao

256th National Meeting and Exposition of the American-Chemical-Society (ACS) - Nanoscience, Nanotechnology and Beyond

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Abstracts of Papers of the American Chemical Society, 2018, **256**: 734

Structural evolution of metal nanoparticles in operando conditions

Gao Yi Zhu Beien

256th National Meeting and Exposition of the American-Chemical-Society (ACS) - Nanoscience, Nanotechnology and Beyond

Abstracts of Papers of the American Chemical Society, 2018, **256**: 27-CATL

Irradiation resistance study of binderless nanopore-isotropic graphite for use in molten salt nuclear reactors

Liu Min Zhang Wenting Song Jinliang Zhang Heyao
Lian Pengfei Gao Yantao Zhang Can He Zhoutong
Liu Zhanjun Zhao Mingwen Xia Huihao
Liu Xiangdong Zhou Xingtai

Key words Nanopore-isotropic graphite, Irradiation stability, Microstructure, Mechanical properties

Binderless nanopore-isotropic graphite (NPIG) produced from mesocarbon microbeads by isostatic pressing method was irradiated with 7 MeV Xe^{26+} to a total peak dose of 0.1, 0.5, 2.5 and 5.0 dpa. The effect of the irradiation on the microstructure and physical properties of NPIG was then evaluated and compared against the performance of isostatic nuclear graphite (IG-110, TOYO TANSO CO., LTD). Ion-irradiation has a different effect on the microstructure (crystallinity, crystallite size) and mechanical properties (hardness, Young's modulus) of NPIG and IG-110 graphite. At lower irradiation doses, the surface morphology of NPIG was fragmented in a similar way to that of IG-110, but the NPIG gradually balled at 5 dpa. X-ray diffraction results show that NPIG has a lower degree of graphitization than IG-110. Raman studies indicated that NPIG reached saturation at lower doses. The nanoindentation showed that the hardness and Young's modulus of the NPIG and IG-110 increased after irradiation. Transmission electron microscopy images also provide clear evidence for an irradiation-induced increase in the number of basal dislocations and defects. Thus, although NPIG is generally more sensitive to irradiation than IG-110, its hardness is actually less affected.

Nuclear Engineering and Design, 2018, **335**: 231

Dynamic characteristics identification of two graphite bricks in molten salt reactor considering fluid-structure interaction

Zhong Yang Yang Xiong Ding Dong Zou Yang Tsang D. K. L.

Key words Nuclear graphite, Fluid-structure interaction, Added mass, Added damping, ABAQUS

Graphite core plays a very important role in thorium molten salt reactor (TMSR) served as a reflector, a moderator as well as a structural material. The whole graphite core is submerged in molten salt during operation and consists of a large number of graphite bricks interconnected with keys and dowels. The molten salt as a fluid will affect the dynamic behavior of the graphite core. This phenomenon is called fluid-structure interaction (FSI). In order to maintain the integrity of the graphite core under a seismic event, it is essential to predict dynamic characteristics of the graphite bricks affected by FSI. In this paper a 1/4 scaled-down test model derived from similarity analysis will be presented. The nonlinear response of the graphite brick under the excitation of the sinusoidal harmonic is regarded as a single degree of freedom system. The dynamic characteristics of added mass and added damping can be obtained by fitting the time history of models' displacement subjected to simple harmonic motion. The experimental results shown that the added mass and the added damping are strongly dependent on the gap size between two bricks. Furthermore, a three-dimensional finite element model has been derived for the dynamic analysis of two graphite bricks with molten salt and the modelling parameters are obtained from the experiment. We found that the results from the numerical method are in good agreement with the experiment.

Nuclear Engineering and Design, 2018, **335**: 409

Unexpected refacetting of palladium nanoparticles under atmospheric N_2 conditions

Zhang Xun Meng Jun Zhu Beien Yuan Wentao Yang Hangsheng Zhang Ze Gao Yi Wang Yong

Key words In-Situ Observation, CO Oxidation, Electron-Microscopy, Copper Nanocrystals, Pd Nanocrystals, Shape Evolution, Hydrogenation, Catalysts, Pressure, Methane

We demonstrate an unexpected refacetting process of Pd nanoparticles, induced by N_2 under atmospheric pressure at elevated temperatures, by in situ TEM observations. The morphology

changes, with a notable increase in the fraction of Pd{110} facets, were visualized by atomic-scale TEM images and further explained by theoretical calculations. Firm evidence and rational understanding revealed that the inert gas N_2 has the ability to modify the structure of metal nanoparticles. This surprising effect should be considered seriously in vast chemical applications that use N_2 as a carrier gas or protective atmosphere.

Chemical Communications, 2018, **54**(62): 8587

Sol-Gel Technology Plus Radiation Curing: A Novel and Facile Technique for Preparing Thick, Large-Area Hyperbranched Polysiloxane Hybrids

Chen Shaoyun Zhuo Dongxian Hu Jiangtao

Key words Epoxy-Resins, Advanced Composites, Thermal-Properties, Surface-Properties, Cyanate Ester, Coatings, Polymers, Polymerization, Nanocomposite, Kinetics

Large-scale shrinkages and holes are the two critical disadvantages of the silicone resin prepared by the sol- gel technology and cured via traditional processes. To simultaneously overcome both problems, sol-gel technology along with gamma-radiation curing is developed for preparing organic- inorganic hybrids with large size and thicknesses. A hyperbranched polysiloxane (H-PMAPS) is successfully synthesized through the controlling hydrolysis of 3-methacryloxypropyltrimethoxysilane and then is subjected to nuclear magnetic resonance (Si NMR) and Fourier transform infrared (FTIR) spectra to characterize its structure. Room-temperature radiation curing followed by thermal curing out-of-the-mold at 170 ℃ for 3h is suitable for curing H-PMAPS (denoted as RC-T/PMAPS). The RC-T/PMAPS hybrid exhibits a homogeneous phase with a riverlike morphology, excellent thermal resistance, and dielectric properties and is optically transparent. These attractive features of the RC-T/PMAPS hybrid suggest that the new approach proposed here is suitable for cutting-edge industries to develop high-performance organic-inorganic hybrids.

Industrial & Engineering Chemistry Research, 2018, **57**(31): 10372

Gain-guided X-ray free-electron laser oscillator

Li Kai Deng Haixiao

Key words Simulation, Facility, Operation, Optics

The X-ray free-electron laser oscillator (XFELO) has recently come to be reconsidered as a promising candidate for producing high-brightness, fully coherent pulses in the hard X-ray regime. This letter proposes a gain-guided XFELO scheme, without the need for the external focusing elements that are required in a conventional configuration. Self-consistent theoretical analysis and three-dimensional numerical simulation results verify that the X-ray transverse mode in such an "unstable" cavity is stable and robust owing to electron beam gain-guiding. The output pulse energy and the transverse and longitudinal coherence are comparable to those from conventional XFELOs. This promising scheme is expected to contribute significantly to the construction and operation of a real XFELO. Published by AIP Publishing.

Applied Physics Letters, 2018, **113**(6): 061106

pH-sensitive microfiltration membrane prepared from polyethersulfone grafted with poly(itaconic acid) synthesized by simultaneous irradiation in homogeneous phase

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Hu Jun Hou Zhengchi

Key words graft polymerization, membrane, pH-sensitive, polyethersulfone, poly(itaconic acid)

Poly(itaconic acid) (PIA) was grafted onto polyethersulfone (PES) by homogeneously phased gamma-ray irradiation. Kinetic polymerization observed was studied by analyzing the effect of irradiation dosages and monomer concentrations. Then, a pH-sensitive microfiltration (MF) membrane was prepared from these PES-g-PIA polymers with different degrees of grafting under phase inversion method. Finally, the contact angles, morphologies, pore sizes, deionized water permeability and filtration performance for aqueous polyethylene glycols solution of the MF membranes were studied. The results show that grafting PIA groups onto PES molecular chains endowed the MF membranes with effective pH-sensitive properties.

Water Science and Technology, 2018, **78**(3): 602

A 1-m non-resonant inelastic x-ray scattering spectrometer at BL15U, Shanghai Synchrotron Radiation Facility

Ni Dongdong Kang Xu Yan Shuai Huang Xinchao Xiong Tao
Liang Dongxu Yang Ke Zhu Linfan

Key words Resolution, Spectroscopy, Performance, Detectors, Analyzer, Beamline

We report the design, construction, and commissioning of a spectrometer for non-resonant inelastic x-ray scattering study installed at BL15U, Shanghai Synchrotron Radiation Facility. It features a 1-m vertical scattering arm. An energy resolution of 1.3 eV is achieved based on the 1m Rowland circle and the diced Si(555) crystal analyzer with a fixed Bragg angle of about 88.8 degrees. The inelastic squared form factors of $2^1S + 2^1P$ of helium with respect to the momentum transfer were measured and compared with the accurate and reliable theoretical calculations in order to verify the spectrometer. Furthermore, the spectrometer is designed to work in the momentum transfer region of 0 $Å^{-1}$ <q< 8.68 $Å^{-1}$ and to initially focus on the non-resonant inelastic x-ray scattering studies on gaseous samples. Published by AIP Publishing.

Review of Scientific Instruments, 2018, **89**(8)

The properties of surface nanobubbles formed on different substrates

Zou Zhenglei Quan Nannan Wang Xingya Wang Shuo
Zhou Limin Hu Jun Zhang Lijuan Dong Yaming

Key words Nanobubbles, Atomic Force Microscopy, Contact Angle, Hydrophobic Modification

The properties and stability of the reported surface nanobubbles are related to the substrate used and the generation method. Here, we design a series of experiments to study the influence of the hydrophobicity of the substrate and the production method on the formation and properties of nanobubbles. We choose three different substrates, dodecyltrichlorosilane (DTS) modified silicon, octadecyltrichlorosilane (OTS) modified silicon, and highly oriented pyrolytic graphite (HOPG) as nanobubble substrates, and two methods of ethanol-water exchange and 4℃ cold water to produce nanobubbles. It is found that using ethanol-water exchange method could produce more and larger nanobubbles than the 4℃ cold water method. The contact angle of nanobubbles produced by ethanol-water exchange depends on the hydrophobicity of substrates, and decreases with the increase of the hydrophobicity of substrates. More interestingly, nanoscopic contact angle

approaches the macroscopic contact angle as the hydrophobicity of substrates increases. It is believed that these results would be very useful to understand the stability of surface nanobubbles.

Chinese Physics B, 2018, **27**(8)

A modular process for the treatment of high level liquid waste (HLLW) using solvent-impregnated graphene aerogel

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Chen Aimei Li Qingnuan Zhang Lan

Key words Graphene aerogel, Solvent impregnated adsorbent, Modular process, HLLW

Graphene aerogel (GA) is a kind of superhydrophobic material with low density, high specific surface area and porosity. It can be used as modular matrix material to be impregnated with extractant due to its excellent organic solvent immobilization performance. In this paper, the modular GA based solvent impregnated adsorbents (GASIA) with various extractants were prepared. The adsorption performance of these adsorbents for typical fission products in high level liquid waste (HLLW) was investigated, and it is found that the adsorption performance is strongly dependent on the impregnated extractants. Based on the batch adsorption experiments, a modular process for the treatment of HLLW was proposed and tested. The results demonstrate that the modular process based GA-SIA possesses advantages of high selectivity, simple operation and low cost.

Hydrometallurgy, 2018, **179**: 167

Stress and thickness calculation of a bolted flat cover with double metal sealing rings

Wang Xiaoyan Zhu Shifeng Wang Xiao Zhang Xiaochun

Key words Thickness calculation equation, Pressure vessel, Bolted flat cover, Double metal sealing rings, Design codes

The design of a bolted flat cover is extremely important for the structural integrity of pressure vessels. The present design codes provide the thickness calculation equations for a bolted flat cover with single metal gasket. However, the rules for a bolted flat cover with double metal sealing rings are not developed to date. In the study, a new thickness calculation equation for the bolted flat cover with double metal sealing rings is proposed. First, the theoretical stress solution for bolted

flat cover with the double metal sealing rings is obtained, based on the theory of simply supported circular plate and then verified using the results from finite element analyses. The results indicate that the influence of double metal sealing ring on the stress of the flat cover is more serious compared to single metal gasket. Second, a more accurate and reasonable equation is proposed to calculate the thickness of bolted flat cover with double metal sealing rings based on the derived theoretical equations of maximum stress. Finally, the influence of linear load and the spacing between rings on the thickness are discussed. Subsequently, a few suggestions are provided to design low-pressure or atmosphere pressure vessels. The study provides a theoretical foundation to develop design codes of pressure vessels in nuclear reactors.

Nuclear Science and Techniques, 2018, **29**(8): 120

Analysis of Th-U breeding capability for an accelerator-driven subcritical molten salt reactor

Zhao Xuechao Cui Deyang Cai Xiangzhou Chen Jingen

Key words Subcritical, Molten salt fuel, Conversion ratio, Net ^{233}U production

Accelerator-driven systems based on molten salt fuel have several unique advantages and features for advanced nuclear fuel utilization. The aim of this work was to study the Th-U breeding capability in such systems, known as "accelerator-driven subcritical molten salt reactors" (ADS-MSRs). Breeding capacities including conversion ratio and net ^{233}U production for various subcriticalities and different minor actinides (MA) loadings were analyzed for an ADS-MSR. The results show that the subcriticality of the core has a considerable effect on the Th-U breeding. A high subcriticality is favorable to improving the conversion ratio, increasing the net ^{233}U production, and reducing the doubling time. Specifically, the doubling time for k_{eff} of 0.99 is larger than 80 years, while the counterpart for k_{eff} of 0.93 is only approximately 22 years. Nevertheless, in an ADS-MSR with a high initial MA loading, MA results in a non-negligible ^{233}U depletion in the first two decades, while increasing the net ^{233}U production compared to reactors without MA loading. During the 50 years of operation, for the subcritical reactor (k_{eff} = 0.97) with MA fraction increasing from 1 to 14% , the net ^{233}U production increases from 3.94 to 8.24t.

Nuclear Science and Techniques, 2018, **29**(8): 121

Helium ion irradiation-induced microstructure evolution on the surfaces of thin nickel foils

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Yang Guo Li Yan

Key words Nickel foil, Helium ion irradiation, Ripple patterns, Compressive stress, Protrusion islands

Polycrystalline nickel foil (sample I) with thickness of ~ 950 nm was irradiated with 0.5-1.2 MeV helium ions at room temperature. Another piece (sample II) with same thickness was mounted behind to receive the irradiation of transmitted helium ions (~0.026-0.537MeV). Morphology evolutions on irradiated surfaces were investigated by scanning electron microscopy (SEM) and atomic force microscopy (AFM). Results show that the open cracks, which were located mainly at grain boundaries, occurred on the surfaces of both irradiated samples. Interestingly, ripple patterns were observed to be regularly arranged on the front surface of sample I. The compressive stress resulting in the sliding on close-packed (111) planes was regarded as the origin of the ripple formation. Moreover, protrusion islands and its surrounding microstructures were observed on the front surface of sample II. The mass transport driven by the lateral stress generated in the helium ion irradiation were discussed as possible reasons.

Nuclear Instruments and Methods in Physics Research Section B: Beam Interactions with Materials and Atoms, 2018, **428**: 24

Spatially correlated coherent diffractive imaging method

Tao Xulei Xu Zijian Liu Haigang Wang Chunpeng
Xing Zhenjiang Wang Yong Tai Renzhong

Coherent diffractive imaging (CDI) is a lensless, high-resolution imaging method that is currently under rapid development by using X-rays, visible light, or electrons. However, its inherent ambiguities and the need of apriori knowledge about objects are limiting applications based on this method. By combining a conventional CDI method with the basic idea of ptychography, the method of spatially correlated CDI, a method fit for multiple sample imaging in single-shot mode, is proposed to enhance the robustness of CDT. In this method, a strong spatial relevancy is built by introducing the same region into each sample, which establishes a strong real-space constraint for image reconstruction. Both simulations and visible-light experiments demonstrated the good imaging quality and robustness of this method, which does not need tight supports.

Applied Optics, 2018, **57**(22): 6527

Solubility of radioactive inorganic salt in supercritical water

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Zhang Hong Wang Kai Liu Xueyang Qian Zhenghua
He Liubin Cai Jun Li Yulan Xia Xiaobin

Key words Solubility, Inorganic salt, Supercritical water, Spent extraction solvent

In order to reduce the deposition of inorganic salt in continuous reactor during the treatment of radioactive spent extraction solvent by supercritical water oxidation, the solubilities of five kinds of radioactive inorganic salts were investigated at temperatures from 390 to 550 °C and pressures from 20 to 25 MPa. The solubilities of inorganic salts were correlated via a semi-empirical approach based on the phase equilibrium between the salt and supercritical water. In addition, parallel hydrolysis of the salts was found as it could be observed from decrease in pH and deviations of anion and cation concentration in the liquid effluent.

Journal of Radioanalytical and Nuclear Chemistry, 2018, **317**(2): 947

Poly-adenine-mediated fluorescent spherical nucleic acid probes for live-cell imaging of endogenous tumor-related mRNA

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Su Shao Li Jiang Wang Lihua Shi Jiye Zuo Xiaolei
Weng Lixing Li Qian Wang Lianhui

Key words Poly-Adenine, Spherical Nucleic Acid Probes, Tumor Related Mrna, Intracellular Detection

Identification of tumor-related mRNA in living cells hold great promise for early cancer diagnosis and pathological research. Herein, we present poly-adenine (polyA)-mediated fluorescent spherical nucleic acid (FSNA) probes for intracellular mRNA detection with regulable sensitivities by programmably adjusting the loading density of DNA on gold nano-interface. Gold nanoparticles (AuNPs) functionalized with polyA-tailed recognition sequences were hybridized to fluorescent "reporter" strands to fabricate fluorescence-quenched FSNA probes. While exposed to target gene, the "reporter" strands were released from FSNA through strand displacement and fluorescence was recovered. With polyA20 tail as the attaching block, the detection limit of FSNA probes was calculated to be 0.31 nM, which is ~55 fold lower than that of thiolated probes without surface density regulation. Quantitative intracellular mRNA detection and imaging could be achieved with

polyA-mediated FSNA probes within 2 hours, indicating their application potential in rapid and sensitive intracellular target imaging.

Nanomedicine-Nanotechnology Biology and Medicine, 2018, **14**(6): 1797

Upgrade of the X-ray pinhole camera system at SSRF

Gao Bo Leng Yongbin Chen Hanjiao Chen Jie Ye Kairong

Key words X-ray pinhole camera, Transverse beam size, Diagnostic beam line, Point spread function, X-ray quasimonochromator

An X-ray pinhole camera has been used to determine the transverse beam size and emittance on the diagnostic beam line of the storage ring at SSRF since 2009. The performance of the beam size measurement is determined by the width of the point spread function of the X-ray pinhole camera. Beam-based calibration was carried in 2012 out by varying the beam size at the source point and measuring the image size. However, this calibration method requires special beam conditions. In order to overcome this limitation, the pinhole camera was upgraded and an X-ray quasi-monochromator was installed. A novel experimental method was introduced by combining the pinhole camera with the monochromator to calibrate the point spread function. The point spread function can be accurately resolved by adjusting the angle of the monochromator and measuring the image size. The X-ray spectrum can also be obtained. In this work, the X-ray quasi-monochromator and the novel beam-based calibration method will be presented in detail.

Nuclear Science and Techniques, 2018, **29**(8): 115

Effects of fuel salt composition on fuel salt temperature coefficient (FSTC) for an under-moderated molten salt reactor (MSR)

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Key words Molten salt reactor (MSR), Fuel salt temperature coefficient (FSTC), Six-factor formula

With respect to a liquid-fueled molten salt reactor (MSR), the temperature coefficient of reactivity mainly includes the moderator temperature coefficient (MTC) and the fuel salt temperature coefficient (FSTC). The FSTC is typically divided into the Doppler coefficient and the density coefficient. In order to compensate for the potentially positive MTC, the FSTC should be

sufficiently negative, and this is mostly optimized in terms of the geometry aspect in pioneering studies. However, the properties of fuel salt also directly influence the FSTC. Thus, the effects of different fuel salt compositions including the ^{235}U enrichment, heavy metal proportion in salt phase (HM proportion), and the ^{7}Li enrichment on FSTC are investigated from the viewpoint of the essential six-factor formula. The analysis is based on an under-moderated MSR. With respect to the Doppler coefficient, the temperature coefficient of the fast fission factors ($\alpha_T(\varepsilon)$) is positive and those of the resonance escape probability ($\alpha_T(p)$), thermal reproduction factor ($\alpha_T(\eta)$), thermal utilization factor ($\alpha_T(f)$), and total non-leakage probability ($\alpha_T(\lambda)$) are negative. With respect to the density coefficient, a $\alpha_T(p)$ and $\alpha_T(\eta)$ are positive, while the others are negative. The results indicate that the effects of the ^{235}U enrichment and HM on FSTC are mainly reflected in $\alpha_T(\varepsilon)$ and $\alpha_T(p)$, which are the dominant factors when the neutron spectrum is relatively hard. Furthermore, the ^{7}Li enrichment influences FSTC by $\alpha_T(f)$ and $\alpha_T(\lambda)$, which are the key factors in a relative soft spectrum. In order to obtain a more negative FSTC for an under-moderated MSR, the possible positive density coefficient, especially its $\alpha_T(p)$, should be suppressed. Thus, a lower ^{235}U enrichment (albeit higher than a certain value, 5 wt% in this article) along with a lower HM proportion and/or a higher ^{7}Li enrichment are recommended. The analyses provide an approach to achieve a more suitable fuel salt composition with a sufficiently negative FSTC.

Nuclear Science and Techniques, 2018, **29**(8): 110

Bunch-by-bunch longitudinal phase monitor at SSRF

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Key words Bunch-by-bunch, Longitudinal phase, Resolution, Pickup signal, Software resampling

Beam signals captured from a button-type pickup contain multidimensional information including the bunch charge, transverse position, bunch length, and longitudinal phase. A bunch phase monitor, which retrieves longitudinal phase information from a pickup signal at a bunch-by-bunch rate, has been developed at the Shanghai Synchrotron Radiation Facility. This paper introduces the basic principles, system setup, data processing method, and preliminary experimental results of this system. The systematic measurement error introduced by the limited system bandwidth, bunch length, and bunch charge variation was studied using simulation data. The random measurement uncertainty was evaluated using experimental beam data. The experimental result shows that the longitudinal phase resolution of this system is better than 1.0 ps. The first application, measuring the relationship between the longitudinal phase and bunch charge to determine the energy loss factor, was implemented, and the preliminary result is also discussed.

Nuclear Science and Techniques, 2018, **29**(8): 113

Visualizing glioma margins by real-time tracking of gamma-glutamyltranspeptidase activity

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Shi Ben Li Jiao Xu Ge Xu Shangchen
Fan Chunhai Zhao Chunchang

Key words Glioma margins, Activatable probe, gamma-Glutamyltranspeptidase, Real-time, Clinical

Distinguishing tumor from adjacent non-cancerous tissue can be problematic during surgical treatment of malignant glioma. Consequently, a novel approach to selective discrimination is required. The goal of this study was to determine whether a fluorescent probe activated by gamma-Glutamyltranspeptidase (GGT), an enzyme that is overexpressed on glioma cell membranes but only minimally expressed in normal brain tissue, could be used to visualize glioma margins. Here, we showed that the GGT-activatable fluorescent probe (NC-B-Cys-γ-Glu) provided real-time in situ tracking of enzyme activity that accurately distinguished glioma from healthy brain tissue. NC-B-Cys-γ-Glu, which featured distinct ratiometric fluorescence responsiveness after interaction with GGT, enabled monitoring of GGT activity in living cells and differentiation between glioma and normal cells. Topical spraying of NC-B-Cys-γ-Glu facilitated real-time *in vivo* identification of orthotopic glioblastomas in a mouse model. Importantly, the tumor, infiltrating area and surrounding normal tissue were distinguished in clinical glioma samples by real-time tracking of GGT activity. When coupled with auto fluorescence bronchoscopy, NC-B-Cys-γ-Glu offered diagnostic value for cancers overexpressing GGT. Therefore, NC-B-Cys-γ-Glu might offer a promising tool to guide maximal yet precise tumor resection while sparing non-cancerous tissue.

Biomaterials, 2018, **173**: 1

Wavelet analysis of extended X-ray absorption fine structure data: Theory, application

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Qu Yongquan Jiang Zheng

Key words EXAFS, Wavelet transform, Local structure, Scattering pathways

Fourier transform (FT) plays an indispensable role in the quantitative analysis of extended X-ray absorption fine structure (EXAFS). The fitting of FT-EXAFS has already solved many scientific issues. However, FT is not well suited for signals which involve transient processes. More

and more complex and obscure systems require to be studied with the development of modern science and technology, especially the complex system showing overlapped single-/multi-scattering pathways in EXAFS spectrum, the unknown system involving atoms with similar atom numbers and some other unusual systems that cannot be solved only by the conventional FT and fitting method. Wavelet transform (WT) of EXAFS spectrums discerns the contribution of each pathway not only in R-space but also in k-space at the same time. The maximums of *k-R* contour map of the WT coefficients' modulus represent the contributions of specific pathways. Together with a priori knowledge or analysis of the system, WT *k-R* map helps us better understand the local structure and improve the fitting model. The most critical issues of WT analysis are how to improve the resolution with the least loss of information, and how to identify the contributions of different pathways quickly and accurately. To meet wider applications in the future, the WT method for EXAFS analysis still need to be improved.

Physica B-Condensed Matter, 2018, **542**: 12

Commentary and introduction to the virtual special issue on nanocarbons for electrochemistry

Yang Nianjun Swain Greg M. Einaga Yasuaki Fan Chunhai

Carbon, 2018, **134**: 539

Facile synthesis of the nitrogen-doped graphene quantum dots at low temperature for cellular labeling

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Key words Graphene quantum dots, Cellular labeling, Cell imaging

A facile one-step approach is developed for the large-scale synthesis of nitrogen doped graphene quantum dot (N-GQDs) at low temperature by using citric acid (CA) as the precursor. The emission wavelength of the N-GQDs is nearly excitation-dependent, which may mirror the effects from particles of different sizes and distribution of different emissive sites on nanoparticles. Moreover, the products are then tested with live Hela cells for the extraordinary biocompatibility. The cellular viability is remained to be 100% even after a 48 h exposure with the high N-GQDs concentration of 200 μg ml^{-1} and this survival rate is really much higher than that have been

repotted previously. The as-prepared N-GQDs with negligible inherent toxicity exhibit excellent biological applications such as bio-imaging and cell tracking.

Materials Research Bulletin, 2018, **104**: 83

Complex silica composite nanomaterials templated with DNA origami

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Li Wei Zhu Bowen Li Jiang Chen Hong Wang Lihua
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Key words Crystal, Nanoscale, Molecules, Nanofabrication, Nanostructure, Orientation, Elasticity, Mechanics, Strategy, Shapes

Genetically encoded protein scaffolds often serve as templates for the mineralization of biocomposite materials with complex yet highly controlled structural features that span from nanometres to the macroscopic scale. Methods developed to mimic these fabrication capabilities can produce synthetic materials with well defined micro-and macro-sized features, but extending control to the nanoscale remains challenging. DNA nanotechnology can deliver a wide range of customized nanoscale two-and three-dimensional assemblies with controlled sizes and shapes. But although DNA has been used to modulate the morphology of inorganic materials and DNA nanostructures have served as moulds and templates, it remains challenging to exploit the potential of DNA nanostructures fully because they require high-ionic-strength solutions to maintain their structure, and this in turn gives rise to surface charging that suppresses the material deposition. Here we report that the Stober method, widely used for producing silica (silicon dioxide) nanostructures, can be adjusted to overcome this difficulty: when synthesis conditions are such that mineral precursor molecules do not deposit directly but first form clusters, DNA-silica hybrid materials that faithfully replicate the complex geometric information of a wide range of different DNA origami scaffolds are readily obtained. We illustrate this approach using frame-like, curved and porous DNA nanostructures, with one-, two- and three-dimensional complex hierarchical architectures that range in size from 10 to 1,000 nanometres. We also show that after coating with an amorphous silica layer, the thickness of which can be tuned by adjusting the growth time, hybrid structures can be up to ten times tougher than the DNA template while maintaining flexibility. These findings establish our approach as a general method for creating biomimetic silica nanostructures.

Nature , 2018, **559**(7715): 593

Effect of plasmonic near field on the emittance of plasmon-enhanced photocathode

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Zhang Meng Gu Qiang

Key words Photocathode, Surface plasmon polaritons, Emittance

The surface plasmon polaritons make the emittance of the electron beam emitted from the photocathode complicated. In this article, numerical investigations are carried out to study the influence of the plasmonic near field (PNF) excited by a square hole array on the beam emittance. The characteristics of the emittance induced by PNF are studied. The coupling between the emittance caused by PNF and the original intrinsic emittance due to the excess energy of electrons and the surface roughness of the cathode is discussed. The results provide insights into the suppression of the emittance caused by PNF and new possibilities to break the limits of the nature of the materials, improving the performance of a photocathode.

Nuclear Instruments and Methods in Physics Research Section A: Accelerators, Spectrometers, Detectors and Associated Equipment, 2018, **897**: 14

Engineering the Coordination Environment of Single-Atom Platinum Anchored on Graphdiyne for Optimizing Electrocatalytic Hydrogen Evolution

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Shu Miao Si Rui Lu Tongbu

Key words Electrocatalysis, Graphdiyne, Hydrogen Evolution, Platinum, Single-Atom Catalysts

Two Pt single-atom catalysts (SACs) of Pt-GDY1 and Pt-GDY2 were prepared on graphdiyne (GDY) supports. The isolated Pt atoms are dispersed on GDY through the coordination interactions between Pt atoms and alkynyl C atoms in GDY, with the formation of five-coordinated C_1-Pt-Cl_4 species in Pt-GDY1 and four-coordinated C_2-Pt-Cl_2 species in Pt-GDY2. Pt-GDY2 shows exceptionally high catalytic activity for the hydrogen evolution reaction (HER), with a mass activity up to 3.3 and 26.9 times more active than Pt-GDY1 and the state-of-the-art commercial Pt/C catalysts, respectively. Pt-GDY2 possesses higher total unoccupied density of states of Pt 5d orbital and close to zero value of Gibbs free energy of the hydrogen adsorption (|ΔGPtH*|) at the Pt

active sites, which are responsible for its excellent catalytic performance. This work can help better understand the structure-catalytic activity relationship in Pt SACs.

Angewandte Chemie International Edition, 2018, **57**(30): 9382

Manipulation of facet orientation in hybrid perovskite polycrystalline films by cation cascade

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Tang Gang Li Runguang Chen Yihua Li Liang Hu Jinsong
Hong Jiawang Chen Qi Gao Xingyu Zhou Huanping

Crystal orientations in multiple orders correlate to the properties of polycrystalline materials, and it is critical to manipulate these microstructural arrangements to enhance device performance. Herein, we report a controllable approach to manipulate the facet orientation within the ABX(3) hybrid perovskites polycrystalline films by cation cascade doping at A-site. Two-dimensional synchrotron radiation grazing incidence wide-angle X-ray scattering is employed to probe the crystal orientations in multiple orders in mixed perovskites thin films, revealing a general pattern to guide crystal planes stacking upon extrinsic doping during crystallization. Different from previous studies, this method enables to adjust the crystal stacking mode of certain crystallographic planes in polycrystalline perovskites. Moreover, the preferred facet orientation is found to facilitate photocarrier transport across the absorber and pertaining interface in the resultant PV device, which provides an exemplary paradigm for further explorations that relate to the microstructures of hybrid perovskite materials and relevant optoelectronics.

Nature Communications, 2018, **9**: 2793

Doping Ti to achieve microstructural refinement and strength enhancement in a high volume fraction Y_2O_3 dispersion strengthened Cu

Zhou Dengshan Wang Xinkai Zeng Wei Yang Chao
Pan Hucheng Li Chenguang Liu Yujie Zhang Deliang

Key words Oxide dispersion strengthened Cu, Microalloying, Yttrium oxide, Microstructural refinement, Strengthening mechanisms, Electrical conductivity

In this work, high volume fraction Y_2O_3 dispersion strengthened Ti-free and Ti-doped Cu samples were prepared by mechanical alloying, high temperature heat treatment and powder compact extrusion to study the role of alloying Ti element on microstructures, mechanical

properties and electrical conductivity of the extruded samples. It is found that the addition of a small amount of 0.4 wt.%Ti effectively suppresses the coarsening of Y_2O_3 particles during material fabrication, which produces smaller and more uniform oxide particles distributed in a homogeneous ultrafine grained Cu matrix. However, a heterogeneous Cu matrix microstructure, consisting of elongated micrometer-scale Cu grains and equiaxed ultrafine Cu grains, is observed in the Ti-free sample due to significant coarsening of the Y_2O_3 particles. The different microstructural features of the two extruded samples lead to distinctively different mechanical behaviors and electrical conductivities. The energy dispersive X-ray spectrometry elemental and high resolution transmission electron microscopy analysis suggest that the stabilizing mechanisms of the Y_2O_3 particles involve both the segregation of Ti atoms to the surface layers of large Y_2O_3 particles and dissolution of Ti atoms into small Y_2O_3 particles to form complex particles.

Journal of Alloys and Compounds, 2018, **753**: 18

Structural and thermodynamic stability of uranyl-deferiprone complexes and the removal efficacy of U(VI) at the cellular level

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Deferiprone (3-hydroxy-1,2-dimethyl-4(1*H*)-pyridone, DFP), which is a drug clinically used for removing heavy metals in vivo, was explored for its removal efficiency towards uranium. The reaction of uranyl nitrate hexahydrate with DFP at room temperature yielded the compound $[(UO_2)(H_2O)(C_7NO_2H_8)_2]4H_2O$ (1), which crystallizes from a mixed solution of methanol and water (pH = 7.0). X-ray diffraction shows that the stable complexation of uranyl occurs from the coordination of two bidentate DFP ligands perpendicular to the O=U=O unit with a fifth coordinating oxygen atom coming from one water molecule, resulting in a pentagonal bipyramidal geometry. The formation constants of uranyl and DFP complexes were measured and the species distribution diagram illustrates that UO_2L_2 (94.6%) is the dominant uranyl-DFP complex in 0.1 M KCl solution at physiological pH = 7.4. The results from both crystallographic and potentiometric studies imply that the metal: ligand ratio is 1:2. The effectiveness of using DFP to remove uranium was examined at the cellular level, and the results suggest that it can significantly reduce the cellular uptake and increase the cellular release of U(VI) in renal proximal tubular epithelial cells (NRK-52E).

Dalton Transactions, 2018, **47**(26): 8764

Equally sloped tomography based X-ray full-field nano-CT at Shanghai Synchrotron Radiation Facility

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Key words X-ray, Full-field, Nano-CT, Equally-sloped tomography

X-ray full-field nano-computed tomography (nano-CT) has non-destructive three-dimensional imaging capabilities with high spatial resolution, and has been widely applied to investigate morphology and structures in various areas. Conventional tomography reconstructs a 3D object from a large number of equal-angle projections. For nano-CT, it takes long collecting time due to the large projection numbers and long exposure time. Here, equallysloped tomography (EST) based nano-CT was implemented and constructed on X-ray imaging beamline at the Shanghai Synchrotron Radiation Facility (SSRF) to overcome or alleviate these difficulties. Preliminary results show that hard TXM with the spatial resolution of 100 nm and the EST-based nano-CT with the ability of 3D nano non-destructive characterization have been realized. This technique promotes hard X-ray imaging capability to nano scales at SSRF and could have applications in many fields including nanomaterials, new energy and life sciences. The study will be helpful for the construction of the new full field X-ray nano-imaging beamline with the spatial resolution of 20 nm at SSRF phase II project.

Nuclear Instruments & Methods in Physics Research Section A-Accelerators Spectrometers Detectors and Associated Equipment, 2018, **896**: 108

Highly Active Surface Structure in Nanosized Spinel Cobalt-Based Oxides for Electrocatalytic Water Splitting

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Lin Xiao Gu Songqi Wu Xiang Weng Tsu-Chien Wang
Jianqiang Zhang Shuo

Spinel cobalt-based oxides are a promising family of materials for water splitting to replace currently used noble-metal catalysts. Identifying the highly active facet and the corresponding coordinated structure of surface redox centers is pivotal for the rational design of low-cost and efficient nanosized catalysts. Using high-resolution transmission electron microscopy and advanced X-ray techniques, as well as ab initio modeling, we found that the activity of Co^{3+} ions exhibits the surface dependence owing to the variability of its electronic configurations. Our calculation shows

that the Co^{3+} site in {100} facet of nanosized $Li_2Co_2O_4$ exhibits an impressive intrinsic activity with low overpotential, far lower than that of the {110} and {111} facets. The unique, well-defined CoO_5 square-pyramidal structure in this nonpolar surface stabilizes the unusual intermediate-spin states of the Co^{3+} ion. Specially, we unraveled that oxygen ion anticipates the redox process via the strong hybridization Co_3d-O_{2p} state, which produces a $3d_z^{21.1}$ filling orbit. Finally, a spin-correlated energy diagram as a function of Co-O distance was devised, showing that the covalency of Co-O significantly affects the spin state of Co^{3+} ions. We suggest that the nonpolar surface that contains CoO_5 units in the edge-sharing systems with the short Co-O bond distance is a potential candidate for alkaline water electrolysis.

Journal of Physical Chemistry C, 2018, **122**(26): 14447

Atomic inner-shell radiation seeded free-electron lasers

Zhang Han Li Kai Yan Jiawei Deng Haixiao Sun Baoyuan

In order to effectively improve the output quality of x-ray free electron laser (XFEL), we theoretically propose an XFEL scheme seeded by atomic inner-shell laser. Atomic inner-shell lasers based on neutral atoms and pumped by XFEL have been experimentally demonstrated [Rohringer *et at.*, Nature (London) 481,488 (2012), Yoneda *et al.*, Nature (London) 524,446 (2015)], which produced sub-femtosecond X-ray pulses with increased temporal coherence. It shows that, by using the inner-shell laser as a seed to modulate the electron bunch, very stable and almost fully-coherent short-wavelength XFEL pulses can be generated. The proposed scheme holds promising prospects in x-ray wavelengths, and even shorter.

Physical Review Accelerators and Beams, 2018, **21**(7): 070701

Highly Durable and Robust Superhydrophobic/Superoleophilic Cotton Fabric with Well-designed Roughness for Oil/Water Separation

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Zhang Maojiang Zhang Kuo Guo Xiaojing
Liu Weihua Wu Guozhong

Key words Superhydrophobicity, Cotton fabric, Oil/water separation, Irradiation grafting, Durability

Herein we report a simple and reproducible method for fabricating highly durable and robust superhydrophobic and superoleophilic cotton fabrics *via* simultaneous radiation-induced graft polymerization of glycidyl methacrylate and subsequent chemical modifications with aminopropyltriethoxysilane and hexamethyldisilazane. The chemical structure and the surface topography of the pristine and the modified cotton fabrics were investigated in detail by ATR-FTIR, XPS, and ^{29}Si NMR, and a grafting layer was successfully immobilized onto the surface of the cotton fabric by forming covalent bonds. Multi-dimensional surface roughness was created by combining micro-sized fibers of the cotton fabric, nanoscaled protuberances of the grafting chain, and molecular level spherical projection points of silicon methyl. The superhydrophobic cotton fabric exhibited long-term stability, ultra-high durability and robustness, and maintained its properties even after 25 wash cycles. The fabric also showed excellent water repellency with a water contact angle of 153° and a high efficiency of oil/water separation (98 %). The superhydrophobic/superoleophilic cotton fabric developed in the present work exhibits important potential applications in superhydrophobic textiles and oil/water separation.

Fibers and Polymers, 2018, **19**(7): 1522

Bifunctional Nitrogen and Cobalt Codoped Hollow Carbon for Electrochemical Syngas Production

Song Xiaokai Zhang Hao Yang Yuqi Zhang Bin Zuo Ming
Cao Xin Sun Jianhua Lin Chao Li Xiaopeng Jiang Zheng

Key words Bifunctional Catalysts, Electrochemical CO_2 Reduction Reaction (CO_2RR), Hydrogen Evolution Reaction (HER), Metal-Organic Frameworks, Single Atom Electrocatalysts

Electrochemical conversion of CO_2 and H_2O into syngas is an attractive route to utilize green electricity. A competitive system economy demands development of cost-effective electrocatalyst with dual active sites for CO_2 reduction reaction (CO_2RR) and hydrogen evolution reaction (HER). Here, a single atom electrocatalyst derived from a metal-organic framework is proposed, in which Co single atoms and N functional groups function as atomic CO_2RR and HER active sites, respectively. The synthesis method is based on pyrolysis of ZnO@ZIF (zeolitic imidazolate framework). The excess in situ Zn evaporation effectively prevents Co single atoms (≈3.4 wt%) from aggregation and maintains appropriate Co/N ratio. The as-prepared electrocatalyst is featured with high graphitic degree of carbon support for rapid electron transport and sponge-like thin carbon shells with hierarchical pore system for facilitating active site exposure and mass transport. Therefore, the electrocatalyst exhibits a nearly 100% Faradic efficiency and a high formation rate of ≈425 mmol g^{-1} h^{-1} at 1.0 V with the gaseous product ratio (CO/H_2) approximating ideal 1/2. With

the assistance of an extensive material characterization and density functional theory (DFT) calculations, it is identified that Co single atoms are uniformly coordinated in the form of Co-C_2N_2 moieties, and act as the major catalytic sites for CO_2 reduction.

Advanced Science, 2018, **5**(7): 1800177

Kinoform and saw-tooth X-ray refractive lenses development at SSRF

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Key words X-ray transport and focusing, Inspection with x-rays

Here we describe the effort made at Shanghai Synchrotron Radiation Facility (SSRF) to develop X-ray refractive lenses for real beamline applications. Fabrication process of silicon and germanium based kinoform lenses are optimized to increase the height-width aspect ratio and decrease the roughness. Saw-tooth lenses made with a new fabrication process based on dry etching are also described. Focusing effect for both kinoform and saw-tooth lenses are tested at Shanghai Synchrotron.

Journal of Instrumentation, 2018, **13**: C07005

Multiple Amplified Electrochemical Detection of MicroRNA-21 Using Hierarchical Flower-like Gold Nanostructures Combined with Gold-enriched Hybridization Chain Reaction

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Key words MicroRNA-21, Electrochemical biosensor, Signal amplification, Hybridization chain reaction

In this work, we present a multiple amplified electrochemical method that can detect target microRNA-21 (miRNA-21) with high sensitivity by using hierarchical flower-like gold nanostructures (HFGNs) and gold-enriched enzyme-free amplification. The HFGNs deposited on ITO conducting glass served as the electrode substrate with large specific surface area, which

allowed the immobilization of large amounts of capture DNA (DNA-1). Then, the gold-enriched hybridization chain reaction (HCR) for signal amplification was attached onto the electrode through target miRNA-mediated sandwich hybridization. The initial strands (I-DNA) enriched on gold nanoparticles (AuNPs) provided plenty of sites for the triggering of the HCR reaction after the addition of H1 and H2 strands, which provided exponential increase of binding sites for the loading of electrochemical signal molecules $[Ru(NH_3)_6]^{3+}$. Therefore, multiple signal amplification could be achieved to reach an ultrasensitive detection of miRNA-21. A wide linear dynamic range from 1fM to 1nM and a detection limit of 0.12fM (S/N=3) was reached with good selectivity. The electrochemical assay method in this work may hold a great potential for clinical diagnosis of genetic disease in the future.

Electroanalysis, 2018, **30**(7): 1349

Elastic squared form factor and binding effect of carbon dioxide studied by the high resolution X-ray scattering

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Key words High resolution X-ray scattering, Elastic squared form factor, Carbon dioxide, Binding effect

The elastic squared form factor of gaseous carbon dioxide was measured for the first time by high resolution Xray scattering to separate the elastic and inelastic scattering. Bond lengths of r(co) = 1.172±0.008 Å and r_{oo} = 2.344 +/- 0.016 Å of CO_2 were determined from the measured elastic squared form factors, which are in good agreement with the NIST benchmark data of r_{co} = 1.1621 Å and r_{oo} = 2.3242 Å. Moreover, the obtained elastic squared form factor difference shows a clear binding effect in the region of small momentum transfers. The present work shows that high resolution X-ray scattering is a powerful tool to study the binding effect of molecules.

Journal of Electron Spectroscopy and Related Phenomena, 2018, **26**: 41

Extraction and structural investigation of jute cellulose nanofibers

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Tian Feng Bian Fenggang Li Hui

Key words Cellulose nanofibril, TEMPO-mediated oxidation, Jute fibers, SR-WAXS

Cellulose nanofibrils (CNFs) are a type of natural nanomaterials extracted from plants and animals that have expanding applications in numerous areas benefiting from their inherent properties of renewability, biodegradability, and sustainability. For energy consumption reduction, CNFs were extracted from raw jute fibers, which were not pretreated in a hot alkali or acid solution, by TEMPOmediated oxidation. Synchrotron radiation wide-angle scattering was performed to realize the crystallization of the CNF crystallites, Fourier transform infrared spectroscopy, transmission electron microscopy, and fieldemission scanning electron microscopy were used to characterize the changes in chemical groups and visualized morphology of CNFs. The simplified preparation and shortened cycle should further help the study of the structure-function relationship of jute CNFs subjected to chemical modification.

Nuclear Science and Techniques, 2018, **29**(7): 106

Immobilization of radioactive fluoride waste in aluminophosphate glass: a molecular dynamics simulation

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Key words Molecular dynamics simulations, Fluoride, Aluminophosphate glasses, Immobilization

Molecular dynamics (MD) simulations were conducted to investigate the structural and chemical environment of aluminum in aluminophosphate glasses. Such glasses have the potential for application in the disposal of radioactive fluoride waste from molten salt reactors (MSR). Due to the risks of studying these materials and the limitations of realistic research conditions, MD simulations were used as an alternative method to study the vitrification of radioactive fluoride waste. In the past decades, aluminophosphate glasses have been studied and they exhibit certain favorable properties for high-level radioactive waste management. This work focuses on the effects of fluorine addition on structural changes in the glass. We observed that glass with composition P_2O_5-Al_2O_3-Na_2O-CaO exhibited a good performance in immobilizing fluoride at low F concentrations (approximately under 25 mol%). Significant changes were observed where PO_3F_2 units replaced PO_3F units in the glass. The four-coordinated AlO_4 units were increasingly converted into five-coordinated $[AlO_xF_y]$ with the increasing F content. The radionuclide Sr in the simulation had the tendency to form six-coordinated octahedrons in the glass. We conclude that the structural changes resulting from the fluoride waste added to aluminophosphate glasses does not adversely affect their chemical stability at relatively low F concentrations, i.e., under 25 mol%. Hence, the use of phosphate glasses is a potential alternative method of fluoride waste disposal.

Nuclear Science and Techniques, 2018, **29**(7): 92

Implantation-decay method to study the beta-delayed charged particle decay

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He Wanbing Huang Meirong Jin Shilun Lin Chengjian
Lu Ming Liu Longxiang Li Yong Ma Peng Ma Junbing
Wang Jiansong Wang Shitao Ye Shaoqiang Yang Yanyun
Zhou Chenglong Zhao Minghui Zhang Huanqiao Ma Yugang
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Key words Implantation-decay method, beta-Delayed proton emission, Proton-rich nuclei, ^{22}Al

In this paper, the implantation-decay method is introduced to study the beta-delayed charged particle decay. A silicon detector array was used for the implantation of the incident beams and for the detection of the emitted particles. An experimental measurement on the beta-delayed particle emission from ^{22}Al was used to demonstrate the method. The half-life value, charged particle spectroscopy, gamma ray spectrum, and gamma particle coincidence for the decay process were obtained and compared with previous experimental results for ^{22}Al. The results show that the implantation-decay method, using a silicon detector array, is a suitable experimental method to study the beta-delayed charged particle decay for proton-rich nuclei.

Nuclear Science and Techniques, 2018, **29**(7): 98

Two-dimensional Na-Cl crystals of unconventional stoichiometries on graphene surface from dilute solution at ambient conditions

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Liang Shanshan Yan Long Li Luhua
Wu Minghong Fang Haiping

NaCl in a 1: 1 stoichiometry is the only known stable form of the Na-Cl crystal under ambient conditions, and non-1: 1 Na-Cl species can only form under extreme conditions, such as high pressures. Here we report the direct observation, under ambient conditions, of Na_2Cl and Na_3Cl as two-dimensional (2D) Na-Cl crystals, together with regular NaCl, on reduced graphene oxide membranes and on the surfaces of natural graphite powders from salt solutions far below the

saturated concentration. Molecular dynamics and density functional theory calculations suggest that this unconventional crystallization process originates from the cation-pi interaction between the ions and the π-conjugated system in the graphitic surface, which promotes the ion-surface adsorption. The strong Na^+-π interaction and charge transfer lead to stoichiometries with an excess of Na^+. With unique electron and spin distributions and bonding, the resulting 2D crystals may have unusual electronic, magnetic, optical and mechanical properties.

Nature Chemistry, 2018, **10**(7): 776

Preparation and adsorption performance of a NiO/MgF_2 composite adsorbent

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Li Yangjuan Dou Qiang Li Qingnuan

Key words MgF_2, MoF_6, Adsorption, Desorption, Extended X-ray absorption fine structure spectroscopy

Fluoride adsorbents have been applied for the purification of UF_6 product from fluorination process. A MgF_2-based adsorbent, NiO/MgF_2, was prepared using NiF_2 as doping agent. The specific surface area of NiO/MgF_2 was 5 times larger than that of MgF_2, its porosity was also larger than that of MgF_2. The saturated adsorption capacity of NiO/MgF_2 for MoF_6 was 21.4±1.9 mg g^{-1}. The desorption behavior was examined by thermogravimetric analysis (TG). The NiO/MgF_2 with adsorbed MoF_6 was investigated using extended X-ray absorption fine structure spectroscopy (EXAFS), which showed no bonding interactions between NiO and MoF_6, while the adsorption of MoF_6 on NiO/MgF_2 was chemisorption via a Mo-F-Mg bond.

Journal of Radioanalytical and Nuclear Chemistry, 2018, **317**(1): 287

Systematic design and three-dimensional simulation of X-ray FEL oscillator for Shanghai Coherent Light Facility

Li Kai Deng Haixiao

Key words XFELO, SCLF, Three-dimensional Bragg diffraction

The Shanghai Coherent Light Facility (SCLF) is a quasi-continuous wave hard X-ray free electron laser facility, which is currently under construction. Due to the high repetition rate and high-quality electron beams, it is straightforward to consider X-ray free electron laser oscillator (XFELO) operation for the SCLF. In this paper, the main processes for XFELO design, and

parameter optimization of the undulator, X-ray cavity, and electron beam are described. A three-dimensional X-ray crystal Bragg diffraction code, named BRIGHT, was introduced for the first time, which can be combined with the GENESIS and OPC codes for the numerical simulations of the XFELO. The performance of the XFELO of the SCLF is investigated and optimized by theoretical analysis and numerical simulation.

Nuclear Instruments & Methods in Physics Research Section A-Accelerators Spectrometers Detectors and Associated Equipment, 2018, **895**: 40

Development and application of optimal burnup estimation methodology for pebble bed reactor

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Key words Pebble bed reactor, Equilibrium cycle, Optimal burnup, Heavy metal utilization

The optimal burnup, which is essential for core design, represents the discharged fuel properties of the core at equilibrium state. The optimal burnup estimation is complex in a pebble bed reactor because the fuel elements are small, numerous and continuously recirculated through the core. In this work, a facilitative method for estimating the optimal burnup of pebble bed reactor is developed. The method employs a single pebble depletion analysis and the neutron non-leakage probability of the core to estimate the attainable burnup of the pebble fuel in the core. With the developed method, the properties of homogeneous mixture fuel of thorium and uranium were analyzed, and the relation of heavy metal utilization with C/HM (graphite-to-heavy metal atom ratio) was also studied. The result shows that, for thorium utilization with homogeneous mixture of seed uranium and thorium fuel, higher enrichment of uranium is preferred. And for a typical pebble design with 20% enriched seed uranium, the heavy metal utilization is about 0.64%, which is equivalent to traditional pressurized water reactor.

Annals of Nuclear Energy, 2018, **117**: 343

Anion photoelectron spectroscopy and chemical bonding of ThO_2^- and ThO_3^-

Li Yanli Zou Jinghan Xiong Xiaogen Xie Hua Tang Zichao
Ge Min Zhao Yafan Liu Hongtao

We conducted a study of electronic structures and chemical bonding of gaseous ThO_2^- and ThO_3^- using velocity-map imaging and ab initio calculations. The electron affinity of neutral ThO_2^-

molecule is reported for the first time with the value of 1.21(5) eV. We obtained a vibrationally resolved photoelectron spectroscopy of ThO_2^- and observed the symmetric stretching frequency of 824(40) cm^{-1} for neutral molecules. One hot band transition is observed in the spectrum of ThO_2^-, which allows the measurement of symmetric stretching mode for ThO2-. The ground state of ThO_2^- is $^2A_1$ with C_{2v} symmetry: the detachment of an electron from the singly occupied molecular orbital (SOMO) results in the ground state of ThO_2. Kohn-Sham molecular orbital analyses reveal an sigma and two weak pi bonds for Th-O multiple bonds in ThO_2. Global minimum search methodology combined with quantum chemical calculations are used to find the minima of ThO_3 and ThO_3^-, and the adiabatic detachment energy of ThO_3^- is calculated to be 3.26 eV at the coupled cluster with singles and doubles plus perturbative triples level. Our theoretical calculations suggest that the ground state of ThO_3^- is $^1A'$ with a symmetry of C_s, while the most stable ThO_3^- is $^2A_1$ with C_{2v} symmetry, thus, the transition from ThO_3^- to ThO_3 undergoes a significant geometry reorganization. Molecular orbital analyses suggest that the SOMO of ThO_3^- is mainly participated by O 2p and O to Th back donation was found in HOMO-2 molecular orbital. This investigation will shed some light on the understanding of covalent bonding in Th-contained molecules. Published by AIP Publishing.

Journal of Chemical Physics, 2018, **148**(24): 244304

Thermally-induced reversible structural isomerization in colloidal semiconductor CdS magic-size clusters

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Structural isomerism of colloidal semiconductor nanocrystals has been largely unexplored. Here, we report one pair of structural isomers identified for colloidal nanocrystals which exhibit thermally-induced reversible transformations behaving like molecular isomerization. The two isomers are CdS magic-size clusters with sharp absorption peaks at 311 and 322 nm. They have identical cluster masses, but slightly different structures. Furthermore, their interconversions follow first-order unimolecular reaction kinetics. We anticipate that such isomeric kinetics are applicable to a variety of small-size functional nanomaterials, and that the methodology developed for our kinetic study will be helpful to investigate and exploit solid-solid transformations in other semiconductor nanocrystals. The findings on structural isomerism should stimulate attention toward advanced design and synthesis of functional nanomaterials enabled by structural transformations.

Nature Communications, 2018, **9**: 2499

β-delayed particle emission from ^{21}Mg

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The β-delayed particle emission from ^{21}Mg was studied at the Radioactive Ion Beam Line in Lanzhou (RIBLL1). Silicon array and high-purity germanium (HPGe) detectors were used to detect the charged particles and gamma-rays emitted from the decay. Half-life time of ^{21}Mg was determined to be 121.9(6) ms. New levels (5.639(26) MeV and 6.644(34) MeV) in the nucleus ^{21}Na were observed. An improved proton spectrum coincident with gamma-rays at 1.633MeV was obtained. A new partial decay scheme was constructed based on the present measurement.

European Physical Journal A, 2018, **54**(6): 107

A general synthetic approach for hexagonal phase tungsten nitride composites and their application in the hydrogen evolution reaction

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Tungsten nitride (WN) materials have shown unique properties in many fields such as energy conversion and storage. Although many studies have been devoted to the synthesis of WN-based materials, the range of materials that can be made is mainly limited to the common cubic beta-WN. Herein, we developed a beta-to delta phase transformation approach by introducing a second transition-metal as a general synthetic method to prepare hexagonal delta-WN and its composites. delta-WN was successfully achieved by introducing Co, Ni or Fe from metal-organic frameworks into tungsten precursors. EXAFS and XRD results confirmed the phase transformation from beta-WN to delta-WN promoted by metallic Co. The delta-WN exhibited superior performance for the hydrogen evolution reaction (HER) compared to beta-WN, *i.e.* 23-fold increase in TOF. The incorporation of Co into δ-WN further increased its activity, for example, δ-WN/$Co_{2.45}$ only required 76 mV overpotential to achieve 10 mA cm^{-2}. XPS analysis and density functional theory calculations revealed that the enhanced activity was due to the synergistic effect between Co and δ-WN which optimized the free energy of hydrogen adsorption and therefore was beneficial to the

HER process. Ni and Fe could also induce the formation of delta-NW, and the as-prepared δ-WN/Ni and δ-WN/Fe both demonstrated satisfactory catalytic activity towards the HER. More importantly, the preparation method introduced in this work may be extended to other metal nitrides or carbides which couldn't be synthesized previously for a variety of potential applications.

Journal of Materials Chemistry A, 2018, **6**(23): 10967

Immobilization of Alkali Metal Fluorides via Recrystallization in a Cationic Lamellar Material, $[Th(MoO_4)(H_2O)_4Cl]Cl\cdot H_2O$

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Searching for cationic extended materials with a capacity for anion exchange resulted in a unique thorium molybdate chloride (TMC) with the formula of $[Th(MoO_4)(H_2O)_4Cl]Cl\cdot H_2O$. The structure of TMC is composed of zigzagging cationic layers$[Th(MoO_4)(H_2O)_4Cl]^{+}$ with Cl^- as interlamellar charge-balancing anions. Instead of performing ion exchange, alkali thorium fluorides were formed after soaking TMC in AF (A = Na, K, and Cs) solutions. The mechanism of AF immobilization is elucidated by the combination of SEM-EDS, PXRD, FTIR, and EXAFS spectroscopy. It was observed that four water molecules coordinating with the Th^{4+} center in TMC are vulnerable to competition with F^-, due to the formation of more favorable Th-F bonds compared to Th-OH_2. This leads to a single crystal-to-polycrystalline transformation *via* a pathway of recrystallization to form alkali thorium fluorides.

Inorganic Chemistry, 2018, **57**(12): 6778

Conceptual design and preliminary performance analysis of a hybrid nuclear-solar power system with molten-salt packed-bed thermal energy storage for on-demand power supply

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Key words Hybrid power system, Concentrating solar power, Small modular reactor, Packed-bed thermal energy storage, Molten-salt, Performance analysis

In support of more efficient utilization of solar and nuclear energy in power generation, the present work proposes a conceptual design of a hybrid nuclear-solar power system (HNSPS) for on-demand power supply, based on a parallel thermal integration of small modular reactors with commercialized molten-salt concentrating solar power tower plants. A cost-effective thermal energy storage system is employed as a thermal coupling and a heat dispatcher to coordinate both nuclear heat and solar heat with power demands. The overall configuration and operation strategy of the hybrid system are elaborated. A numerical model of the hybrid system is developed based on the circulation of molten-salt. Using the model, a 7-day performance analysis of the hybrid system with different considerations are conducted. Effects of key design parameters on system performances are investigated by a parametric study. A customized evaluation parameter, named as "design score", is defined to assess the suitability of the designed configurations. The performance analysis shows that the integration of nuclear power with concentrating solar power allows the system to be less dependent on heat dispatch to achieve required power regulations, comparing to a standalone CSP plant with an equivalent power capacity. The parametric study indicates that a higher heat generation utilization of the hybrid system requires a larger TES and a smaller heliostats field, while a higher power supply efficiency of the hybrid system is accompanied with a larger TES, a larger heliostats field, and a higher nuclear power capacity proportion. The optimum design configuration of a 200 MWe HNSPS is estimated to have a nuclear power capacity proportion of 50%, a theoretical thermal energy storage duration of 14.8 h, and a heliostats field with a solar multiple of 1.27. This configuration can completely satisfy the power demand without any heat generation curtailment during the 7-day operation. The obtained results allow the HNSPS to be considered as a promising non-carbon-emitting power generation system for on-demand power supply.

Energy Conversion and Management, 2018, **166**: 174

A Rechargeable High-Temperature Molten Salt Iron-Oxygen Battery

Peng Cheng Guan Chengzhi Lin Jun Zhang Shiyu Bao Hongliang Wang Yu Xiao Guoping Chen George Zheng Wang Jianqiang

Key words energy storage, iron-oxygen battery, molten salt, rechargeable, zirconia

The energy and power density of conventional batteries are far lower than their theoretical expectations, primarily because of slow reaction kinetics that are often observed under ambient conditions. Here we describe a low-cost and high-temperature rechargeable iron-oxygen battery

containing a bi-phase electrolyte of molten carbonate and solid oxide. This new design merges the merits of a solid-oxide fuel cell and molten metal-air battery, offering significantly improved battery reaction kinetics and power capability without compromising the energy capacity. The as-fabricated battery prototype can be charged at high current density, and exhibits excellent stability and security in the highly charged state. It typically exhibits specific energy, specific power, energy density, and power density of 129.1 Wh kg^{-1}, 2.8 kW kg^{-1}, 388.1 Wh L^{-1}, and 21.0 kW L^{-1}, respectively, based on the mass and volume of the molten salt.

ChemSusChem, 2018, **11**(11): 1880

A remark on the sign change of the four-particle azimuthal cumulant in small systems

Bzdak Adam Ma Guoliang

The azimuthal cumulants, $c_2\{2\}$ and $c_2\{4\}$, originating from the global conservation of transverse momentum in the presence of hydro-like elliptic flow are calculated. We observe the sign change of $c_2\{4\}$ for small number of produced particles. This is in a qualitative agreement with the recent ATLAS measurement of multi-particle azimuthal correlations with the subevent cumulant method.

Physics Letters B, 2018, **781**: 117

In Situ Reduction from Uranyl Ion into a Tetravalent Uranium Trimer and Hexamer Featuring Ion-Exchange Properties and the Alexandrite Effect

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By utilizing zinc amalgam as an in situ reductant and pH regulator, mild hydrothermal reaction between $UO_2(CH_3COO)_2{\cdot}2H_2O$, H_2SO_4, and Cs_2CO_3 or between $UO_2(CH_3COO)_2{\cdot}2H_2O$, $C_2H_4(SO_3H)_2$, and K_2CO_3 yielded a novel cesium U^{IV} sulfate trimer $Cs_4[U_3O(SO_4)_7]{\cdot}2.2H_2O$ (**1**) and a new potassium U^{IV} disulfonic hexamer $K[U_6O_4(OH)_5(H_2O)_5][C_2H_4(SO_3)_2]_6{\cdot}6H_2O$ (**2**), respectively. Compound **1** features a lamellar structure with a honeycomb lattice, and it represents an unprecedented trimeric U^{IV} cluster composed of purely inorganic moieties. Complex **2** is built

from hexanuclear U^{4+} cores and K^+ ions interconnected by μ_5-$[C_2H_4(SO_3)_2]^{2-}$ groups, leading to the construction of an extended framework rather than commonly observed discrete, neutral molecular sulfonate clusters. The various binding modes of the sulfate and disulfonate groups, especially the multidentate ones, enable additional bridging between metal ions, which promotes oligomerization and isolation of polynuclear species. Furthermore, compound **1** exhibits both ion-exchange properties and the Alexandrite effect, and it is the second example of a uranium complex without chromic functional ligands displaying the latter feature.

Inorganic Chemistry, 2018, **57**(11): 6753

The effect of Ar ion beam irradiation on mesocarbon microbead-densified graphite as the matrix of fuel elements in molten-salt nuclear reactors

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Key words Molten salt reactor, Fuel element, Graphite matrix, Ion irradiation, Nanoindentation

Mesocarbon microbeads (MCMBs) were added to the precursors of a traditional matrix A3-3 graphite to increase its density for use as the matrix of fuel elements to inhibit the impregnation of liquid fluoride salt in molten salt reactors. The physical properties of the densified graphite (MDG) obtained using MCMBs with different sizes were compared with those of the A3-3 graphite. Ar ion-beam irradiation by a 4 MV accelerator was used to obtain surface damage to similar to 1 μm depth in the specimens. Results show that the median pore sizes of the MDGs increase from 530 to 644 nm with the size of MCMBs increasing from 2 to 16 μm, but all are smaller than that of the A3-3 graphite (924 nm) . The density is increased by adding MCMBs. The MDG prepared from MCMBs with a size of 2 μm has the highest resistance to irradiation hardening. Both the A3-3 graphite and the MDGs become amorphous at an Ar ion beam dose of 1.47 dpa.

New Carbon Materials, 2018, **33**(3): 268

Thermodynamic Evaluation of NaF-MFn(M=Be, U, Th) Systems for Molten Salt Reactor

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Key words Molten salt, Thermodynamic modeling, Phase diagram

The phase diagrams of $NaF-BeF_2$, $NaF-ThF_4$ and $NaF-UF_4$ systems were assessed based on thermodynamic principles, and diverse thermodynamic models were adapted to different systems. Associate solution model (ASM) was used to describe the Gibbs energies of liquid phase of the $NaF-BeF_2$ system, whereas other systems($NaF-ThF_4$ and $NaF-UF_4$) were treated with the substitutional solution model(SSM) and intermediate compounds were described as stoichiometric compounds according to the Neumann-Kopp rule. All the thermodynamic model parameters were optimized by the least squares procedure until good coincidence was achieved between the calculated results and the experimental data. The derived thermodynamic parameters will be merged into the $NaF-BeF_2-ThF_4-UF_4$ database to develop the thorium molten salt reactor(TMSR) project.

Chemical Research in Chinese Universities, 2018, **34**(3): 457

Experimental Investigation and Thermodynamic Modeling of the $NaCl-NaNO_3-Na_2SO_4$ Ternary System

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Key words Thermodynamics modeling, Molten salt, Thermal energy storage, Phase diagram

Molten salts as heat transfer and storage materials have been used to nuclear energy and concentrated solar power(CSP) applications. In this work, the system of molten salt mixture based on thermodynamic principles was designed as thermal energy storage(TES) materials. The substitutional solution model can be employed to describe the Gibbs energies of all liquid phase. Thermodynamic model parameters for the $NaCl-NaNO_3-Na_2SO_4$ subsystems were conducted by thermodynamic evaluation and optimization based on experimental phase-equilibria data. Thus, a set of self-consistent thermodynamic database was eventually obtained to reliably calculate the whole phase diagram and thermodynamic properties for the $NaCl-NaNO_3-Na_2SO_4$ternary system. The results manifest that the eutectic point of theternary system located at T=280 ℃ and x_{NaCl}=8.4%, x_{NaNO3}=86.3% and x_{Na2SO4}=5.3%. Moreover, the results predicted were verified experimentally using differential scanning calorimetry(DSC) and the agreement between the measured value[T=(287±2) ℃] and predicted value(T=280 ℃) was satisfactory. Thus, the thermodynamic calculation method will be used to design and develop novel molten salt mixture as thermal energy storage materials.

Chemical Research in Chinese Universities, 2018, **34**(3): 475

Phosphate-Based Ultrahigh Molecular Weight Polyethylene Fibers for Efficient Removal of Uranium from Carbonate Solution Containing Fluoride Ions

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Key words ultrahigh molecular weight polyethylene fibers, radiation induced graft polymerization, glycidyl methacrylate, phosphate group, removal of uranium from carbonate solution

This work provides a cost-effective approach for preparing functional polymeric fibers used for removing uranium (U(VI)) from carbonate solution containing NaF. Phosphate-based ultrahigh molecular weight polyethylene (UHMWPE-g-PO_4) fibers were developed by grafting of glycidyl methacrylate, and ring-opening reaction using phosphoric acid. Uranium (U(VI)) adsorption capacity of UHMWPE-g-PO_4 fibers was dependent on the density of phosphate groups (DPO, $mmol \cdot g^{-1}$). UHMWPE-g-PO_4 fibers with a DPO of 2.01 $mmol \cdot g^{-1}$ removed 99.5% of U(VI) from a Na_2CO_3 solution without the presence of NaF. In addition, when NaF concentration was 3 $g \cdot L^{-1}$, 150 times larger than that of U(VI), the U(VI) removal ratio was still able to reach 92%. The adsorption process was proved to follow pseudo-second-order kinetics and Langmuir isotherm model. The experimental maximum U(VI) adsorption capacity (Qmax) of UHMWPE-g-PO_4 fibers reached 110.7 $mg \cdot g^{-1}$, which is close to the calculated Qmax (117.1 $mg \cdot g^{-1}$) by Langmuir equation. Compared to F^-, Cl^-, NO_3^-, and SO_4^{2-} did not influence U(VI) removal ratio, but, $H_2PO_4^-$ and CO_3^{2-} significantly reduced U(VI) removal ratio in the order of $F^- > H_2PO_4^- > CO_3^{2-}$. Cyclic U(VI) sorption-desorption tests suggested that UHMWPE-g-PO_4 fibers were reusable. These results support that UHMWPE-g-PO_4 fibers can efficiently remove U(VI) from carbonate solutions containing NaF.

Molecules, 2018, **23**(6): 1245

Emerging Characterizing Techniques in the Fine Structure Observation of Metal Halide Perovskite Crystal

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Key words organic-inorganic crystal, surface structure, STM, calculation

Driven by its appealing application in the energy harvesting industry, metal halide perovskite solar cells are attracting increasing attention from various fields, such as chemistry, materials,

physics, and energy-related industries. While the energy conversion efficiency of the perovskite solar cell is being investigated often by various research groups, the relationship between the surface structure and the property is still ambiguous and, therefore, becomes an urgent topic due to its wide application in the real environment. Recently, the fine structure characterization of perovskite crystals has been analysed by varying techniques, such as XRD, synchrotron-based grazing incidence XRD, XAFS, and STM, in addition to others. In this review article, we will summarize recent progresses in the monitoring of fine nanostructures of the surface and crystal structures of perovskite films, mainly by XAFS, XRD, and STM, focusing on the discussion of the relationship between the properties and the stability of perovskite solar cells. Furthermore, a prospective is given for the development of experimental approaches towards fine structure characterization.

Crystals, 2018, **8**(6): 232

Enhancement of water self-diffusion at super-hydrophilic surface with ordered water

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Key words ordered water layer, self-diffusion, dipole correlation, hydrogen bond

It has been well acknowledged that molecular water structures at the interface play an important role in the surface properties, such as wetting behavior or surface frictions. Using molecular dynamics simulation, we show that the water self-diffusion on the top of the first ordered water layer can be enhanced near a super-hydrophilic solid surface. This is attributed to the fewer number of hydrogen bonds between the first ordered water layer and water molecules above this layer, where the ordered water structures induce much slower relaxation behavior of water dipole and longer lifetime of hydrogen bonds formed within the first layer.

Chinese Physics B, 2018, **27**(6): 060101

Pt Single Atoms Embedded in the Surface of Ni Nanocrystals as Highly Active Catalysts for Selective Hydrogenation of Nitro Compounds

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Li Hongliang Wang Xu Zheng Xusheng Zhu Junfa Li Zhenyu
Si Rui Zeng Jie

Key words Platinum, nickel, single atoms, selective hydrogenation, hydrogen diffusion

Single-atom catalysts exhibit high selectivity in hydrogenation due to their isolated active sites, which ensure uniform adsorption configurations of substrate molecules. Compared with the achievement in catalytic selectivity, there is still a long way to go in exploiting the catalytic activity of single-atom catalysts. Herein, we developed highly active and selective catalysts in selective hydrogenation by embedding Pt single atoms in the surface of Ni nanocrystals (denoted as Pt_1/Ni nanocrystals). During the hydrogenation of 3-nitrostyrene, the TOF numbers based on surface Pt atoms of Pt_1/Ni nanocrystals reached ~1800 h^{-1} under 3 atm of H_2 at 40 °C, much higher than that of Pt single atoms supported on active carbon, TiO_2, SiO_2, and ZSM-5. Mechanistic studies reveal that the remarkable activity of Pt_1/Ni nanocrystals derived from sufficient hydrogen supply because of spontaneous dissociation of H_2 on both Pt and Ni atoms as well as facile diffusion of H atoms on Pt_1/Ni nanocrystals. Moreover, the ensemble composed of the Pt single atom and nearby Ni atoms in Pt_1/Ni nanocrystals leads to the adsorption configuration of 3-nitrostyrene favorable for the activation of nitro groups, accounting for the high selectivity for 3-vinylaniline.

Nano Letters, 2018, **18**(6): 3785

Bunch-by-bunch beam size measurement during injection at Shanghai Synchrotron Radiation Facility

Chen Hanjiao Chen Jie Gao Bo Leng Yongbin

Fast beam profile measurement is important in fast beam dynamic behavior investigations. A bunch-by-bunch beam size measurement system, which is presently used to measure horizontal profile, has been developed at the Shanghai Synchrotron Radiation Facility (SSRF) and is capable of measuring bunches within a separation of 2 ns. The system is based on a direct-imaging optical system and high-speed photomultiplier array detector. A high-bandwidth linear signal amplifier and acquisition module have also been designed to process bunch-by-bunch multi-channel signals from the detector. The software resampling technique and principal component analysis method were developed to obtain the synchronized data and enhance the signal-to-noise ratio. The fast injection of transients was successfully captured and analyzed. Moreover, the bunch-by-bunch positions and sizes exhibited strong oscillation after the injection at the horizontal betatron oscillation frequency of the SSRF storage ring, and this demonstrated the bunch-by-bunch measurement capability of our system.

Nuclear Science and Techniques, 2018, **29**(6): 79

Study of the crosstalk evaluation for cavity BPM

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Lai Longwei Yuan Renxian

Key words Crosstalk, Pill-box cavity BPM, PCA, Harmonic analysis, Resolution

In order to pursue high-precision beam position measurements for free-electron laser facilities, a cavity beam position monitor (CBPM) is employed to measure the transverse position that can meet the requirement of position resolution at a sub-micrometer or even nanometer scale. However, for the pill-box cavity BPM, crosstalk between the cavities will have an effect on the accurate measurement of beam position. To reduce the effect of crosstalk on CBPM performance and ease the measurement of the isolation between the cavities, the cavities with a slight difference in resonant frequency were designed and applied in the Dalian coherent light source and Shanghai soft X-ray free-electron laser facilities. Furthermore, two methods, the principal component analysis method and the method of harmonic analysis, are proposed in this paper to evaluate the crosstalk. The results demonstrate that the two methods are feasible in evaluating the crosstalk between the cavities.

Nuclear Science and Techniques, 2018, **29**(6): 83

X-ray fluorescence microtomography based on polycapillary-focused X-rays from laboratory source

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Deng Biao Xiao Tiqiao

Key words X-ray fluorescence microtomography, Polycapillary, Laboratory X-ray source

X-ray fluorescence microtomography (mu XFCT) is a nondestructive analytical technique and has been widely used to nondestructively detect and quantify the elemental composition and distributions in samples. Usually, synchrotron radiation X-rays are used for mu XFCT, due to its high flux density. In this paper, a laboratory-sourcebased mu XFCT system was developed, in which a polycapillary lens is employed to focus the X-ray beam and improve the flux density. The maximum likelihood expectation maximization algorithm was used to reconstruct the computed tomography slices at a limited number of projections. The experimental results demonstrated that the developed system could reveal the elemental distribution inside the test sample, with an elemental sensitivity of 1000 ppm.

Nuclear Science and Techniques, 2018, **29**(6): 85

A density functional theory study on the interaction between UO_2^{2+} and the carbamoylphosphoramidic acid ligand for uranium extraction from seawater

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Key words Uranium extraction, Adsorption, Density functional theory

Phosphorylurea molecules, which contain both phosphoryl and carbonyl groups, are considered efficient extractants for UO_2^{2+}. This study aims to explain the complexation of UO_2^{2+} with carbamoylphosphoramidic acid (CPO), a simple model for phosphorylurea, for ligand design for uranium recovery from seawater using density functional theory calculations, natural bond order analysis, and the quantum theory of atoms in molecules. The results showed that, when CPO acts as a monodentate ligand, the affinity of phosphoryl for UO_2^{2+} is stronger than that of carbonyl, and CPO coordinates with UO_2^{2+} through the phosphoryl oxygen atom. When CPO serves as a bidentate ligand, both the phosphoryl and carbonyl oxygen atoms connect to UO_2^{2+}, and the U–O(carbonyl) bond plays a more important role than the U–O(phosphoryl) bond in the interaction between UO_2^{2+} and CPO. This paradox may be caused by the significant charge transfer from the U–O(carbonyl) π bond orbital to the C–N σ antibond orbital of the bidentate CPO. The NH spacer between the phosphoryl and carbonyl groups could ensure the delocalization of the electron system of the molecule. The bidentate binding motif is favored by entropy and opposed by enthalpy, while the monodentate binding motif is favored by enthalpy and opposed by entropy. Ultimately, the bidentate binding motif is more favorable than the monodentate one. As expected, the interaction between UO_2^{2+} and the deprotonated CPO is stronger than that between UO_2^{2+} and the neutral CPO. Comparing the interaction between UO_2^{2+} and CPO with that between UO_2^{2+} and *N*-phenylcarbamoylphosphoramidic acid (PhCPO), formed by replacing one hydrogen atom from the terminal nitrogen atom of CPO with a phenyl group, the phenyl substituent at the terminal nitrogen atom of PhCPO shows a slightly negative effect on the interaction between UO_2^{2+} and PhCPO.

Nuclear Science and Techniques, 2018, **29**(6): 90

Electron-beam radiation effects on the structure and properties of polypropylene at low dose rates

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Zhang Cong Li Linfan Li Jingye

Key words Electron beam, Radiation effect, Low dose rate, Polypropylene

While the high-energy radiation effects on polypropylene, which are crucial for the cable industry for nuclear power plants, have been thoroughly studied, the property changes of PP at low-dose-rate electron-beam irradiation are far from elucidated. Herein, the influence of electron-beam irradiation on the structure and properties of PP was examined. The static EB irradiation conditions were 1.2 MeV at a low dose rate of 20 kGy/h to achieve absorbed doses ranging from 45, to 60, 100, and 200 kGy. The molecular structure was first evaluated by measuring the carboxyl index and the relative radical concentrations via Fourier transform infrared spectroscopy and electron spin resonance, respectively. Mechanical, differential scanning colorimetric, and rheological tests were carried out to further investigate the changes in the properties (tensile, crystalizing, and viscoelastic properties) of irradiated PP, which showed good agreement with the structural analysis results. We found that radio-oxidative degradation (chain scission) was predominant, which can be due to the low dose rate facilitating oxygen diffusion into the PP matrix during electron-beam irradiation.

Nuclear Science and Techniques, 2018, **29**(6): 87

Study on neutronics design of ordered-pebble-bed fluoride-salt-cooled high-temperature experimental reactor

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Peng Honghua Liu Yafen Dai Ye Ji Ruiming Kang Xuzhong
Chen Xingwei Li Minghai Yu Xiaohan

Key words Ordered-pebble-bed fluoride-salt-cooled high-temperature experimental reactor, Neutronics design, Reactive control, Neutron spectrum, Temperature coefficient

This paper presents a neutronics design of a 10 MW ordered-pebble-bed fluoride-salt-cooled high-temperature experimental reactor. Through delicate layout, a core with ordered arranged pebble bed can be formed, which can keep core stability and meet the space requirements for thermal hydraulics and neutronics measurements. Overall, objectives of the core include inherent safety and sufficient excess reactivity providing 120 effective full power days for experiments.

Considering the requirements above, the reactive control system is designed to consist of 16 control rods distributed in the graphite reflector. Combining the large control rods worth about 18000-20000 pcm, molten salt drain supplementary means (- 6980 to - 3651 pcm) and negative temperature coefficient (- 6.32 to - 3.80 pcm/K) feedback of the whole core, the reactor can realize sufficient shutdown margin and safety under steady state. Besides, some main physical properties, such as reactivity control, neutron spectrum and flux, power density distribution, and reactivity coefficient, have been calculated and analyzed in this study. In addition, some special problems in molten salt coolant are also considered, including ^{6}Li depletion and tritium production.

Nuclear Science and Techniques, 2018, **29**(6): 81

2.856 GHz microwave signal extraction from mode-locked Er-fiber lasers with sub-100 femtosecond timing jitter

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Key words BOMPD, 3 x 3 coupler, Timing jitter, Mode-locked Er-fiber laser, SXFEL

A balanced optical microwave phase detector (BOMPD) based on a 3 x 3 coupler is presented. This system was developed to extract ultra-low-jitter microwave signals from optical pulse trains emitted by mode-locked Er-fiber lasers, and synchronized microwave and laser systems. We demonstrate that the BOMPD achieves a precision of synchronization of less than 100 femtosecond of timing jitter. The experimental setup can be applied to the soft X-ray free-electron laser located on the campus of the Shanghai synchrotron radiation facility. A microwave signal with a 2.856 GHz frequency is extracted from a 238 MHz mode-locked Er-laser, with an absolute timing jitter of 34 fs in the 10 Hz-10 MHz frequency offset range. In addition, the microwave and 238 MHz optical pulse signals are synchronized with a relative timing jitter of 16 fs at the same frequency offset range.

Nuclear Science and Techniques, 2018, **29**(6): 91

Decay modes of highly excited nuclei

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Key words Excited nuclei, IQMD model, GEMINI model, Deexcitation

The deexcitation of single excited ^{112}Sn nuclei at T = 1–30 MeV is simulated using the isospin-dependent quantum molecular dynamics (IQMD) model and GEMINI model. The

fragmentation mechanism, critical behavior, and kinematic characteristics are investigated within these two models. The results show that the IQMD model can be applied to the analysis of fragmentation processes, critical points, and slope temperature extraction. The results of IQMD are generally consistent with experimental □ M_{IMF}□ −Z_{bound} data. However, GEMINI can reproduce the experimental data better than IQMD for isotopic distributions.

Nuclear Science and Techniques, 2018, **29**(6): 78

Enormously improved $CH_3NH_3PbI_3$ film surface for environmentally stable planar perovskite solar cells with PCE exceeding 19.9%

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Key words Perovskite solar cells, Surface crystallization phase purity, In-situ stretching synchrotron-based XRD, Structural stability

One of the most important factors governing the photovoltaic efficiency and environmental stability of Perovskite Solar Cells (PSCs) is the quality of their perovskite films. However, the present study demonstrates that $CH_3NH_3PbI_3$ perovskite films after anti-solvent washing are far from perfect on the surface, where the crystallization degree is quite low with complex multi-phases associated with numerous defects and notable chemical inhomogeneity. Herein, we report a novel anti-solvent washing treatment simply using Hydrogen Iodide (HI) additive in chlorobenzene (CB) which can enormously improve $CH_3NH_3PbI_3$ films surface with high crystallization phase purity and chemical homogeneity, leading to excellent structural stability under humidity, heat and even tensile force. Based on such high quality films with defect-less surface, fabricated planar PSCs with an architecture of ITO/TiO_2/$CH_3NH_3PbI_3$/Spiro-OMeTAD/MoO_x/Au present a champion PCE of 19.94% and improved stability under humidity. Moreover, fabricated flexible planar PSCs on PET/ITO substrates with a champion PCE of 17.32% are shown to be more robust under tensile force than their control devices. The present study thus not only provides more insight into the facile defects passivation process on the surface achieved *via* balancing halide ions, but also provides a practical but efficient treatment which can be widely used to fabricate high quality $CH_3NH_3PbI_3$ films for environmentally stable high performance device applications.

Nano Energy, 2018, **48**: 10

Functional reliability analysis of a molten salt natural circulation system

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Key words Functional reliability, Failure probability, Molten salt natural circulation

The functional reliability evaluation of a molten salt natural circulation system, the nitrate natural circulation loop, was performed. Improved procedures based on the RMPS were applied, considering all the uncertainties to avoid a mass of epistemic uncertainties for an innovative system and introducing a systematic sensitivity analysis process. The system was modeled using Relap5-MS. An uncertainty analysis package of molten salt fluid, named NCUAPackage, was developed to deal with the source correlation parameters and model uncertainties inside the code. 229 samples of 43 input uncertainty parameters were propagated through Relap5-MS. The result functional failure probability of is 0.039 including two failure modes. Sensitivity analysis screened out the most important parameters and revealed that the observables and input parameters follow good linear relationships. An important finding is that the model uncertainty of the heat coefficient of NDHX shell side contributes a lot to the failure probability. It is necessary to consider the model uncertainty for the design and reliability analysis.

Nuclear Engineering and Design, 2018, **332**: 127

A novel atmospheric tritium sampling system

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Key words Atmospheric tritium, HTO, HT, CH_3T, Hydrogen supply module, Methane supply module

The health hazard of tritium is related to its chemical form. Sampling different chemical forms of tritium simultaneously becomes significant. Here a novel atmospheric tritium sampling system (TS-212) was developed to collect the tritiated water (HTO), tritiated hydrogen (HT) and tritiated methane (CH_3T) simultaneously. It consisted of an air inlet system, three parallel connected sampling channels, a hydrogen supply module, a methane supply module and a remote control system. It worked at air flow rate of 1 L/min to 5 L/min, with temperature of catalyst furnace at 200 °C for HT sampling and 400 °C for CH_3T sampling. Conversion rates of both HT and CH_3T to HTO were larger than 99%. The collecting efficiency of the two-stage trap sets for HTO was larger than 96% in 12 h working-time without being blocked. Therefore, the collected efficiencies of

TS-212 are larger than 95% for tritium with different chemical forms in environment. Besides, the remote control system made sampling more intelligent, reducing the operator's work intensity. Based on the performance parameters described above, the TS-212 can be used to sample atmospheric tritium in different chemical forms.

Nuclear Instruments & Methods in Physics Research Section A-Accelerators Spectrometers Detectors and Associated Equipment, 2018, **892**: 127

Theoretical study of $ZrCoH_3$ and the anti-disproportionation ability of alloying elements

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Cheng Hongwei Yin Huiqin Qian Nan Huang Yu Wu Xijun
Liu Wei Li Yan

Key words Tritium storage, First-principles calculation, $ZrCoH_3$, ZrCo, Alloying element, Hydrogen-induced, disproportionation

First-principles calculations were performed to investigate the bonding characteristics of the undoped and doped $ZrCoH_3$ and predict the anti-disproportionation abilities of alloying elements (i.e. Y, V, Nb, Ta, Zr, Cr, Mn, Ru, Rh, Pd and Zn). The binding between H and Zr (or its substitute elements) shows strong ionic and weak covalent feature, and that between H and Co (or its substitute elements) displays the opposite characteristic. The H diffusion process, the size of the 8e site and the corresponding Zr-H distance were calculated, and the substitute elements of Zr (i.e. Nb, Ta and especially V) are predicted to be helpful to improve the ZrCo alloy against the hydrogen-induced disproportionation, and the substitute elements of Co may be not suitable.

International Journal of Hydrogen Energy, 2018, **43**(22): 10410

Chemically activating MoS_2 via spontaneous atomic palladium interfacial doping towards efficient hydrogen evolution

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Ge Junjie Jiang Zheng Wang Jinlan Tang Daiming
Cao Xinzhong Liu Changpeng Xing Wei

Lacking strategies to simultaneously address the intrinsic activity, site density, electrical transport, and stability problems of chalcogels is restricting their application in catalytic hydrogen production. Herein, we resolve these challenges concurrently through chemically activating the

molybdenum disulfide (MoS_2) surface basal plane by doping with a low content of atomic palladium using a spontaneous interfacial redox technique. Palladium substitution occurs at the molybdenum site, simultaneously introducing sulfur vacancy and converting the 2H into the stabilized 1T structure. Theoretical calculations demonstrate the sulfur atoms next to the palladium sites exhibit low hydrogen adsorption energy at –0.02 eV. The final MoS_2 doped with only 1wt% of palladium demonstrates exchange current density of 805 μA cm^{-2} and 78 mV overpotential at 10 mA cm^{-2}, accompanied by a good stability. The combined advantages of our surface activating technique open the possibility of manipulating the catalytic performance of MoS_2 to rival platinum.

Nature Communications, 2018, **9**: 2120

Reconstruction of Supported Metal Nanoparticles in Reaction Conditions

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Key words density functional calculations, heterogeneous catalysis, supported nanoparticles, surface chemistry, transmission electron microscopy

Metal nanoparticles (NPs) dispersed on a high surface-area support are normally used as heterogeneous catalysts. Recent in situ experiments have shown that structure reconstruction of the NP occurs in real catalysis. However, the role played by supports in these processes is still unclear. Supports can be very important in real catalysis because of the new active sites at the perimeter interface between nano particles and supports. Herein, using a developed multiscale model coupled with in situ spherical aberration corrected (Cs-corrected) TEM experiments, we show that the interaction between the support and the gas environment greatly changes the contact surface between the metal and support, which further leads to the critical change in the perimeter interface. The dynamic changes chcnzges of the interface in reactive environments can thus be predicted and be included in the rational design of Supported metal nanocatalysts. In particular, our multiscale model shows quantitative consistency with experimental observations This work offers possibilities for obtaining atomic scale structures and insights beyond the experimental limits.

Angewandte Chemie International Edition, 2018, **57**(22): 6464

Synergistic effects on microstructural evolution and hardening of the Hastelloy N alloy under subsequent He and Xe ion irradiation

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Synergistic effects in the evolution of He bubbles and dislocation loops in Hastelloy N alloy were investigated using transmission electron microscopy and nanoindentation. Results show that the sizes of both He bubbles and dislocation loops induced by the He and Xe irradiation were larger than those in the individual irradiation cases. The corresponding hardening degree of irradiated sample was also measured to be higher than the combined hardening value of two individual irradiation cases. The underlying physics controlling the synergistic effects have revealed that the vacancies are preferentially captured by pre-existed He bubbles as compared to their annihilation with the interstitial atoms during the subsequent Xe irradiation.

Journal of Applied Physics, 2018, **123**(20): 205901

The structural isomerism in gold nanoclusters

Xu Wen Wu Zeng Xiao Cheng Gao Yi

The isomerism in thiolate-protected gold (Au) nanoclusters is important for the understanding of structure–property correlations and the design of Au nanoclusters with specific structures and properties. Although recent studies have identified stereoisomerism, the understanding of structural isomerism is still lacking. Herein, we identified three distinct mechanisms of structural isomerism (i.e., core isomerism, staple isomerism, and complex isomerism) based on the crystallized isomers of thiolate-protected Au nanoclusters, and these mechanisms can be viewed as analogous to those of the structural isomerism in organic molecules (i.e., chain isomerism, point isomerism, and functional isomerism). Using the discovered core isomerism and staple isomerism, two $Au_{28}(SR)_{20}$ isomers are predicted and their synthesis feasibilities are illuminated. These new insights into the structural isomerism can facilitate rational design of new isomers of thiolate-protected Au nanoclusters and guide future experimental synthesis.

Nanoscale, 2018, **10**(20): 9476

Formation of nano-sized M_2C carbides in Si-free GH3535 alloy

Jiang Li Wang Yinling Hu Rui Liu Renduo Ye Xiangxi
Li Zhijun Zhou Xingtai

GH3535 alloy is one of the most promising structural materials for molten salt reactors (MSRs). Its microstructure is characterized by equiaxed grains and coarser primary M_6C carbide strings. In this study, stable nano-sized M_2C carbides were obtained in GH3535 alloy by the removal of Si and thermal exposure at 650 °C. Nano-sized M_2C carbide particles precipitate preferentially at grain boundaries during the initial stage of thermal exposure and then spread all over the grain interior in two forms, namely, arrays along the {1 1 1} planes and randomly distributed particles. The precipitate-free zones (PFZs) and the precipitate-enriched zones (PEZs) of the M_2C carbides were found to coexist in the vicinity of the grain boundaries. All M_2C carbides possess one certain orientation relationship (OR) with the matrix. Based on microstructural characterizations, the formation process of M_2C carbides with different morphologies was discussed. The results suggested that the more-stable morphology and OR of M_2C carbides in the Si-free alloy provide higher hardness and better post-irradiation properties, as reported previously. Our results indicate the preferential application of Si-free GH3535 alloy for the low-temperature components in MSRs.

Scientific Reports, 2018, **8**: 8158

The effect of He bubbles on the swelling and hardening of UNS N10003 alloy

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Yan Long Tang Ming

Key words Nickel based alloy, Ion irradiation, He bubbles, Swelling, Irradiation hardening

In order to investigate the effect of He bubbles on the swelling and hardening of nickel based alloys, 1.2 MeV He ion irradiation was performed on UNS N10003 alloy at 650 °C. The number densities and sizes of He bubbles increase with increasing irradiation dose. Neither "black spots" nor dislocation loops were observed in TEM images of the as-irradiated samples. Irradiation dose up to 6.18 displacements per atom (dpa) causes a swelling of 2.67%, which is mainly ascribed to He bubbles. He bubbles induced hardening increases with increasing irradiation dose. The

irradiation hardening behavior was compared with heavy ion irradiation. The result reveals that the obstacle strength of He bubbles is less than that of the saturated heavy ion induced irradiation defects.

Journal of Alloys and Compounds, 2018, **746**: 153

Angiopep-2-conjugated Ag_2S Quantum Dot for NIR-II Imaging of Brain Tumors

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Fan Chunhai Gao Jimin Sun Yanhong

Key words Ag_2S quantum dot, brain-targeting, angiopep-2, NIR-II imaging

Ag_2S quantum dot with excellent NIR-Ⅱ fluorescence can provide deeper tissue penetration (>1.1 cm) and higher spatiotemporal resolution (25 μm, 50 ms) in comparison to the conventional fluorophore. In this study, we designed a NIR-Ⅱ probe based Ag_2S quantum dot for imaging of brain tumor. Angiopep-2 was used to modify Ag_2S quantum dot, which is a 19-mer peptide exhibiting high binding efficiency with low-density lipoprotein receptor-related protein-1 (LRP-1) of blood brain barrier and glioma. Due to the surface of Ag_2S quantum dots with carboxyl groups and angiopep-2 peptide with amino groups, Ag_2S was conjugated with Angiopep-2 (Ag_2S-ANG) through the condensation reaction of amino and carboxyl groups mediated by EDC and NHS. The structure, size and spectral properties of Ag_2S-ANG were characterized by agarose electrophoresis, dynamic light scattering transmission, electron microscope (TEM), UV-vis spectrometer and NIR fluorescence spectrometer, respectively. Results showed that Ag_2S-ANG had a short migration distance compared with Ag_2S in the agarose gel electrophoresis. The hydrate particle size of Ag_2S was approximately 6 nm, Ag_2S-ANG was approximately 8 nm and its zeta potential exhibited electropositive reinforcement, zeta potential of Ag_2S is -11.47±1.56 mV and Ag_2S-ANG is +28.7±1.35 mV. Ag_2S-ANG exhibited similar absorbance and fluorescence spectra to Ag_2S, except a slight enhancement of emission peak. These results indicated that Ag_2S-ANG was synthesized successfully. We further observed its cell cytotoxicity, distribution and uptake in Uppsala 87 Malignant Glioma cells(U87MG), and *in vivo* distribution in the solid tumor-bearing mouse. Ag_2S-ANG had no obvious cytotoxicity when the concentration is inferior to 100 μg/mL and had more uptake in U87MG cells than that of Ag_2S. In animal experiments, glioma tumor-bearing mice were used to investigate the distribution and tumor targeting of Ag_2S-ANG. Results showed that Ag_2S-ANG can distribute and accumulate in subcutaneous tumor site, indicating that Ag_2S-ANG had the potential of targeting the glioma cells.

Acta Chimica Sinica, 2018, **76**(5): 393

Systematic Study in Mammalian Cells Showing No Adverse Response to Tetrahedral DNA Nanostructure

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Ma Jifei Cui Rongrong Zhang Yu Shi Jiye Li Qian Lv Min
Sun Yanhong Wang Lihua Li Jiang Zhu Ying

Key words tetrahedral DNA nanostructures (TDNs), cell, interaction, biocompatibility, cell cycle

The advent of DNA technology has demonstrated great potential in a wide range of applications, especially in the field of biology and biomedicine. However, current understanding of the toxicological effects and cellular responses of DNA nanostructures remains to be improved. Here, we chose tetrahedral DNA nanostructures (TDNs), a type of nanocarriers for delivering molecular drugs, as a model for systematic live-cell analysis of the biocompatibility of TDNs to normal bronchial epithelial cells, carcinoma cells, and macrophage. We found that the interaction behaviors of TDNs in different cell lines were very different, whereas after internalization, most of the TDNs in diverse cell lines were positioned to lysosomes. By a systematic assessment of cell responses after TDN exposure to various cells, we demonstrate that internalized TDNs have good innate biocompatibility. Interestingly, we found that TDN-bearing cells would not affect the cell cycle progression and accompany cell division and that TDNs were separated equally into two daughter cells. This study improves our understanding of the interaction of DNA nanostructures with living systems and their biocompatibility, which will be helpful for further designing DNA nanostructures for biomedical applications.

ACS Applied Materials & Interfaces, 2018, **10**(18): 15442

Evaporation of nanoscale water on a uniformly complete wetting surface at different temperatures

Guo Yuwei Wan Rongzheng

The evaporation of nanoscale water films on surfaces affects many processes in nature and industry. Using molecular dynamics (MD) simulations, we show the evaporation of a nanoscale water film on a uniformly complete wetting surface at different temperatures. With the increase in temperature, the growth of the water evaporation rate becomes slow. Analyses show that the hydrogen bond (H-bond) lifetimes and orientational autocorrelation times of the outermost water film decrease slowly with the increase in temperature. Compared to a thicker water film, the

H-bond lifetimes and orientational autocorrelation times of a monolayer water film are much slower. This suggests that the lower evaporation rate of the monolayer water film on a uniformly complete wetting surface may be caused by the constriction of the water rotation due to the substrate. This finding may be helpful for controlling nanoscale water evaporation within a certain range of temperatures.

Physical Chemistry Chemical Physics, 2018, **20**(17): 12272

Charge Neutralization Drives the Shape Reconfiguration of DNA Nanotubes

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Li Qian Wang Lihua Yang Sichun Fan Chunhai Lin Jianping

Key words DNA nanotechnology, molecular channels, molecular dynamics, SAXS, shape reconfiguration

Reconfiguration of membrane protein channels for gated transport is highly regulated under physiological conditions. However, a mechanistic understanding of such channels remains challenging owing to the difficulty in probing subtle gating-associated structural changes. Herein, we show that charge neutralization can drive the shape reconfiguration of a biomimetic 6-helix bundle DNA nanotube (6HB). Specifically, 6HB adopts a compact state when its charge is neutralized by Mg^{2+}, whereas Na^{+} switches it to the expanded state, as revealed by MD simulations, small-angle X-ray scattering (SAXS), and FRET characterization. Furthermore, partial neutralization of the DNA backbone charges by chemical modification renders 6HB compact and insensitive to ions, suggesting an interplay between electrostatic and hydrophobic forces in the channels. This system provides a platform for understanding the structure-function relationship of biological channels and designing rules for the shape control of DNA nanostructures in biomedical applications.

Angewandte Chemie International Edition, 2018, **57**(19): 5418

An ATP-Responsive Linear DNA Hydrogel

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Qu Xiangmeng Wang Lihua Pei Hao

Key words DNA, Hydrogel, Aptamer

A single-stranded DNA with adenosine triphosphate (ATP) aptamer sequence and a single-stranded DNA with cohesive end were designed for the formation of linear DNA hydrogel.

First, a double-stranded DNA monomer was formed by the hybridization of sticky ends. Then this monomer self-assembled to form a long linear DNA polymer and further form a DNA hydrogel by physically cross-linking The formation of the hydrogel was characterized by rheological tests and the transition from the gel state to the solution state was observed by stress scanning. Using methylene blue (MB) as a marker, the responsive dynamics of the DNA hydrogel to ATP was characterized by UV absorption spectroscopy. Within 15 min after the addition of ATP, the absorbance of the DNA hydrogel at 664 nm rose rapidly and reached a plateau, indicating that the DNA hydrogel can respond quickly to ATP. Moreover, the absorbance of the DNA hydrogel at 664 nm has a good linear correlation with ATP concentration. For comparison, ATP, thymidine triphosphate (TTP), cytidine triphosphate (CTP) and guanosine triphosphate (GTP) were added to the DNA hydrogel, respectively. The UV absorption spectrum test showed that only the ATP-containing DNA hydrogel was depolymerized and MB was released, indicating that the DNA hydrogel has good stability and its response to ATP was specific.

Acta Polymerica Sinica, 2018, **5**: 553

One-Dimensional Zinc Oxide Nanomaterials for Application in High-Performance Advanced Optoelectronic Devices

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Zeng Leyong Xie Lina Zhao Hongbin

Key words zinc oxide, one-dimensional nanostructure, light-emitting diode, photodetector, localized surface plasmon, piezo-phototronic effect

Unlike conventional bulk or film materials, one-dimensional (1D) semiconducting zinc oxide (ZnO) nanostructures exhibit excellent photoelectric properties including ultrahigh intrinsic photoelectric gain, multiple light confinement, and subwavelength size effects. Compared with polycrystalline thin films, nanowires usually have high phase purity, no grain boundaries, and long-distance order, making them attractive for carrier transport in advanced optoelectronic devices. The properties of one-dimensional nanowires—such as strong optical absorption, light emission, and photoconductive gain—could improve the performance of light-emitting diodes (LEDs), photodetectors, solar cells, nanogenerators, field-effect transistors, and sensors. For example, ZnO nanowires behave as carrier transport channels in photoelectric devices, decreasing the loss of the light-generated carrier. The performance of LEDs and photoelectric detectors based on nanowires can be improved compared with that of devices based on polycrystalline thin films. This article reviews the fabrication methods of 1D ZnO nanostructures—including chemical vapor deposition, hydrothermal reaction, and electrochemical deposition—and the influence of the growth parameters

on the growth rate and morphology. Important applications of 1D ZnO nanostructures in optoelectronic devices are described. Several approaches to improve the performance of 1D ZnO-based devices, including surface passivation, localized surface plasmons, and the piezo-phototronic effect, are summarized.

Crystals, 2018, **8**(5): 223

Ionic Liquids Incorporating Polyamide 6: Miscibility and Physical Properties

Zheng Xin Lin Qingqing Jiang Pan Li Yongjin Li Jingye

Key words PA6, ionic liquid, homogenous blends, physical connection, dynamic rheological behaviors

The effects of 1-vinyl-3-butyl imidazole chloride (VBIM) on the structure and properties of Polyamide 6 (PA6) were investigated systematically. It was found that PA6/VBIM blends were homogeneous without phase separation. The glass transition temperature (Tg) of PA6 increased with small VBIM loadings followed by the decreasing in Tg with further increasing the amount of VBIM. The crystallization temperature decreased with the addition of VBIM because of the strong interactions between VBIM and the PA6 matrix, as well as the dilution effect when large amounts of VBIM was introduced to the matrix. According to rheological testing, small amounts of VBIM enhanced the storage modulus and melt viscosity of PA6. Tensile tests also show an increase in strength and modulus at relatively low loadings of VBIM. The strength of PA6 with only 1 wt % VBIM improved by 108% compared to that of neat PA6. Fourier transform infrared (FTIR) investigations revealed that the ions of VBIM preferred to form hydrogen bonds with amide groups in PA6. Therefore, VBIM acts as physical connection point for the neighboring PA6 molecular chains. The specific interactions between VBIM and PA6 account not only for the enhanced melt viscosity of PA6, but also for the improved mechanical properties. Moreover, outstanding antistatic property was also observed. The surface resistivity of the sample with 1 wt % VBIM was 1.50 $\times 10^{10}$/sq, which means good electric dissipation property

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Polymers, 2018, **10**(5): 562

Framework-Nucleic-Acid-Enabled Biosensor Development

Yang Fan Li Qian Wang Lihua Zhang Guoun Fan Chunhai

Key words biosensor, DNA nanostructures, framework nucleic acids, *in vitro* detection, intracellular sensing

Nucleic acids have been actively exploited to develop various exquisite nanostructures due to their unparalleled programmability. Especially, framework nucleic acids (FNAs) with tailorable functionality and precise addressability hold great promise for biomedical applications. In this review, we summarize recent progress of FNA-enabled biosensing in homogeneous solutions, on heterogeneous surfaces, and inside cells. We describe the strategies to translate the structural order and rigidity of FNAs to interfacial engineering with high controllability, and approaches to realize multiplexing for highly parallel *in vitro* detection. We also envision the marriage of the currently available FNA tool sets with other emerging technologies to develop a new generation of biosensors for precision diagnosis and bioimaging.

ACS Sensors, 2018, **3**(5): 903

Intergranular stress study of TC11 titanium alloy after laser shock peening by synchrotron-based high-energy X-ray diffraction

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Zhou X. Wang J.

The distribution of residual lattice strain as a function of depth were carefully investigated by synchrotron-based high energy X-ray diffraction (HEXRD) in TC11 titanium alloy after laser shock peening (LSP). The results presented big compressive residual lattice strains at surface and subsurface, then tensile residual lattice strains in deeper region, and finally close to zero lattice strains in further deep interior with no plastic deformation thereafter. These evolutions in residual lattice strains were attributed to the balance of direct load effect from laser shock wave and the derivative restriction force effect from surrounding material. Significant intergranular stress was evidenced in the processed sample. The intergranular stress exhibited the largest value at surface, and rapidly decreased with depth increase. The magnitude of intergranular stress was proportional to the severity of the plastic deformation caused by LSP. Two shocks generated larger intergranular stress than one shock.

AIP Advances, 2018, **8**(5): 055126

Sub-picosecond electron bunch length measurement using coherent transition radiation at SXFEL

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Longitudinal electron bunch length plays a significant role in single-pass free-electron lasers (FEL), as the high-gain FEL process depends strongly on the high peak current of electron bunches. Longitudinal electron bunch length was measured by detecting the interferogram of coherent transition radiation generated by electron bunches using a THz interferometer and a Golay cell (spectral range 0.02–20 THz) at Shanghai X-ray free-electron laser. The detailed process of measurement and data analysis are discussed herein. Furthermore, the electron bunch length was estimated based on the dispersive strength R56R56 of the bunch compressor and the energy spread δ of electron bunches, which were obtained via experiments. The comparison showed that the measured bunch length was consistent with the estimated bunch length.

Nuclear Science and Techniques, 2018, **29**(5): 74

Tritium concentrations in precipitation in Shanghai

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Zhang Qin Liu Jiayu Yao Jian Liu Wei

Key words Tritium, Precipitation, Seasonality, Origin

Tritium concentrations in precipitation can be used as a criterion to evaluate the tritium baseline of the environment. The tritium concentration in precipitation in Shanghai during 2014–2015 was determined. Values ranged from 0.68 ± 0.04 to 4.11 ± 0.39 Bq/L, and it showed a decreasing trend compared with historical data, however, the values were slightly higher than the natural background tritium level. Additionally, the tritium concentration shows a seasonal variation: It was higher in autumn and winter and lower in summer and spring. A comparison of concentrations in precipitation in Shanghai and around the Qinshan Nuclear Power Plant reveals no correlation, implying that the nuclear power plant operations may not affect the environment of Shanghai. Thus, the raised tritium concentrations in Shanghai might be due to the effects of monsoons, spring leak, raindrop, or other activities that generate tritium there. Those activities may include chemistry research that uses tritium as a tracer.

Nuclear Science and Techniques, 2018, **29**(5): 63

Upgrade of macromolecular crystallography beamline BL17U1 at SSRF

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Pan Qiangyan Liu Ke Sun Bo Zhou Huan Li Minjun
Xu Qin Xu Chunyan Yu Feng He Jianhua

Key words Shanghai Synchrotron Radiation Facility, Macromolecular crystallography, Endstation, Goniometer, Fine-phi slicing

Beamline BL17U1 at Shanghai Synchrotron Radiation Facility is an energy-tunable macromolecular crystallography beamline that has been in user operation since 2009. Growing demand from the user community for a small beam and related experimental methods have motivated upgrades of the devices in the endstation. Minibeam modes have already been developed for operation. A self-integrated diffractometer reduces the sphere of confusion of the rotatory axis to 1 mu m. The new diffractometer is equipped with an upgraded on-axis viewing system that can improve the resolving power. Additionally, the area detector was also upgraded to the newest generation of detectors, the EIGER X 16M, which can collect data at 133 Hz. After these upgrades, the endstation became virtually new. This paper covers the upgrade of the endstation devices and gives the first data collection results.

Nuclear Science and Techniques, 2018, **29**(5): 68

Coexistence of Polaronic States and Superconductivity in Iron-Pnictide Compound $Ba_2Ti_2Fe_2As_4O$

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Cao Guanghan Zhang Xiangzhi Ma Junzhang Shi Ming
Huang Yaobo Qian Tian Ding Hong Tai Renzhong

The electronic structure of iron-pnictide compound superconductor $Ba_2Ti_2Fe_2As_4O$, which has metallic intermediate Ti_2O layers, is studied using angle-resolved photoemission spectroscopy. The Ti-related bands show a 'peak-dip-hump' line shape with two branches of dispersion associated with the polaronic states at temperatures below around 120 K. This change in the spectra occurs along with the resistivity anomaly that was not clearly understood in a previous study. Moreover, an energy gap induced by the superconducting proximity effect opens in the polaronic bands at temperatures below Tc (~21 K). Our study provides the spectroscopic evidence that superconductivity coexists with polarons in the same bands near the Fermi level, which provides a

suitable platform to study interactions between charge, lattice and spin freedoms in a correlated system.

Chinese Physics Letters, 2018, **35**(5): 057401

Deciphering active biocompatibility of iron oxide nanoparticles from their intrinsic antagonism

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Li Jiang Song Haiyun Shi Jiye Ling Daishun Wang Lihua
Chen Nan Fan Chunhai

Key words catalase-like activity, iron oxide nanoparticles, autophagy, cytotoxicity, reactive oxygen species

Magnetite nanoparticles (Fe_3O_4 NPs) are a well proven biocompatible nanomaterial, which hold great promise in various biomedical applications. Interestingly, unlike conventional biocompatible materials (e.g., polyethylene glycol (PEG)) that are chemically and biologically inert in nature, Fe_3O_4 NPs are known to be catalytically active and exhibit prominent physiological effects. Herein, we report an “active”, dynamic equilibrium mechanism for maintaining the cellular amenity of Fe_3O_4 NPs. We examined the effects of two types of iron oxide (magnetite and hematite) NPs in rat pheochromocytoma (PC12) cells and found that both induced stress responses. However, only Fe_2O_3 NPs caused significant programmed cell death, whereas Fe_3O_4 NPs are amenable to cells. We found that intrinsic catalase-like activity of Fe_3O_4 NPs antagonized the accumulation of toxic reactive oxygen species (ROS) induced by themselves, and thereby modulated the extent of cellular oxidative stress, autophagic activity, and programmed cell death. In line with this observation, we effectively reversed severe autophagy and cell death caused by Fe_2O_3 NPs via co-treatment with natural catalase. This study not only deciphers the distinct intrinsic antagonism of Fe_3O_4 NPs, but opens new routes to designing biocompatible theranostic nanoparticles with novel mechanisms.

Nano Research, 2018, **11**(5): 2746

The dynamic micro computed tomography at SSRF

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Key words Computerized Tomography (CT) and Computed Radiography (CR), Image reconstruction in medical imaging, Inspection with x-rays, Data compression

Synchrotron radiation micro-computed tomography (SR-mu CT) is a critical technique for quantitative characterizing the 3D internal structure of samples, recently the dynamic SR-mu CT has been attracting vast attention since it can evaluate the three-dimensional structure evolution of a sample. A dynamic mu CT method, which is based on monochromatic beam, was developed at the X-ray Imaging and Biomedical Application Beamline at Shanghai Synchrotron Radiation Facility, by combining the compressed sensing based CT reconstruction algorithm and hardware upgrade. The monochromatic beam based method can achieve quantitative information, and lower dose than the white beam base method in which the lower energy beam is absorbed by the sample rather than contribute to the final imaging signal. The developed method is successfully used to investigate the compression of the air sac during respiration in a bell cricket, providing new knowledge for further research on the insect respiratory system.

Journal of Instrumentation, 2018, **13**: C05006

Nanoscale delivery systems for cancer immunotherapy

Wang Zejun Liu Wenhan Shi Jiye Chen Nan Fan Chunhai

Increased understanding of tumor immunology has prompted rapid development of cancer immunotherapy in the past few years. The recent clinical success of immunotherapeutic approaches, such as immune checkpoint blockade and chimeric antigen receptor T cells, demonstrates their potential as a cancer terminator. Nevertheless, strategies to improve the overall efficiency and to reduce the side effects of immunotherapy are highly demanded. Nano-delivery systems hold great promise in biomedical applications due to their unique physiochemical properties and advantages in efficient tissue-specific delivery, enhanced cellular uptake and responsiveness to physiological and environmental stimuli. Immuno-nanomedicine opens a new field in cancer treatment and has attracted broad interest. In this review, we present recent advances in the field of cancer immunotherapy and focus on the nanocarrier-mediated delivery of immunomodulators as well as manipulation of immune cells. Applications of various types of nanomaterials (inorganic, polymers, liposomes, DNA-based, biomimetic and bio-derived nanoparticles) are summarized. Challenges and opportunities of nanovehicles in cancer immuno-oncology are also discussed.

Materials Horizons, 2018, **5**(3): 344

A sagittally confined high-resolution spectrometer in the 'water window'

Li Zhuo Li Bin

Key words X-ray spectrometers, water window, geometric optics, ray tracing, diffraction principle, optical aberration analysis and optimization

The authors report a novel scheme for a grazing-incidence spectrometer forming an excellent meridional flat field in its detector domain to deliver the desired spectral resolution throughout the full designated spectral range, while reducing the sagittal astigmatism substantially to enhance the spectral intensity. The optical properties of the system are thoroughly investigated and optimized, and the detector plane is fitted well to the meridional or sagittal focal curves. The authors demonstrated that a resolving power of 6000-18000 could be achieved within the `water window' (2-5 nm) for an effective meridional source size of 200 μm (r.m.s.), and it would be further improved to 20000-40000 if the source size was confined to 50 μm (r.m.s.).

Journal of Synchrotron Radiation, 2018, **25**: 738

Thickness-dependent structural characteristics for a sputtering-deposited chromium monolayer and Cr/C and Cr/Sc multilayers

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Tian Naxi Li Aiguo

Key words X-ray multilayer, chromium, interface, growth, ligand

The interior structure, morphology and ligand surrounding of a sputtering-deposited chromium monolayer and Cr/C and Cr/Sc multilayers are determined by various hard X-ray techniques in order to reveal the growth characteristics of Cr-based thin films. A Cr monolayer presents a three-stage growth mode with sudden changes occurring at a layer thickness of ~ 2 nm and beyond 6 nm. Cr-based multilayers are proven to have denser structures due to interfacial diffusion and layer growth mode. Cr/C and Cr/Sc multilayers have different interfacial widths resulting from asymmetry, degree of crystallinity and thermal stability. Cr/Sc multilayers present similar ligand surroundings to Cr foil, whereas Cr/C multilayers are similar to Cr monolayers. The aim of this study is to help understand the structural evolution regulation versus layer thickness and to improve

the deposition technology of Cr-based thin films, in particular for obtaining stable Cr-based multilayers with ultra-short periods.

Journal of Synchrotron Radiation, 2018, **25**: 785

Thermodynamic modeling of LiF-NaF-KF-CrF_3 system

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Wu Shuang Wu Xijun Liu Wenguan Xie Leidong

Key words KF-CrF_3, NaF-CrF_3, CALPHAD, First-principles, LiF-NaF-KF-CrF_3, Solubility

The thermodynamic evaluation and optimizations of the KF-CrF_3 and NaF-CrF_3 systems were carried out within the framework of CALPHAD (CALculation of PHAse of Diagrams) approach. The liquid phase was described by the associated solution model, and the intermediate phase were treated as stoichiometric compound model. All the model parameters were optimized based on the experimental phase equilibria data from experimental measurements and theoretical predictions (First-principles calculation and empirical equation). A set of self-consistent and reliable thermodynamic parameters was obtained, which can well describe the phase equilibria and thermodynamic properties of the KF-CrF_3 and NaF-CrF_3 system. Furthermore, the database for the LiF-NaF-KF-CrF_3 quaternary system was preliminarily established using Muggianu extrapolation model. Meanwhile, the solubility of CrF_3 in FLiNaK at different temperatures was obtained. The calculated value is in good agreement with the reported measurements by ORNL, considering kinetic factor of K_3CrF_6 involved in FLiNaK.

Journal of Fluorine Chemistry, 2018, **209**: 6

Microstructure, hardness and modulus of carbon-ion-irradiated new SiC fiber (601-4)

Huang Qing Lei Guanhong Liu Renduo Li Jianjian Yan Long
Li Cheng Liu Weihua Wang Mouhua

Two types of SiC fibers, one is low-oxygen and carbon-rich fiber denoted by 601-4 and the other is low-oxygen and near-stoichiometric Tyranno SA, were irradiated with 450 keV C^+ ions at room temperature. The Raman spectra indicate that irradiation induced distortion and amorphization of SiC crystallites in fibers. TEM characterization of Tyranno SA suggests that SiC crystallites undergo a continued fragmentation into smaller crystalline islands and a continued increase of surrounding amorphous structure. The SiC nano-crystallites (<15 nm) in 601-4 fiber are

more likely to be amorphized than larger crystallites (~200 nm) in Tyranno SA. The hardness and modulus of 601-4 continuously decreases with increasing fluence, while that of Tyranno SA first increases and then decreases.

Journal of Nuclear Materials, 2018, **503**: 91

Influence of graphite-alloy interactions on corrosion of Ni-Mo-Cr alloy in molten fluorides

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Li Xiaoyun Yu Guojun Zhou Xingtai Wang Jianqiang

Key words Ni-base alloy, Molten salt, EPMA, Weight loss, De-alloying, High temperature corrosion

In this study, the effects of graphite-alloy interaction on corrosion of Ni-Mo-Cr alloy in molten FLiNaK salt were investigated. The corrosion tests of Ni-Mo-Cr alloys were conducted in graphite crucibles, to examine the differences of test specimens in conditions of electric contact and isolated with graphite, respectively. The corrosion attack is severer with more weight loss and deeper Cr depletion layer in samples electric contact with graphite than those isolated with graphite. The occurrence of galvanic corrosion between alloy specimens and graphite container was confirmed by electrochemical measurement. The corrosion is controlled by nonelectric transfer in isolated test while electrochemical reaction accelerated corrosion in electric contact test.

Journal of Nuclear Materials, 2018, **503**: 116

Phase-retrieval-based synchrotron X-ray micro-tomography for 3D structural characterization and quantitative analysis of agalloch eaglewood

Liu Huiqiang Lin Fanghua Lin Jianhuan Sulaiman Kaisa
Xiao Tiqiao Sun Yun Pang Yuan Liu Haigang

The propagation-based phase-contrast computed micro-tomography (PPCT) dominates the nondestructive three-dimensional inner structure measurement in biological and soft material research, especially for the synchrotron-based application. It is essential for botanic assessments in plant physiology and eco-physiology to quantitatively visualize microstructures and tiny density variations in wood tissues. An experimental study of synchrotron-based X-ray PPCT combined

with the presented phase-attenuation-duality phase retrieval (PR) algorithm was implemented with the agalloch eaglewood specimens at different stages. Due to the striking contrast-to-noise ratio and density resolution of the PR-PPCT technique, the experimental results successfully visualized the three-dimensional morphological characterization of different tissues of agalloch eaglewood specimens, and the feature distribution of eaglewood resin was quantitatively segmented and measured for statistic analysis of component volume and size of eaglewood growth. It was demonstrated that the PR-PPCT technique has a great potential for 3D visualization and quantitative analysis of structural characteristics of agalloch eaglewood, associated with resin formation and distribution in specimens, and it is helpful for the wood science and application.

Wood Science and Technology, 2018, **52**(3): 839

Experimental investigation of the bed structure in liquid salt cooled pebble bed reactor

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Yan Rui Zou Yang Cai Xiangzhou

Key words Liquid salt, Pebble bed, Packing factor, Vibration

Based on the advanced high temperature reactor (AHTR), which is an advanced concept combining attractive attributes by adopting liquid salt and coated particle fuel, more and more reactor designs that use fuel pebbles are developed. The bed structure in liquid salt cooled pebble bed reactor is important for reactor design. To investigate the bed structure in the reactor, the Pebble Recirculation Experiment Device (PRED) and the Pebble Bed Dense Experiment facility (PBDE), which were mock-ups for TMSR-SF (Thorium-based Molten Salt Reactor with Solid Fuel) were developed. Packing experiments were performed under different conditions. The results show that, the packing factor of TMSR-SF is supposed to be about 0.574, which is much less than 0.60 in gaseous environment, the loading rate of pebbles and the velocity of inlet flow has great effect on the bottom shape of the pebble bed, the structure of the pebble bed remains stable during normal operation and changes under accident conditions, loss of the coolant in the core may cause rearrangement of pebble bed, increase in packing factor that caused by strong vibration may induce reactivity in reactor core. The pebble bed behavior under different conditions that investigated in this paper provides the basis phenomenological analysis for reactor design. Moreover, the running of PRED demonstrates the feasibility of the methods for pebble loading and defueling in liquid salted cooled pebble bed reactors.

Nuclear Engineering and Design, 2018, **331**: 24

X-ray absorption spectroscopy study of synthetic cobalt blue pigments similar to Kangxi blue and white porcelain

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Key words cobalt, cobalt compounds, microstructure, pigment, spinels, X-ray methods

A series of cobalt blue pigments, which were synthesized based on the chemical compositions of the blue pigments in Kangxi blue and white porcelain, were investigated by Co, Mn, and Fe K-edge and $L_{2,3}$-edge X-ray absorption spectroscopy to determine the oxidation states and species of the elements and to discern their impact on the blue color. The results reveal that Co is bivalent and mainly located at tetrahedral sites, which is the main parameter controlling the blue color. Mn is mainly present as Mn^{2+}, or $Co_xZn_{1-x}Al_2O_4$ and Fe is mainly present as Fe^{3+}. In particular, Fe^{3+} substitutes the Al in $CoAl_2O_4$ and occupies octahedral sites with a high Mn content. All the synthetic cobalt blue pigments can form a solid solution with various end-members or an intermediate solution spinel. The spectroscopic determination of the oxidation states and speciation of Co, Mn, and Fe furthers understanding of the coloration of blue pigments in blue and white porcelain.

Journal of the American Ceramic Society, 2018, **101**(5): 2130

Adsorption behavior of thorium on N,N,N ',N '-tetraoctyldiglycolamide (TODGA) impregnated graphene aerogel

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Li Qingnuan Zhang Lan

Key words Graphene aerogel, TODGA, Solvent impregnated adsorbent, Thorium

As a kind of three-dimensional graphene architecture material with superhydrophobic, low density, high specific surface area and porosity, graphene aerogel (GA) can be used to immobilize extractant to constitute the solvent impregnated adsorbent. In this paper, the N,N,N′,N′-tetraoctyldiglycolamide impregnated graphene aerogel (GA-TODGA) was prepared to remove the thorium from aqueous solution. It is found that the adsorption of thorium on GA-TODGA is strongly dependent on the concentration of TODGA in GA and HNO_3 in aqueous solution. Compared with other solvent impregnated adsorbents, the adsorption capacity of

GA-TODGA is much higher due to the high immobilization capacity of GA for TODGA. Furthermore, the GA-TODGA also possesses excellent stability and reusability, ensuring the application potential of using GA-TODGA in large scale.

Talanta, 2018, **181**: 311

Preparation of highly fluorescent sulfur doped graphene quantum dots for live cell imaging

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Niu Yongyan Li Xiaolong

Key words Sulfur doping, Graphene quantum dots, Cell bio-imaging

Herein, we reported a facile one-step hydrothermal strategy to synthesize stable, strong blue fluorescence and water-soluble sulfur doped graphene quantum dots (S-GQDs) with the citric acid (CA) and powdered sulfur (S) as the precursors. The results indicated that S atoms were successfully introduced into the structure of graphene, and sulfur doping indeed improved the intensity of blue emission of GQDs. The as-prepared S-GQDs, as the effective cell-imaging material, would easily penetrated into the cell membranes of Hela cell and exhibited relatively low cytotoxicity. When treated with the typical bacteria medium (*Staphylococcus aureus LZ-01 and Escherichia coli DH5α*), it also did not show the conspicuous antiseptic qualities. Therefore, the S-GQDs would have potential applications in the bio-imaging.

Journal of Luminescence, 2018, **197**: 147

Sharing of Na^+ by Three -COO^- Groups at Deprotonated Carboxyl-Terminated Self-Assembled Monolayer-Charged Aqueous Interface

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Tian Chuanshan Shen Y. Ron Wen Yu-Chieh
Shi Guosheng Fang Haiping

By combining theoretical calculations and experimental observations, we show that Na^+ can be shared by three charged $-COO^-$ groups of the deprotonated carboxyl-terminated self-assembled monolayers in aqueous solution at lipid–aqueous interface. This is similar to the sharing structure of

Na^+ usually found in crystals. Notably, this ionic configuration leads to a hydroxyl orientation distribution of interfacial water molecules, showing a maximum toward the bulk solution, in addition to the maximum toward the charged surface expected based on the structure of one-to-one ion-pair formation between Na^+ and $-COO^-$. Our results provide new insights for a better understanding of electrochemically and biologically related charged interfaces at the molecular level and should be helpful to design the nanodevices and bioinspired human-made nanomaterials.

Journal of Physical Chemistry C, 2018, **122**(16): 9111

Facet-specific interaction between methanol and TiO2 probed by sum-frequency vibrational spectroscopy

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Gao Yi Shen Y. Ron Liu Wei-Tao

Key words titanium dioxide, facet effect, adsorption configuration, sum-frequency vibration spectroscopy, Fermi resonance

The facet-specific interaction between molecules and crystalline catalysts, such as titanium dioxides (TiO_2), has attracted much attention due to possible facet-dependent reactivity. Using surface-sensitive sum-frequency vibrational spectroscopy, we have studied how methanol interacts with different common facets of crystalline TiO_2, including rutile(110), (001), (100), and anatase(101), under ambient temperature and pressure. We found that methanol adsorbs predominantly in the molecular form on all of the four surfaces, while spontaneous dissociation into methoxy occurs preferentially when these surfaces become defective. Extraction of Fermi resonance coupling between stretch and bending modes of the methyl group in analyzing adsorbed methanol spectra allows determination of the methanol adsorption isotherm. The isotherms obtained for the four surfaces are nearly the same, yielding two adsorbed Gibbs free energies associated with two different adsorption configurations singled out by ab initio calculations. They are (i) ∼−20 kJ/mol for methanol with its oxygen attached to a low-coordinated surface titanium, and (ii) ∼−5 kJ/mol for methanol hydrogen-bonded to a surface oxygen and a neighboring methanol molecule. Despite similar adsorption energetics, the Fermi resonance coupling strength for adsorbed methanol appears to depend sensitively on the surface facet and coverage.

Proceedings of the National Academy of Sciences of the United States of America, 2018, **115**(17): E3888

High brightness fully coherent x-ray amplifier seeded by a free-electron laser oscillator

Li Kai Yan Jiawei Feng Chao Zhang Meng Deng Haixiao

X-ray free-electron laser oscillator (XFELO) is expected to be a cutting-edge tool for fully coherent x-ray laser generation, and undulator taper technique is well-known for considerably increasing the efficiency of free-electron lasers (FELs). In order to combine the advantages of these two schemes, FEL amplifier seeded by XFELO is proposed by simply using a chirped electron beam. With the right choice of the beam parameters, the bunch tail is within the gain bandwidth of XFELO, and lase to saturation, which will be served as a seeding for further amplification. Meanwhile, the bunch head which is outside the gain bandwidth of XFELO, is preserved and used in the following FEL amplifier. It is found that the natural "double-horn" beam current, as well as residual energy chirp from chicane compressor, are quite suitable for the new scheme. Inheriting the advantages from XFELO seeding and undulator tapering, it is feasible to generate nearly terawatt level, fully coherent x-ray pulses with unprecedented shot-to-shot stability, which might open up new scientific opportunities in various research fields.

Physical Review Accelerators and Beams, 2018, **21**(4): 040702

The irradiation hardening of Ni-Mo-Cr and Ni-W-Cr alloy under Xe^{26+} ion irradiation

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Li Jianjian Xue Wandong Wang Wanxia Tang Ming Yan Long
Yin Wen Zhou Xingtai

Key words Nickel-based alloy, Irradiation hardening, Nix-Gao model, Transmission electron microscopy (TEM)

The irradiation hardening of Ni-Mo-Cr and Ni-W-Cr alloy was investigated. 7 MeV Xe^{26+} ion irradiation was performed at room temperature and 650 °C with peak damage dose from 0.05 to 10 dpa. With the increase of damage dose, the hardness of Ni-Mo-Cr and Ni-W-Cr alloy increases, and reaches saturation at damage dose ≥1 dpa. Moreover, the damage dose dependence of hardness in both alloys can be described by the Makin and Minter's equation, where the effective critical volume of obstacles can be used to represent irradiation hardening resistance of the alloys. Our results also show that Ni-W-Cr alloy has better irradiation hardening resistance than Ni-Mo-Cr

alloy. This is ascribed to the fact that the W, instead of Mo in the alloy, can suppress the formation of defects under ion irradiation.

Nuclear Instruments and Methods in Physics Research Section B: Beam Interactions with Materials and Atoms, 2018, **421**: 50

Transition to thorium fuel cycle for TMSR

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Key words TMSR, In-core transition, Ex-core transition, Negative feedback coefficient, Thorium fuel cycle

Molten Salt Reactor (MSR) has been recognized as one of the reference reactors of the Generation IV International Forum (GIF) with the unique potential (inherent safety, no fuel fabrication, online fuel reprocessing, etc). A thermal MSR based on $^{232}Th/^{233}U$ fuel cycle can be designed to be a breeder with low fissile inventory and leads to a short doubling time and low transuranic (TRU) inventory. However, the fissile fuel supply is one of the unresolved problems since there is no available ^{233}U. It is therefore needed to use existing fissile materials such as ^{235}U or Plutonium to produce ^{233}U. In this paper, two ways for the thorium fuel cycle transition are proposed. One is that the TMSR is started with existing fissile material as starting fuel and thorium as fertile fuel. The bred ^{233}U from thorium is reinjected into the core for critical operation to achieve the transition to thorium fuel cycle gradually in the core (in-core transition). The other also adopts the same starting fuel as the in-core transition but stores the bred ^{233}U out of the core for starting a new TMSR which is then operated with $^{232}Th/^{233}U$ fuel cycle (ex-core transition). The transition performances for the two ways are analyzed based on a thermal TMSR configuration with negative coefficient and BR greater than 1.0. The results show that the transition capacity with Pu or TRU fuel is attractive. For the in-core transition mode, the thorium fuel cycle is quickly evoked and the characteristics of the TMSR turn out to be equivalent to the ^{233}U started TMSR after about 15-year operation. For the ex-core transition mode, the ^{233}U production is appreciable which needs less than 5 years to restart a new TMSR. Besides, the temperature feedback coefficients for the two ways are all negative during the entire operation. Finally, the preliminary characteristics of the thorium fuel cycle deployment are illustrated, which reveals that a thorium nuclear energy park containing various TMSRs as a TMSR fleet can provide sustainable nuclear energy with low production of long-life nuclear wastes.

Nuclear Engineering and Design, 2018, **330:** 420

Nucleic acid-based electrochemical nanobiosensors

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Key words DNA, Aptamer, Nanomaterial, Electrochemical biosensor, Biomarker

The detection of biomarkers using sensitive and selective analytical devices is critically important for the early stage diagnosis and treatment of diseases. The synergy between the high specificity of nucleic acid recognition units and the great sensitivity of electrochemical signal transductions has already shown promise for the development of efficient biosensing platforms. Yet nucleic-acid based electrochemical biosensors often rely on target amplification strategies (e.g., polymerase chain reactions) to detect analytes at clinically relevant concentration ranges. The complexity and time-consuming nature of these amplification methods impede moving nucleic acid-based electrochemical biosensors from laboratory-based to point-of-care test settings. Fortunately, advancements in nanotechnology have provided growing evidence that the recruitment of nanoscaled materials and structures can enhance the biosensing performance (particularly in terms of sensitivity and response time) to the level suitable for use in point-of-care diagnostic tools. This Review highlights the significant progress in the field of nucleic acid-based electrochemical nanobiosensing with the focus on the works published during the last five years.

Biosensors & Bioelectronics, 2018, **102**: 479

Functionalization of cotton fabrics with highly durable polysiloxane-TiO_2 hybrid layers: potential applications for photo-induced water-oil separation, UV shielding, and self-cleaning

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Zhang Maojiang Zhang Kuo Liu Weihua Wu Guozhong

Using a facile strategy to prepare multifunctional cotton fabrics with switchable superhydrophobicity–superhydrophilicity, UV-resistance, photo-induced water–oil separation, and self-cleaning properties is an important and urgent issue in the sustainable development of natural fibers. Herein, a new type of surface modified cotton fabric with a polysiloxane–TiO_2 hybridized coating (Cot-*g*-PMAPS/TiO_2) was prepared through radiation-induced graft polymerization and sol–gel technology. The hybridized coating was composed of two sub-layers: an inner part consisting of an organic–inorganic hybrid layer to address the issue of self-degradation of

TiO_2-loaded polymeric materials while simultaneously improving the adhesion of the TiO_2 film to its support, and an outer part consisting of nanocrystalline anatase TiO_2 to endow the cotton fabric with multifunctionality. The influence of the polysiloxane–TiO_2 on the structure and integrated performance of Cot-*g*-PMAPS/TiO_2 was systematically studied. The results showed that the polysiloxane–TiO_2 coating improved the UV absorption capacity 5.6-fold compared with that of the untreated cotton fabric. In addition, the retention of the break strength of Cot-*g*-PMAPS/TiO_2 was 95.6% after 192 h of UV irradiation. Since the polysiloxane–TiO_2 coating is chemically bound to the cotton fibers, the Cot-*g*-PMAPS/TiO_2 fabric possesses long-term stability, ultra-high durability, and robustness. After 20 commercial or domestic launderings, the UV absorption intensity and WCAs were almost the same as those of the newly fabricated material. The Cot-*g*-PMAPS/TiO_2 also exhibits photo-induced water–oil separation and self-cleaning based on the switchable superhydrophobicity–superhydrophilicity and the photoactivity of TiO_2. This study provides an interesting insight into the design of a novel functional material based on a controllable surface structure.

Journal of Materials Chemistry A, 2018, **6**(14): 6085

Electrostatic force spectroscopy revealing the degree of reduction of individual graphene oxide sheets

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Hu Jun Zhang Yi

Key words degree of reduction, dielectric property, electrostatic force microscopy, electrostatic force spectroscopy, graphene oxide

Electrostatic force spectroscopy (EFS) is a method for monitoring the electrostatic force microscopy (EFM) phase with high resolution as a function of the electrical direct current bias applied either to the probe or sample. Based on the dielectric constant difference of graphene oxide (GO) sheets (reduced using various methods), EFS can be used to characterize the degree of reduction of uniformly reduced one-atom-thick GO sheets at the nanoscale. In this paper, using thermally or chemically reduced individual GO sheets on mica substrates as examples, we characterize their degree of reduction at the nanoscale using EFS. For the reduced graphene oxide (rGO) sheets with a given degree of reduction (sample n), the EFS curve is very close to a parabola within a restricted area. We found that the change in parabola opening direction (or sign the parabola opening value) indicates the onset of reduction on GO sheets. Moreover, the parabola opening value, the peak bias value (tip bias leads to the peak or valley EFM phases) and the EFM phase contrast at a certain tip bias less than the peak value can all indicate the degree of reduction of rGO samples, which is positively correlated with the dielectric constant. In addition, we gave the

ranking of degree for reduction on thermally or chemically reduced GO sheets and evaluated the effects of the reducing conditions. The identification of the degree of reduction of GO sheets using EFS is important for reduction strategy optimization and mass application of GO, which is highly desired owing to its mechanical, thermal, optical and electronic applications. Furthermore, as a general and quantitative technique for evaluating the small differences in the dielectric properties of nanomaterials, the EFS technique will extend and facilitate its nanoscale electronic devices applications in the future.

Beilstein Journal of Nanotechnology, 2018, **9**: 1146

Terahertz time-domain spectroscopy of L-histidine hydrochloride monohydrate

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Zhang Jianbing Qi Wenpeng Han Jiaguang Zhao Hongwei

Key words L-histidine hydrochloride monohydrate, Low-frequency vibration, Terahertz absorption spectrum, Temperature effect

The low-frequency absorption spectrum of l-histidine hydrochloride monohydrate (LHHM) over 0.5–4.0 THz was measured by terahertz time-domain spectroscopy (THz-TDS). The comparison between the THz absorption spectra of LHHM and l-histidine (LHis) was made. The two distinctive THz spectra of LHHM and LHis indicate that THz spectroscopy is sensitive to different specimens. The low-temperature THz spectral features of LHHM presented the blue-shift and splitting as the temperature decreased. Solid-state density functional theory (DFT) calculation of the vibrational modes of LHHM was performed for better understanding the THz characteristic spectrum, and the validity of the calculation modes was confirmed by comparing with the experimental observations. Powder X-ray diffraction (PXRD) was also carried out to check the structures of LHHM and LHis.

Journal of Molecular Structure, 2018, **1157**: 486

Elimination technology of noise introduced by top-up injection in synchrotron radiation infrared beamline

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Key words synchrotron radiation infrared source, constant current injection, elimination technology of noise, zone median filtering

In order to enhance the photon flux and brightness of a synchrotron source, and improve the thermal stability of optical elements, synchrotron radiation source often operates in the qusi-constant current injection (Top-Up) mode. The Top-Up mode can maintain a stable beam current in the storage ring of Synchrotron Source. When the electron is injected into the storage ring from the booster, a noise induced by the instantaneous fluctuation of the beam current in the storage ring will cause a large fluctuation on the interferogram, which can be observed by the FUR spectrometer used in IR experimental endstation. The median filtering algorithm is not sufficient to filter the noise according to the noise characteristics. Therefore, a zone median filter method is proposed to eliminate the noise introduced by the Top-Up mode. A set of the processes of zone median filtering algorithm is designed, which can eliminate the Top-Up mode induced noise on the interferogram automatically. Simulation results show that: the filtering algorithm can be applied to eliminate the noise on the interferogram introduced by the Top-Up mode effectively, so the method can be used to enhance the spectral SNR of the spectrum in the Top-Up mode.

Journal of Infrared and Millimeter Waves, 2018, **37**(2): 251

An efficient and reusable quaternary ammonium fabric adsorbent prepared by radiation grafting for removal of Cr(VI) from wastewater

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Wu Guozhong

Key words Hexavalent chromium, Polyethylene, Nonwoven fabrics, Radiation grafting, Removal, Reusable

A novel quaternary ammonium polyethylene nonwoven fabric for removing chromium ions from water was prepared via radiation-induced grafting of glycidyl methacrylate and further modification with N,N'-dimethylethylenediamine. The structural and morphological characteristics of the adsorbent were analyzed using Fourier transform infrared spectroscopy (FTIR), thermogravimetry and differential thermogravimetry (TG/DTG), scanning electron microscopy (SEM), and X-ray photoelectron spectroscopy (XPS). The influences of several principal factors, including pH value, initial Cr(VI) concentration, contact time, and coexisting anions (including SO_4^{2-}, CO_3^{2-}, NO_3^-, PO_4^{3-}, and Cl^-), on adsorption performance were investigated via batch tests. The results showed that the optimum removal efficiency was 99.2% at pH 3 and the maximum adsorption quantity for Cr(VI) at 25 °C was 336 mg/g. The adsorption kinetic parameters were better fitted with the pseudo-second-order kinetic model, and the equilibrium data were described

very well by the Freundlich isotherm model. Furthermore, the as-synthesized adsorbent exhibited excellent regeneration and recyclability while maintaining high adsorption performance after five adsorption/desorption cycles.

Environmental Science and Pollution Research, 2018, **25**(11): 11045

Corrosion of Incoloy 800H alloys with nickel cladding in FLiNaK salts at 850 ℃

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Liang Jianping Yu Kun Leng Bin Li Zhijun Zhou Xingtai

Key words Nickel, Superalloys, EPMA, Alkaline corrosion, High temperature corrosion, Welding

The corrosion of 800H alloy with and without Ni-cladding, as well as GH3535 alloy, in molten FLiNaK salts at 850 °C has been investigated. Results show that Cr and Fe are depleted from the alloys surface and grain boundaries, where “diffusion paths” are formed. The corrosion process is mainly controlled by the redox reaction of impurity metal ions with Fe and Cr at the alloy surface, and an alloy or cladding layer chemistry criterion is suggested as $Fe + Cr \leq 11$ wt.%. Cr element is found to be hardly depleted from Σ3 type grain boundaries.

Corrosion Science, 2018, **133**: 349

Magnetic field stability of PrFeB magnets developed by GBD for cryogenic permanent magnet undulators

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Key words PrFeB, Grain boundary diffusion, Undulator, Irreversible demagnetization, Rare earths

The magnetic field stability of the PrFeB magnets is one of the key points which affect its application in such devices as cryogenic permanent magnet undulators. In this study, the magnetic properties and microstructure of PrFeB magnets, which were developed by the grain boundary diffusion, were examined. The demagnetizing field distribution of the cryogenic permanent magnet undulator made using the PrFeB magnets was simulated by Radia, and the change mechanism of the irreversible demagnetization following treatments at high temperatures was experimentally studied. The results show that the intrinsic coercivity of the PrFeB magnets can be increased by diffusion of Tb. Meanwhile, the remanence of the magnets displays almost no loss, and the

increasing range is closely related to the orientation thickness of the PrFeB magnet. Therefore, the PrFeB magnets developed using grain boundary diffusion are found to have extremely high comprehensive magnetic properties. The irreversible demagnetization of the PrFeB magnets developed by grain boundary diffusion for the CPMU is determined to be significantly improved following high-temperature treatments.

Journal of Rare Earths, 2018, **36**(4): 385

Study on inherent neutron sources in MSR

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Zou Yang Liu Guimin

Key words MSR, Fuel salt, Inherent neutron source, Photoneutron, Alpha-induced neutron

The molten salt reactor (MSR) has received much recent attention. The presence of beryllium and the mixing of actinides with light nuclei in the fuel salt result in a relatively strong neutron source that can affect the surveillance at subcritical and transient characteristics during operation. In this study, we predict the inherent neutron sources based on a MSR model. The calculation shows that in the fresh core, the inherent neutron sources are mainly from alpha-induced neutrons. After power operation, the inherent neutron sources become remarkably stronger due to photoneutrons. Although being an insignificant part in the total neutron population during operation, the inherent neutron sources can be used as the installed neutron source after shutdown. If the MSR has continuously operated at full power (2 MWt) for 10 days, then there would be no need for the installed source within 80 days after shutdown. After operating constantly for 500 days, the installed neutron source can be eliminated within 2 years after shutdown.

Nuclear Science and Techniques, 2018, **29**(4): 47

Ω and ϕ production in Au + Au collisions at $\sqrt{s_{NN}}$=11.5 and 7.7 GeV in a dynamical quark coalescence model

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Zhang ChunJian Zhong Chen

Key words QCD phase transition, Multi-strangeness particles, Elliptic flow, AMPT

The Ω and ϕ production in relativistic heavy-ion collisions is studied in a dynamical quark coalescence model using the phase space information of strange quarks from a multiphase transport (AMPT) model. Enhanced local parton density fluctuation is implemented in the AMPT to simulate

the QCD phase transition dynamics. By studying the transverse momentum p_T spectra and the elliptic flow of the multi-strangeness particles, such as Ω and ϕ, and the Ω/ϕ ratio as a function of p_T in the AMPT, we find that the new development improves the description of experimental data. The study motivates further experimental investigations of Ω and ϕ production in phase II of the Beam Energy Scan program at RHIC.

Nuclear Science and Techniques, 2018, **29**(4): 54

The effect of ball-milling time and annealing temperature on fracture toughness of Ni-3 wt.% SiC using small punch testing

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Key words Ni-SiC, Small punch, Transmission electron microscopy, Powder metallurgy, Molten salt reactor

A set of dispersion strengthened Ni-3 wt.% SiC samples have been prepared via a powder metallurgy route for an application in molten salt reactor (MSR) systems. A mixture of 97 wt.% Ni and 3 wt.% SiC powder was prepared by varying the ball-milling time (8, 24, 36 and 48 h). The ball-milling process was followed by powder consolidation using spark plasma sintering (SPS) and rapid cooling to room temperature. The samples were then annealed at different temperatures (300 °C, 700 °C and 850 °C). The fracture behaviour of the Ni-3 wt.% SiC samples was investigated using the Small Punch Test (SPT). A scanning electron microscope (SEM) with energy dispersive spectrometer (EDS) and electron back-scatter diffraction (EBSD), as well as transmission electron microscopy (TEM) were employed to examine the microstructure of the tested Ni-3 wt.% SiC samples. The obtained results show that the SPT fracture energy is strongly dependent on the grain size of Ni matrix, which is affected by ball-milling times and annealing temperature. It has been further found that the segregation of large SiC particles at grain boundaries promotes intergranular fracture and thus significantly reduces the fracture energy. The results indicate that the distribution and size of SiC particles at grain boundary is mainly affected by the ball-milling time. Hence, the ball-milling time governs the fracture toughness of Ni-3 wt.% SiC samples.

Materials Characterization, 2018, **138**: 289

The control of magnetic vortex state in rectangular nanomagnet

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Zhu Fangyuan Tai Renzhong

We study the magnetic vortex states in rectangular nanomagnet with aspect ratio close to two by micro-magnetic simulations and experiments comparatively, and propose a simple way to manipulate both the chirality and polarity independently by tuning the direction of the in-plane magnetic field. There are always two vortices which have opposite chirality with Neel type wall and identical polarity for the rectangular nanomagnet with aspect ratio close to two. Four stable vortex states can be genetated from the uniformly magnetized state by in-plane magnetic field, and specific vortex states depend on the direction of the initial magnetization. The phenomenont of the formation of vortex states was explained based on the vortex dynamics. Also the reliability of proposed method was confirmed by domain structure using magnetic force microscopy (MFM) in experiment.

Journal of Magnetism and Magnetic Materials, 2018, **451**: 379

Electron-beam-induced post-grafting polymerization of acrylic acid onto the surface of Kevlar fibers

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Key words Electron beam, Irradiation, Grafting, Kevlar fiber, Acrylic acid

The surface of Kevlar fibers was successfully modified by electron beam (EB)-induced post-grafting of acrylic acid (AA). The generation of radicals in the fibers was confirmed by electron spin resonance (ESR) measurements, and the concentration of radicals was shown to increase as the absorbed dose increased, but decrease with increasing temperature. The influence of the synthesis conditions on the degree of grafting was also investigated. The surface microstructure and chemical composition of the modified Kevlar fibers were characterized by scanning electron microscopy (SEM) and X-ray photoelectron spectroscopy (XPS). The SEM images revealed that the surface of the grafted fibers was rougher than those of the pristine and irradiated fibers. XPS analysis confirmed an increase in C(O)OH groups on the surface of the Kevlar fibers, suggesting successful grafting of AA. These results indicate that EB-induced post-grafting polymerization is effective for modifying the surface properties of Kevlar fibers.

Radiation Physics and Chemistry, 2018, **145**: 74

Identification of binuclear Co2N5 active sites for oxygen reduction reaction with more than one magnitude higher activity than single atom CoN4 site

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Gao Liqin Jin Zhao Ge Junjie Jiang Zheng Chen Shengli
Liu Changpeng Xing Wei

Key words Binuclear active site, Oxygen reduction reaction, Electrocatalyst, X-ray absorption spectroscopy, Fuel cells

Herein, a novel binuclear active site structure, $Co_2N_xC_y$, is intentionally designed and successfully fabricated to efficiently catalyze the oxygen reduction reaction (ORR), which is achieved by precisely controlling the atomic scale structure of bimetal-organic frameworks before pyrolysis. Through discovering a two-atom site with Co-Co distance at 2.1–2.2 Å from aberration-corrected scanning transmission electron microscopy (STEM), as well as a novel shortened Co-Co path (2.12 Å) from the X-ray absorption spectroscopy, we for the first time identified the binuclear Co_2N_X site in the pyrolyzed catalyst. Combined with density functional theory (DFT) calculation, the structure is further confirmed as Co_2N_5. Excitingly, the Co_2N_5 site performs approximately 12 times higher activity than the conventional CoN_4 site and the corresponding catalyst shows unprecedented catalytic activity in acidic electrolyte with half-wave potential of 0.79 V, approaching the commercial Pt/C catalyst and presenting the best one among the Co-N-C catalysts. Theoretical density functional theory calculations reveal that the novel binuclear site exhibits considerably reduced thermodynamic barrier towards ORR, thus contributing to the much higher intrinsic activity. Our finding opens up a new path to design efficient M-N_x/C catalysts, thus pushing the fuel cell industry field one step ahead.

Nano Energy, 2018, **46**: 396

A special coarsening mechanism for intergranular helium bubbles upon heating: A combined experimental and numerical study

Gao Jie Huang Hefei Liu Xiang Wang Chengbin
Stubbins James F. Li Yan

Key words lntergranular helium bubbles, Coarsening mechanism, In situ TEM heating, Analytical modelling

Here, by using in situ transmission electron microcopy, we discovered a special mechanism governing the coarsening of intergranular helium bubbles, which exhibit pancake-like growth along grain boundaries to achieve coalescence with another bubble upon heating at 673 K. The developed analytical model, addressing the stress field induced by the bubble internal pressure, well reproduced the observed shape evolution during the bubble growth. Moreover, we show that the coalescing rate of intergranular bubbles was controlled by the surface diffusion and can be accelerated by the pressure gradient between bubbles.

Scripta Materialia, 2018, **147**: 93

Direct Growth of Graphene on Silicon by Metal-Free Chemical Vapor Deposition

Tai Lixuan Zhu Daming Liu Xing Yang Tieying
Wang Lei Wang Rui Jiang Sheng Chen Zhenhua
Xu Zhongmin Li Xiaolong

Key words Graphene, Silicon, Metal-free CVD, Domain growth

The metal-free synthesis of graphene on single-crystal silicon substrates, the most common commercial semiconductor, is of paramount significance for many technological applications. In this work, we report the growth of graphene directly on an upside-down placed, single-crystal silicon substrate using metal-free, ambient-pressure chemical vapor deposition. By controlling the growth temperature, in-plane propagation, edge-propagation, and core-propagation, the process of graphene growth on silicon can be identified. This process produces atomically flat monolayer or bilayer graphene domains, concave bilayer graphene domains, and bulging few-layer graphene domains. This work would be a significant step toward the synthesis of large-area and layer-controlled, high-quality graphene on single-crystal silicon substrates.

Nano-Micro Letters, 2018, **10**(2): 20

pH and thermal-dependent ultrafiltration membranes prepared from poly (methacrylic acid) grafted onto polyethersulfone synthesized by simultaneous irradiation in homogenous phase

Fan Kai Huang Jianxia Yang Haijun Lu Runsan Sun Xueqing
Hu Jun Hou Zhengchi

Key words Membrane, Polyethersulfone, Graft polymerization, γ-ray irradiation, PH- and thermal-dependent

Polyethersulfone (PES) and monomer methacrylic acid (MAA) were chosen to synthesize the grafted polymer PES-g-PMAA by simultaneous γ-ray irradiation in homogenous phase. Membranes prepared from pristine PES and PES-g-PMAA with different degrees of grafting (DGs), have been obtained. The kinetics of grafting reaction and the DG values were studied through sulphur elemental analysis. The morphology study of the membranes showed formation of sponge-like structure in the sub-layer of membrane, along with grafting PMAA onto the PES chains. By ultrafiltration experiments, a regular pH-dependent permeability and thermal-dependent permeability of PES-g-PMAA membranes was demonstrated through introduction of PMAA onto the PES which reduced the water flux of the membranes. The pH-dependent permeability could be attributed to pH-sensitive reconfiguration of PMAA molecule chains on the surface of membrane pore, while thermal-dependent permeability might be caused by better thermal-sensibility of PMAA chains inside the membrane.

Journal of Membrane Science, 2018, **551**: 222

Possible scenarios for the transition to thorium fuel cycle in molten salt reactor by using enriched uranium

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Key words Molten salt reactor, Fuel cycle, Enriched uranium, Thorium

Molten Salt Reactor (MSR) with Th-^{233}U fuel cycle attracts more and more attention with its excellent performance such as desirable breeding capacity, low waste production and high inherent safety. Considering the fact that there is no available ^{233}U in the nature, it is necessary to analyze the fuel transition from enriched ^{235}U/Th to ^{233}U/Th and then give a flexible transition scenario for a graphite-moderated MSR. By employing an in-house developed tool which is based on SCALE6.1, two scenarios, a Breeding and Burning (B&B) scenario and a Pre-breeding scenario, are studied. The evolution of the inventories of main nuclides, net ^{233}U production and isothermal temperature coefficient are presented and discussed in the B&B scenario. It is found that the fuel transition can be achieved smoothly by using enriched uranium with greater than 40% concentration of ^{235}U. The fuel transition can still be accomplished with 20% enriched uranium but takes a long double time of about 79 years. Meanwhile, we perform an analysis of the Pre-breeding scenario and conclude that it is efficient to produce ^{233}U and the double time ranges from 2.07 years for the 10-day reprocessing to 10.7 years for the 180-day reprocessing. A comparison of these two scenarios is conducted, which indicates that the B&B scenario is more favorable than the Pre-breeding scenario from the aspect of resource utilization efficiency. Finally, a combined three-stage program for developing Th-based MSRs is proposed.

Progress in Nuclear Energy, 2018, **10**: 75

The Scanning Magnets for Proton Therapy Designed by SINAP

Jia Bolei Zhao Zhentang Ouyang Lianhua

Key words Proton therapy scanning system, dipole magnets, dynamic magnetic field, scanning scope, eddy current

A new proton therapy scanning system for the treatment of cancer has been accomplished at the Shanghai Institute of Applied Physics (China). It is mainly comprised of two separate dipole magnets, which have been fabricated and now are under commission. According to the design requirements, we have confirmed the dimensions of the magnets and optimized the local and integrated field quality. The static electromagnetic field analysis has been completed in OPERA 3D, including the spatial distribution and interference of themagnetic fields, the optimization of the pole, the verification of the scanning scope. The dynamic behaviors of the two dipole magnets were analyzed respectively and approaches to reduce the effects of the eddy currents were integrated into the design. In addition, the static and dynamic magnetic field measurements were finished. Compared with the simulated magnetic fields, the measurement results indicate that the design of the scanning magnets reaches the design targets. All the specific design results of the scanning magnets are concluded in this paper.

IEEE Transactions on Applied Superconductivity, 2018, **28**(3): 4400904

The Design and Magnetic Measurement of a SuperBend Dipole Magnet at SSRF

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Key words Accelerator magnets, electromagnets, magnetic field measurement

In order to increase the critical photon energy, and to save space for accommodating more insertion devices, four normal bend magnets will be replaced by high field ones during the phase-II beamline project of the Shanghai Synchrotron Radiation Facility (SSRF). The design of these superbends has been finished, the first one has been manufactured and measured recently at SSRF. This water-cooled resistive magnet has a total length of 1000 mm and a steering field of 2.32 T. An air slot in the magnet pole was used to control the uniformity of the field integral distribution. The design as well as the magnetic measurement results are presented. Also presented is a newly developed field shimming method, which has been verified as effective and convenient in the field integral shimming of a magnet with straight air slots in the poles.

IEEE Transactions on Applied Superconductivity, 2018, **28**(3): 4002403

Comparison of heavy-ion transport simulations: Collision integral in a box

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Simulations by transport codes are indispensable to extract valuable physical information from heavy-ion collisions. In order to understand the origins of discrepancies among different widely used transport codes, we compare 15 such codes under controlled conditions of a system confined to a box with periodic boundary, initialized with Fermi-Dirac distributions at saturation density and temperatures of either 0 or 5 MeV. In such calculations, one is able to check separately the different ingredients of a transport code. In this second publication of the code evaluation project, we only consider the two-body collision term, i.e., we perform cascade calculations. When the Pauli blocking is artificially suppressed, the collision rates are found to be consistent for most codes (to within 1% or better) with analytical results, or completely controlled results of a basic cascade code. In order to reach that goal, it was necessary to eliminate correlations within the same pair of colliding particles that can be present depending on the adopted collision prescription. In calculations with active Pauli blocking, the blocking probability was found to deviate from the expected reference values. The reason is found in substantial phase-space fluctuations and smearing tied to numerical algorithms and model assumptions in the representation of phase space. This results in the reduction of the blocking probability in most transport codes, so that the simulated system gradually evolves away from the Fermi-Dirac toward a Boltzmann distribution. Since the numerical fluctuations are weaker in the Boltzmann-Uehling-Uhlenbeck codes, the Fermi-Dirac statistics is maintained there for a longer time than in the quantum molecular dynamics codes. As a result of this investigation, we are able to make judgements about the most effective strategies in transport simulations for determining the collision probabilities and the Pauli blocking. Investigation in a similar vein of other ingredients in transport calculations, like the mean-field propagation or the production of nucleon resonances and mesons, will be discussed in the future publications.

Physical Review C, 2018, **97**(3): 034625

Investigation on Molecular Structures of Electron-Beam-Irradiated Low-Density Polyethylene by Rheology Measurements

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While the effect of high-energy irradiation on low-density polyethylene (LDPE) has been extensively investigated, the molecular structure changes under different irradiation conditions are less well understood. In this work, we have made systematic investigations on the molecular structure of electron beam irradiated LDPE under various irradiation conditions. The microstructures have been mainly characterized by rheological measurements using small amplitude oscillatory shear (SAOS) and analyzed by a weighted relaxation spectrum and a van Gurp–Palmen plot. It was found that the linear viscoelasticity of LDPE exhibited a strong dependence on the radiation atmosphere due to oxidative degradation in the presence of oxygen. An improved/destroyed network structure could be acquired when LDPE was irradiated in a nitrogen/oxygen environment, as compared with that in air. Differences became more significant when LDPE was irradiated at higher temperature (80 °C) due to the facilitated diffusion of free radicals within the polymer matrix. For the first time, the effects of electron beam on LDPE under various irradiating conditions have been clarified.

Industrial & Engineering Chemistry Research, 2018, **57**(12): 4298

Imaging of Colorectal Cancers Using Activatable Nanoprobes with Second Near-Infrared Window Emission

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Shi Ben Wang Rongchen Chen Jian Gao Wei Shi Ping
Fan Chunhai Zhao Chunchang Tian He

Key words colon cancer, fluorescence, invivo imaging, nanoprobes, second near-infrared window

Fluorescent probes in the second near-infrared window (NIR-II) allow high-resolution bioimaging with deep-tissue penetration. However, existing NIR-II materials often have poor signal-to-background ratios because of the lack of target specificity. Herein, an activatable NIR-II nanoprobe for visualizing colorectal cancers was devised. This designed probe displays

H_2S-activated ratiometric fluorescence and light-up NIR-II emission at 900–1300 nm. By using this activatable and target specific probe for deep-tissue imaging of H_2S-rich colon cancer cells, accurate identification of colorectal tumors in animal models were performed. It is anticipated that the development of activatable NIR-II probes will find widespread applications in biological and clinical systems.

Angewandte Chemie International Edition, 2018, **57**(14): 3626

Effect of in-medium nucleon-nucleon cross section on proton-proton momentum correlation in intermediate-energy heavy-ion collisions

Wang Tingting Ma Yugang Zhang Chunjian Zhang Zhengqiao

The proton-proton momentum correlation function from different rapidity regions is systematically investigated for the Au + Au collisions at different impact parameters and different energies from 400 A MeV to 1500 A MeV in the framework of the isospin-dependent quantum molecular dynamics model complemented by the Lednický-Lyuboshitz analytical method. In particular, the in-medium nucleon-nucleon cross-section dependence of the correlation function is brought into focus, while the impact parameter and energy dependence of the momentum correlation function are also explored. The sizes of the emission source are extracted by fitting the momentum correlation functions using the Gaussian source method. We find that the in-medium nucleon-nucleon cross section obviously influences the proton-proton momentum correlation function, which is from the whole-rapidity or projectile or target rapidity region at smaller impact parameters, but there is no effect on the mid-rapidity proton-proton momentum correlation function, which indicates that the emission mechanism differs between projectile or target rapidity and mid-rapidity protons.

Physical Review C, 2018, **97**(3): 034617

Shape Evolution of Metal Nanoparticles in Binary Gas Environment

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To control the shape and structure of metal nanoparticle (NP) is a crucial strategy to improve its catalytic properties, but the understanding and quantitative description of the structure reconstruction of the catalysts under reaction conditions has not been achieved. Previous works are mostly focused on the single gas conditions, which is apparently not the case in the real catalytic

reactions. In this work, a multi-scale structure reconstruction model is established to describe the equilibrium structures of metal NPs in mixed gas environment quantitatively. Taking NO and CO reaction as a model system, the structures of the Pd, Pt and Rh NPs in a large range of temperature and pressure are fully presented. Moreover, we show the variation of P_NO: P_CO plays the critical role in determining the structures and therefore the number of active sites of the NPs at certain conditions. This work provides an efficient model to guide the future experiments in the real reactions.

Journal of Physical Chemistry C, 2018, **122**(11): 6144

Reactivating Catalytic Surface: Insights into the Role of Hot Holes in Plasmonic Catalysis

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Key words catalysis, DFT, hot holes, nanoplasmonic, X-ray absorption spectra

Surface plasmon resonance of coinage metal nanoparticles is extensively exploited to promote catalytic reactions via harvesting solar energy. Previous efforts on elucidating the mechanisms of enhanced catalysis are devoted to hot electron-induced photothermal conversion and direct charge transfer to the adsorbed reactants. However, little attention is paid to roles of hot holes that are generated concomitantly with hot electrons. In this work, 13 nm spherical Au nanoparticles with small absorption cross-section are employed to catalyze a well-studied glucose oxidation reaction. Density functional theory calculation and X-ray absorption spectrum analysis reveal that hot holes energetically favor transferring catalytic intermediates to product molecules and then desorbing from the surface of plasmonic catalysts, resulting in the recovery of their catalytic activities. The studies shed new light on the use of the synergy of hot holes and hot electrons for plasmon-promoted catalysis.

Small, 2018, **14**(12): 1703510

An overview on the research of Sr_2IrO_4-based system probed by X-ray absorption spectroscopy

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Key words Sr_2IrO_4, XAS, spin-orbit coupling, valence changes, local structure

Investigations of materials with 5*d* transition metal ions have opened up new paradigms in condensed-matter physics because of their large spin-orbit coupling (SOC) interactions. The typical compound is Sr_2IrO_4, which attracted much attention due to its similarities to the parent compound

of high-T_c cuprate superconductor La_2CuO_4. Theoretical calculations predicted that the unconventional superconductivity can occur in carrier doped-Sr_2IrO_4 system. Until now, hundreds of experimental methods were devoted to investigate the carrier doping effect on Sr_2IrO_4. Synchrotron radiation-based X-ray absorption spectroscopy (XAS) made great contributions to the local lattice and electronic structure, and also the intimate relationship between the local structure and physical properties induced by carrier doping. The aim of this review is a short introduction to the progress of research on Sr_2IrO_4-based system probed by the unique technique — XAS, including the strength of the SOC, valence changes upon doping and even local lattice structure with atomic level for this Sr_2IrO_4-based family.

Modern Physics Letters B, 2018, **32**(8): 1850094

Nanoscale mapping of dielectric properties based on surface adhesion force measurements

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Key words adhesion, atomic force microscopy (AFM), graphene oxide (GO), nanoscale dielectric properties, reduced graphene oxide (RGO)

The detection of local dielectric properties is of great importance in a wide variety of scientific studies and applications. Here, we report a novel method for the characterization of local dielectric distributions based on surface adhesion mapping by atomic force microscopy (AFM). The two-dimensional (2D) materials graphene oxide (GO), and partially reduced graphene oxide (RGO), which have similar thicknesses but large differences in their dielectric properties, were studied as model systems. Through direct imaging of the samples with a biased AFM tip in PeakForce Quantitative Nano-Mechanics (PF-QNM) mode, the local dielectric properties of GO and RGO were revealed by mapping their surface adhesion forces. Thus, GO and RGO could be conveniently differentiated. This method provides a simple and general approach for the fast characterization of the local dielectric properties of graphene-based materials and will further facilitate their applications in energy generation and storage devices.

Beilstein Journal of Nanotechnology, 2018, **9**: 900

Unraveling the oxygen vacancy structures at the reduced CeO_2(111) surface

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Veronica Ganduglia-Pirovano M. Gao Yi

Oxygen vacancies at ceria (CeO_2) surfaces play an essential role in catalytic applications. However, during the past decade, the near-surface vacancy structures at CeO_2(111) have been questioned due to the contradictory results from experiments and theoretical simulations. Whether surface vacancies agglomerate, and which is the most stable vacancy structure for varying vacancy concentration and temperature, are being heatedly debated. By combining density functional theory calculations and Monte Carlo simulations, we proposed a unified model to explain all conflicting experimental observations and theoretical results. We find a novel trimeric vacancy structure which is more stable than any other one previously reported, which perfectly reproduces the characteristics of the double linear surface oxygen vacancy clusters observed by STM. Monte Carlo simulations show that at low temperature and low vacancy concentrations, vacancies prefer subsurface sites with a local (2 × 2) ordering, whereas mostly linear surface vacancy clusters do form with increased temperature and degree of reduction. These results well explain the disputes about the stable vacancy structure and surface vacancy clustering at CeO_2(111), and provide a foundation for the understanding of the redox and catalytic chemistry of metal oxides.

Physical Review Materials, 2018, **2**(3): 035802

Comprehensive Understanding of the Spatial Configurations of CeO_2 in NiO for the Electrocatalytic Oxygen Evolution Reaction: Embedded or Surface-Loaded

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Key words CeO_2, electocatalysis, NiO, oxygen evolution, spatial configurations

Introducing cerium (Ce) species into electrocatalysts has been recently developed as an effective approach to improve their oxygen evolution reaction (OER) performance. Importantly, the spatial distribution of Ce species in the hosts can determine the availability of Ce species either as additives or as co-catalysts, which would dictate their different contributions to the enhanced electrocatalytic performance. Herein, the comprehensive investigations on two different catalyst

configurations, namely CeO_2-embedded NiO (Ce-NiO-E) and CeO_2-surface-loaded NiO (Ce-NiO-L), are performed to understand the effect of their specific spatial arrangements on OER characteristics. The Ce-NiO-E catalysts exhibit a smaller overpotential of 382 mV for 10 mA cm^{-2} and a lower Tafel slope of 118.7 mV dec^{-1}, demonstrating the benefits of the embedded configuration for OER, as compared with those of Ce-NiO-L (426 mV and 131.6 mV dec^{-1}) and pure NiO (467 mV and 140.7 mV dec^{-1}), respectively. The improved OER property of Ce-NiO-E originates from embedding small-sized CeO_2 clusters into the host for the larger specific surface area, richer surface defects, higher oxygen adsorption capacity, and better optimized electronic structures of the surface active sites, as compared with Ce-NiO-L. Above findings provide a valuable guideline for and insight in designing catalysts with different spatial configurations for enhanced catalytic properties.

ADVANCED FUNCTIONAL MATERIALS, 2018, **28**(11): 1706056

Investigating the quark flavor dependence of the chiral magnetic effect with a multiphase transport model

Huang Ling Ma Chunwang Ma Guoliang

Because the properties of the QCD phase transition and the chiral magnetic effect (CME) depend on the number of quark flavors (Nf) and quark mass, relativistic heavy-ion collisions provide a natural environment to investigate the flavor features if quark deconfinement occurs. We introduce an initial two-flavor or three-flavor dipole charge separation into a multiphase transport (AMPT) model to investigate the flavor dependence of the CME. By taking advantage of the recent ALICE data of charge azimuthal correlations with identified hadrons, we attempt to disentangle two-flavor and three-flavor CME scenarios in Pb+Pb collisions at 2.76 TeV. We find that the experimental data show a certain potential to distinguish the two scenarios, therefore we further suggest to collect more data to clarify the possible flavor dependence in future experiments.

Physical Review C, 2018, **97**(3): 034909

Bandwidth broadening of X-ray free electron laser pulses with the natural gradient of planar undulator

Song Minghao Yan Jiawei Li Kai Feng Chao Deng Haixiao

Key words Large bandwidth, Deflecting cavity, Corrugated structure, Natural gradient

Besides the target to pursue the narrow bandwidth X-ray pulses, the large bandwidth free-electron laser pulses are also strongly demanded to satisfy a wide range of scientific user

experiments. In this paper, using the transversely tilt beam enabled by deflecting cavity and/or corrugated structure, the potential of large bandwidth X-ray free-electron lasers generation with the natural gradient of the planar undulator are discussed. Theoretical predictions and numerical simulations demonstrated that X-ray bandwidth exceeding 5% can be observed with the optimized free-electron laser parameters.

Nuclear Instruments and Methods in Physics Research Section A: Accelerators, Spectrometers, Detectors and Associated Equipment, 2018, **884**: 11

MoS_2 Nanoprobe for MicroRNA Quantification Based on Duplex-Specific Nuclease Signal Amplification

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Li Li Qu Xiangmeng Shen Xizhong Li Jiang

Key words multiplexed detection, microRNA, MoS_2, molecular beacons, DSN

MicroRNAs (miRNAs) play significant regulatory roles in physiologic and pathologic processes and are considered as important biomarkers for disease diagnostics and therapeutics. Simple, fast, sensitive, and selective detection of miRNAs, however, is challenged by their short length, low abundance, susceptibility to degradation, and homogenous sequence. Here, we report a novel design of nanoprobes for highly sensitive and selective detection of miRNAs based on MoS_2-loaded molecular beacons (MBs) and duplex-specific nuclease (DSN)-mediated signal amplification (DSNMSA). We show that MoS_2 nanosheets not only exhibit high affinity toward MBs but also act as an efficient quencher for absorbed MBs. The strong fluorescence-quenching ability of MoS_2 in combination with cyclic DSNMSA contributes to the superior sensitivity of our method, with a limit of detection 4 orders of magnitude lower than that of traditional hybridization methods. Moreover, the nanoprobes also show high selectivity for discriminating homogenous miRNA sequences with one-base differences because of the discrimination ability of MBs and DSN. Furthermore, we demonstrate that the MoS_2-loaded MB nanoprobes can be utilized for multiplexed detection of miRNAs. Given its high sensitivity and specificity, as well as the multiplexed function, this novel method as an effective tool shows a great promise for simultaneous quantitative analysis of multiple miRNAs in biomedical research and clinical diagnosis.

ACS Applied Materials & Interfaces, 2018, **10**(9): 7825

Efficient selection methods for black phosphorene nanoribbons

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Black phosphorene (BP) has shown anisotropic, electronic, mechanical, and thermal properties for various promising applications in recent years. To take full advantage of this unique anisotropy in its further functional design and application, it is of paramount importance to separate BP with well-defined chirality quickly and precisely. In this paper, we propose three efficient methods to separate BP ribbons with different chiralities by utilizing their strong chirality-dependent bending stiffness. Our results show that the bending stiffness in the zigzag direction is 4 times larger than that in the armchair direction. The mechanical anisotropy and bending–binding competition are used to realize chirality-dependent design. To fold, wrap or scroll the BP nanoribbons, it is necessary to overcome the bending stiffness by applying the binding energy between the BP nanoribbons and the contact surfaces. Due to the mechanical anisotropy, the BP nanoribbons could easily be folded, wrapped and scrolled along the armchair direction rather than the zigzag direction. Therefore, we introduce this characteristic in our chirality separation designs as, the self-folding model to fold up the armchair BP nanoribbons by nanoparticles, the suspension-bridge sieve model to pull down the armchair BP nanoribbons, and the nanorod-roller model to scroll up the armchair nanoribbons. Our separation methods in this research can be extended to other 2D materials with anisotropic mechanical properties. We hope our findings would offer a novel route for the manufacturing of BP-based electronic devices and self-assembly of nano-devices.

Nanoscale, 2018, **10**(9): 4385

Experimental study of heat transfer enhancement for molten salt with transversely grooved tube heat exchanger in laminar-transition-turbulent regimes

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Key words Molten salt, Convective heat transfer, Transversely grooved tube, Heat exchanger, Enhanced heat transfer

In an effort to develop a heat transfer enhancement technique for molten salt in heat exchanger, experiments are carried out to evaluate the heat transfer performance of transversely grooved tube using molten salt as the hot fluid flowing through the inner concentric tube within the Reynolds

number from 300 to 60,000 and Prandtl number from 11 to 27. The effects of Reynolds number and Prandtl number on the thermal-hydraulic behavior in laminar, transition and turbulent flow are studied. Results show that transversely grooved tube will significantly enhance the heat transfer performance of molten salt and meanwhile decrease the critical Reynolds numbers of the transition from laminar flow to turbulent flow. For laminar flow and transition flow, heat transfer enhancement ratio relative to the smooth tube varies with the changing of Reynolds number and Prandtl number. While for the turbulent flow, the enhancement effect is almost independent on Reynolds number and Prandtl number. Finally, heat transfer correlations of molten salt in transversely grooved tube are proposed depending upon the flow regime and have good agreement with experiment data. Experimental results will provide valuable reference and greatly contribute to the practical design of molten salt heat exchanger with heat transfer enhancement techniques.

Applied Thermal Engineering, 2018, **132**: 95

Experimental investigation and thermodynamic modeling of the $LiNO_3$-$RbNO_3$-$AgNO_3$ system and its subsystems

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Key words Molten salts, Computational thermodynamics, Phase diagrams

Computational thermodynamics approach based on experimental values is applied to evaluation and optimization of the $LiNO_3$-$RbNO_3$-$AgNO_3$ system and its subsystems in this work. The substitutional solution model (SSM) was used to describe all liquid phase. All the intermediate compounds were treated as stoichiometric of which Gibbs energies comply with the Neumann-Kopp rule. A set of self-consistent database with thermodynamic model parameters obtained for the $LiNO_3$-$RbNO_3$-$AgNO_3$ subsystems and this database were used to predict thermodynamic properties of the $LiNO_3$-$RbNO_3$-$AgNO_3$ ternary system. The calculated results were verified experimentally using differential scanning calorimetry (DSC) and X-ray diffraction (XRD) techniques, and the agreement between the experimental values and predicted values is satisfactory. The phase diagram of the $LiNO_3$-$RbNO_3$-$AgNO_3$ ternary system contain two eutectic types: one eutectic (Liquid ↔ α-$AgNO_3$ + $LiRb(NO_3)_2$ + $AgRb(NO_3)_2$) at 385.3 ± 1.5 K and another eutectic (Liquid ↔ $LiRb(NO_3)_2$ + $AgRb(NO_3)_2$ + $AgRb_2(NO_3)_3$) at 398.8 ± 1.5 K. Through computational thermodynamics approach, a multi-component system was successfully predicted and this approach will be applied to design and develop multi-component molten salt mixtures as thermal energy storage (TES) materials.

Journal of Alloys and Compounds, 2018, **746**: 124

Laser test of the prototype of CEE time projection chamber

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Peng Liu Chen Jinhui Zhang Song Zhong Chen Wu Chen
Li Qite Zang Hongliang Ge Yucheng Lin Chengjian
Jia Huiming Ma Nanru Wang Dongxi Ma Peng Xu Jun
Fang Deqing Ma Yugang

Key words TPC, Thick GEM, Laser test, Track resolution, Energy resolution

A prototype thick-GEM-based cooling storage ring external-target experiment (CEE) time projection chamber (TPC) is constructed and tested with the pulsed ultraviolet laser beams. The results indicate that the prototype TPC has a good performance in three-dimensional track resolution. In *X* direction the position resolution is about 0.2 mm, and in *Y* direction the position resolution is about 0.5 mm. The results also determine that the energy resolution is about 5.4%, which achieve the requirements of the CEE experiment and can be used to study the nuclear state equation and the quantum chromo dynamics.

Nuclear Science and Techniques, 2018, **29**(3): 41

Preliminary design of a femtosecond timing system for large accelerator facilities

Liu Ming Dai Xiaolei Yin Chongxian Zhao Binqing

Key words Timing system, Large accelerator facilities, Synchronization in femtoseconds

Large accelerator facilities require clocks and triggers with high accuracy to synchronize equipment and devices. A new femtosecond timing system was designed to meet the demands of new facilities. In this system, the radio-frequency signal is modulated in a continuous-wave laser carrier with frequency stabilization, and timing events are distributed in the same fiber. The phase drift is detected precisely, based on the principle of the Michelson interferometer. The phase drift is compensated with coarse and fine correctors afterward. We aim to realize the stable transmission of the RF signal and timing events for a long distance and duration, with the phase drift and additive jitter in femtoseconds. After the extension, the system will become a complete solution for the clock-and-trigger distribution of synchrotron radiation facilities, free-electron lasers, and other accelerators. The physics design, simulation analysis, and preliminary results are included in the paper.

Nuclear Science and Techniques, 2018, 29(3): 32

Determination of boron concentration in uranium fuel samples by ICP-OES following a separation step by cation exchange resin

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Cao Changqing Zhou Wei Zhao Zhongqi

Key words Boron determination, ICP-OES, Boron evaporation, Memory effect, Matrix match method, Resin separation

The boron content of uranium fuel samples with boron concentrations in the range of 0.05–10 μg/g was determined using inductively coupled plasma optical emission spectrometry (ICP-OES) after the uranium was separated by cation exchange. The samples were dissolved in 3 M HNO_3 on a hot plate at 150 °C and evaporated to near dryness. The residues were redissolved in 0.2 M HNO_3 and passed through a column loaded with Dowex 50WX8-400 resin. Uranium was adsorbed on the resin, while boron was easily eluted with 0.2 M HNO_3. The boron content of the effluent was determined using ICP-OES. Several strategies were employed to improve the reliability of the experimentally determined boron content. The addition of mannitol and proper control of the evaporation process were shown to be effective in preventing boron loss during sample dissolution and evaporation. The memory effect was eliminated by flushing the system with 1.5% ammonia for 30 s between successive sample runs, and the matrix match method was used to eliminate the matrix effect arising from mannitol during the ICP-OES analysis. The accuracy of the results of the analysis was determined by addition recovery tests and by comparison with the results of three Chinese certified reference materials (GBW04242, GBW04243, and GBW04232). Using the method we developed, the limit of detection for boron was as low as 0.05 μg/g in uranium fuel samples, and the relative standard deviations for 0.1–0.5 g uranium samples with 0.05–2 μg/g of boron were within 9%.

Nuclear Science and Techniques, 2018, 29(3): 44

Study on Nondestructive Testing for CuAz Preservative-Treated Bamboo with Synchrotron Radiation X-Ray

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Xie Honglan Deng Biao Du Guohao Tong Yajun Xiao Tiqiao

Key words CuAz preservative, Bamboo, Synchrotron radiation, Dual energy subtraction imaging, Phase contrast imaging

The third-generation synchrotron radiation X-ray has many advantages such as high brightness, continuous spectrum, wide spectral range, high spatial resolution and high resolution and so on, which helps to realize the adjustable energy and precise calculation of its spectrum. And it also has the competitive advantage of obtaining the edge enhancement image for high contrast imaging of low Z materials. In this paper, the Cu distribution was obtained by dual energy subtraction imaging and the characteristic microstructures of CuAz preservative treated bamboo were investigated systemically with XPCM at Shanghai Synchrotron Radiation Facility (SSRF). The results showed the testing techniques were expected to the important precision nondestructive methods for preservative treated bamboo.

Spectroscopy and Spectral Analysis, 2018, 38(2): 901

Hydrophobic nanochannel self-assembled by amphipathic Janus particles confined in aqueous nano-space

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Yao Jun Zhuang Wei Fang Haiping

Key words amphipathic Janus particle, self-assembly, uninterrupted hydrophobic channel, water blockage

Hydrophobic nanochannel plays a significant role in many physical, biological, and geological phenomena and exhibits impressive applications due to both its ubiquitous distribution and great ability to transport hydrophobic molecules, including various oils and gases. Based on theoretical modeling, we herein reveal that the amphipathic Janus nanoparticles have a large probability to self-assemble into uninterrupted hydrophobic nanochannels inside the aqueous nano-space, although there are large portions of the Janus nanoparticles to be hydrophilic. The key to this observation is the attractions between the hydrophobic regimes on neighboring amphipathic Janus particles through hydrophobic interaction in aqueous nano-space. More surprisingly, the permeation efficiency of hydrophobic molecules through the uninterrupted hydrophobic channel in Janus particles aggregate is even higher than that in the aggregate of hydrophobic particles. We note that the proposed amphipathic Janus particles can be transported to the appropriate positions by the water since the hydrophilic regimes still remain a strong particle-water interaction. We also note that most natural subsurface rocks are not completely hydrophobic or hydrophilic but have complex surfaces with inhomogeneous wetting property. Our work therefore provides a detailed molecular level understanding of the formation of underground strata as well as the new insight for constructing the artificial hydrophobic channels for various applications, such as the design of proppants to enhance the recovery of the unconventional oil/gas.

Chinese Physics B, 2018, 27(3): 030505

Nucleon effective masses in neutron-rich matter

Li Baoan Cai Baojun Chen Liewen Xu Jun

Key words Nucleon effective mass, Equation of state, Neutron-rich matter, Nuclear symmetry energy, Optical potential, Short-range correlation

Various kinds of isovector nucleon effective masses are used in the literature to characterize the momentum/energy dependence of the nucleon symmetry potential or self-energy due to the space/time non-locality of the underlying isovector strong interaction in neutron-rich nucleonic matter. The multifaceted studies on nucleon isovector effective masses are multi-disciplinary in nature. Besides structures, masses and low-lying excited states of nuclei as well as nuclear reactions, studies of the isospin dependence of short-range correlations in nuclei from scatterings of high-energy electrons and protons on heavy nuclei also help understand nucleon effective masses especially the so-called E-mass in neutron-rich matter. A thorough understanding of all kinds of nucleon effective masses has multiple impacts on many interesting issues in both nuclear physics and astrophysics. Indeed, essentially all microscopic many-body theories and phenomenological models with various nuclear forces available in the literature have been used to calculate single-nucleon potentials and the associated nucleon effective masses in neutron-rich matter. There are also fundamental principles connecting different aspects and impacts of isovector strong interactions. In particular, the Hugenholtz–Van Hove theorem connects analytically nuclear symmetry energy with both isoscalar and isovector nucleon effective masses as well as their own momentum dependences. It also reveals how the isospin-quartic term in the equation of state of neutron-rich matter depends on the high-order momentum-derivatives of both isoscalar and isovector nucleon potentials. The Migdal–Luttinger theorem facilitates the extraction of nucleon E-mass and its isospin dependence from experimentally constrained single-nucleon momentum distributions. The momentum/energy dependence of the symmetry potential and the corresponding neutron–proton effective mass splitting also affect transport properties and the liquid–gas phase transition in neutron-rich matter. Moreover, they influence the dynamics and isospin-sensitive observables of heavy-ion collisions through both the Vlasov term and the collision integrals of the Boltzmann–Uehling–Uhlenbeck transport equation. We review here some of the significant progresses made in recent years by the nuclear physics community in resolving some of the hotly debated and longstanding issues regarding nucleon effective masses especially in dense neutron-rich matter. We also point out some of the remaining key issues requiring further investigations in the era of high precision experiments using advanced rare isotope beams.

Progress in Particle and Nuclear Physics, 2018, 99: 29

Shannon information entropy in heavy-ion collisions

Ma Chunwang Ma Yugang

Key words Shannon information entropy, Nuclear liquid-gas transition, Nuclear reaction model, Asymmetric nucleus, Heavy ion physics

The general idea of information entropy provided by C.E. Shannon “hangs over everything we do” and can be applied to a great variety of problems once the connection between a distribution and the quantities of interest is found. The Shannon information entropy essentially quantify the information of a quantity with its specific distribution, for which the information entropy based methods have been deeply developed in many scientific areas including physics. The dynamical properties of heavy-ion collisions (HICs) process make it difficult and complex to study the nuclear matter and its evolution, for which Shannon information entropy theory can provide new methods and observables to understand the physical phenomena both theoretically and experimentally. To better understand the processes of HICs, the main characteristics of typical models, including the quantum molecular dynamics models, thermodynamics models, and statistical models, etc., are briefly introduced. The typical applications of Shannon information theory in HICs are collected, which cover the chaotic behavior in branching process of hadron collisions, the liquid–gas phase transition in HICs, and the isobaric difference scaling phenomenon for intermediate mass fragments produced in HICs of neutron-rich systems. Even though the present applications in heavy-ion collision physics are still relatively simple, it would shed light on key questions we are seeking for. It is suggested to further develop the information entropy methods in nuclear reactions models, as well as to develop new analysis methods to study the properties of nuclear matters in HICs, especially the evolution of dynamics system.

Progress in Particle and Nuclear Physics, 2018, 99: 120

Functionalized polyethylene fibers for the selective capture of palladium ions from aqueous solution

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Key words Polyethylene fiber, Palladium, Adsorption, EXAFS, Selectivity

An innovative ultrahigh molecular weight polyethylene (UHMWPE) fibrous adsorbent was successfully synthesized via radiation grafting and applied to the selective capture of palladium

ions from dilute aqueous solutions. The influence of the pH, initial Pd(II) concentration, and temperature on the adsorption performance was examined in a batch adsorption experiment. Pd K-edge extended X-ray absorption fine structure (EXAFS) spectra indicated that Pd(II) was immobilized on the adsorbent surface via a ligand exchange reaction that formed a stable UHMWPE-PMDA-Pd complex. Although the concentrations of coexisting ions (Cu(II), Zn(II), Cr(VI), Fe(III), and Ni(II)) in the solution were much higher than that of Pd(II), the adsorption capacity for Pd(II) of the as-prepared absorbent was significantly greater than that for other metal ions. Kinetic studies showed good correlation with the pseudo-second-order model. The maximum capacity for Pd(II) adsorption was approximately 221.8 $mg \cdot g^{-1}$ at 298 K. The adsorption behavior conformed to the Langmuir isotherm model. Thermodynamic studies revealed that the adsorption of Pd(II) was a feasible, spontaneous, and endothermic process.

Applied Surface Science, 2018, 433: 116

A First-Principles Study on the Vibrational and Electronic Properties of Zr-C MXenes

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Zeng Guangli Zhang Wei Ren Cuilan Han Han Huai Ping

Key words first-principles study, Zr-C MXenes, phonon spectra, density of states

Within the framework of density functional theory calculations, the structural, vibrational, and electronic properties of Zr_nC_{n-1} (n = 2, 3, and 4) and their functionalized MXenes have been investigated. We find that the most stable configurations for Zr-C MXene are the ones that the terminal groups F, O, and OH locate on the common hollow site of the superficial Zr layer and its adjacent C layer. F and OH-terminated Zr_3C_2 and Zr_4C_3 have small imaginary acoustic phonon branches around Γ point while the others have no negative phonon modes. The pristine MXenes (Zr_2C, Zr_3C_2 and Zr_4C_3) are all metallic with large DOS contributed by the Zr atom at the Fermi energy. When functionalized by F, O and OH, new hybridization states appear and the DOS at the Fermi level are reduced. Moreover, we find that their metallic characteristic increases with an increase in n. For $(Zr_nC_{n-1})O_2$, Zr_2CO_2 is a semiconductor, $Zr_3C_2O_2$ is a semimetal, and $Zr_4C_3O_2$ becomes a metal.

Communications in Theoretical Physics, 2018, 69(3): 336

Tris-amidoximate uranyl complexes via η^2 binding mode coordinated in aqueous solution shown by X-ray absorption spectroscopy and density functional theory methods

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Zhou Jing Li Jiong Wang Yu Yang Shitong
Wang Shuao Li Jingye Wu Guozhong Wang Jianqiang

Key words uranyl speciation, X-ray absorption near-edge structure, XANES, extended X-ray absorption fine structure, EXAFS, local coordination structure, amidoxime ligand, DFT calculations

The present study sheds some light on the long-standing debate concerning the coordination properties between uranyl ions and the amidoxime ligand, which is a key ingredient for achieving efficient extraction of uranium. Using X-ray absorption fine structure combined with theoretical simulation methods, the binding mode and bonding nature of a uranyl-amidoxime complex in aqueous solution were determined for the first time. The results show that in a highly concentrated amidoxime solution the preferred binding mode between UO_2^{2+} and the amidoxime ligand is η^2 coordination with tris-amidoximate species. In such a uranyl-amidoximate complex with η^2 binding motif, strong covalent interaction and orbital hybridization between U 5f/6d and (N, O) 2p should be responsible for the excellent binding ability of the amidoximate ligand to uranyl. The study was performed directly in aqueous solution to avoid the possible binding mode differences caused by crystallization of a single-crystal sample. This work also is an example of the simultaneous study of local structure and electronic structure in solution systems using combined diagnostic tools.

Journal of Synchrotron Radiation, 2018, 25: 514

Radiolysis products and degradation mechanism studies on tri-isoamyl phosphate (TiAP)

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Wang Jinhua Zhang Lan Li Qinguan

Key words Tri-isoamyl phosphate (TiAP irradiation stability, radiolysis products, radiolysis mechanism

Di-1-methyl heptyl methyl phosphonate (DMHMP) is a promising alternative extractant for

Th-U fuel reprocessing, in which the irradiation stability of extractant should be systematically studied. In this paper, the radiolysis products of DMHMP were analyzed qualitatively and quantitatively with gas and ion chromatograph, the possible radiolysis mechanism of DMHMP was also concluded. Moreover, the effect of structure on the radiolysis products and irradiation stability of neutral organophosphorus compound extractant was also discussed.

Radiochimica Acta, 2018, 106(3): 239

Effect of Ti additions on structure and phase stability of Sb_2Te_3 thin films by experimental and theoretical methods

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Influence of Ti additions in Sb_2Te_3 thin films on structure and phase stability was studied by experiments together with theoretical calculations. The incorporation of Ti atoms in the Sb_2Te_3 thin films caused formation of finer grains. By X-ray photoelectron spectroscopy and ab initio calculation, both the Sb and Te atoms are likely to be replaced by the Ti atoms to form Ti–Sb and Ti–Te covalent bonds. It suggests that the Ti atoms locate in Te1 position and interstice of the lattice.

Journal of Materials Science-Materials in Electronics, 2018, 29(6): 4704

Synergistic effects between hydroxyl radicals and hydrated electrons on strengthening decomposition of an s-triazine compound: A combined experimental and theoretical study

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Jia Chengtao Wu Minghong

Key words s-Triazine, Cyanuric acid, Electron beam, Photo-degradation, Decomposition mechanisms, Theoretical calculations

The decomposition of an environmentally recalcitrant *s*-triazine compound, prometry (PMT), was carried out by experimental and theoretical approaches to study the combined effects of hydroxyl radicals ($^{\bullet}OH$) and hydrated electrons (e_{aq}^{-}). With the participation of strongly oxidative radicals $^{\bullet}OH$ and reductive radicals e_{aq}^{-} induced by electron beam (EB), PMT obtained a

good decomposition performance, which was obviously better than those methods simply using ·OH as the single active species. The evolution of cyanuric acid (CA) during the EB and UV irradiation processes elucidate that former method could efficiently decompose such chemically stable intermediate. The experiments of radical scavengers further suggest that ·OH was the predominant radical during PMT degradation, while e_{aq}^- was beneficial to further decomposition and mineralization. Combined with the results of density functional theory (DFT) calculations, the strengthened synergistic effects between ·OH and e_{aq}^- were proven. The calculations illustrated ·OH could attack the carbon-branch-chains of *s*-trazine ring and form OH-adducts rather than nitrogen oxides. Moreover, the presence of e_{aq}^- could not only greatly change the geometry of the *s*-triazine ring, but also help cleaving alkyl chain on ring, thus facilitate the complete mineralization.

Chemosphere, 2018, 195: 365

Evaluation of thermal physical properties of molten nitrate salts with low melting temperature

Zhang Peng Cheng Jinhui Jin Yuan An Xuehui

Key words Molten nitrate salt, Heat transfer fluid, Thermal energy storage, Thermal physical properties

$NaNO_3$-KNO_3 (60–40 wt%, Solar salt) has been used as medium for TES and HTF in the CSP system. One of the key challenges using Solar salt is its high melting temperature, which may freeze and block the pipeline. In this work, a novel eutectic nitrate molten salt of the $LiNO_3$-$NaNO_3$-KNO_3-$CsNO_3$ system with low melting temperature of 368 K is designed using Calphad method. Its thermal physical properties, as well as that of Solar salt, $LiNO_3$-$NaNO_3$-KNO_3, $NaNO_3$-KNO_3-$CsNO_3$, $NaNO_3$-KNO_3-$Ca(NO_3)_2$, and $LiNO_3$-$NaNO_3$-KNO_3-$CsNO_3$-$Ca(NO_3)_2$ molten salts are comprehensively determined and evaluated for better understanding their thermal storage and heat transfer performances, such as the melting temperature, thermal stability, specific heat capacity, thermal diffusivity, density and viscosity. The energy storage capacities and figures of merit of the six molten nitrate salts are calculated based on their thermophysical properties to evaluate their TES and HTF performances. This work not only provides the basic engineering data for CSP system, but is useful for choosing media of TES and HTF.

Solar Energy Materials and Solar Cells, 2018, 176: 36

Bacterial Analysis Using an Electrochemical DNA Biosensor with Poly-Adenine-Mediated DNA Self-Assembly

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Ding Min Aldalbahi Ali Ge Zhilei Wang Lihua Yan Juan
Lu Na Li Jiang Wen Yanli Liu Gang

Key words self-assembly monolayer poly-adenine DNA probe electrochemical biosensor modification-free E. coli genome

The spatial arrangement of DNA probes on the electrode surface is of critical significance for the performance of electrochemical biosensors. However, rational control of the probe surface remains challenging. In this work, we develop a capture probe carrying a poly-adenine anchoring block to construct a programmable self-assembled monolayer for a “sandwich-type” electrochemical biosensor. We show that with a co-assembling strategy using a polyA capture probe and 6-mercapto-1-hexanol, the density of the probes on the gold electrode can be simply adjusted by the length of polyA. The electron-transfer effect and thus the hybridization efficiency can as well be optimized by tuning the polyA length. As a result, we obtained an excellent biosensor performance with a limit of detection as low as 5 fM for a synthetic DNA target. We demonstrate the practicability of this system by analyzing a PCR product from *Escherichia coli* genomic DNA (0.2 pg/μL). On the basis of the ideal electrochemical interface, our polyA-based biosensor exhibited excellent reusability and stability, which is important for potential applications in the onsite analysis for a wide range of targets.

ACS Applied Materials & Interfaces, 2018, 10(8): 6895

Eliminating the microbunching-instability-induced sideband in a soft x-ray self-seeding free-electron laser

Zhang Kaiqing Zeng Li Qi Zheng Feng Chao Wang Dong

Key words Sideband, Microbunching instability, Longitudinal coherence, Self-seeding

Soft x-ray self-seeding has been proved to be a feasible method to improve the longitudinal coherence of high gain free-electron laser. However, a pedestal-like sideband in the spectrum has been observed in the experiment, which generally limits the purity of the radiation pulse and the user’s application. The previous theoretical study indicates that the pedestal-like sideband is mainly induced by microbunching instability generated from LINAC. In this paper, three dimensional simulations have been performed to confirm the analytical results and show the formation process

of the spectral sideband. A probable method is proposed to eliminate the pedestal-like sideband by simply inserting a magnetic chicane before the self-seeding FEL undulator. Theoretical and numerical simulations have been performed and the results show that the proposed method can efficiently eliminate the microbunching-instability-induced sideband in a soft x-ray self-seeding FEL.

Nuclear Instruments & Methods in Physics Research Section A-Accelerators Spectrometers Detectors and Associated Equipment, 2018, 882: 22

Temperature dependence of spherical micelles of PS3000-b-PAA(5000) studied by in-situ small angle X-ray scattering

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Key words block copolymer, small angle X-ray scattering, temperature effect, synchrotron

Amphiphilic block copolymer has a character that it spontaneously self-assembles into various micellar morphologies when dissolved in selective solvents with different proportions. Amphiphilic block copolymer has wide potential applications in drug delivery such as the targeting delivery, controlled release, molecular recognition, etc. Poly (styrene)block-poly (acrylic acid) (PS-b-PAA) is a representative amphiphilic block copolymer whose self-assembly in the selective solvents has been widely studied during the past years. Micellar morphology of PS-b-PAA sensitive to temperature, and temperature effect of PS-b-PAA are of great importance for the drug delivery. However, the micellar morphologies of PS-b-PAA have been investigated mainly at the room temperature so far. The understanding is still limited to micellar morphology of PS-b-PAA in the varying temperature processes. In the present work, an investigation of the relationship between micellar morphology of PS-b-PAA and the temperature is conducted by using in-situ small-angle X-ray scattering (in-situ SAXS). The SAXS experiments are performed on the BL19U2 beamline of Shanghai Synchrotron Radiation Facility. The energy is selected to be 10 keV and the wave length is 0.1033 nm. The two-dimensional (2D) SAXS patterns are recorded by Pilatus 1 M with a pixel size of 172 μm × 172 μm. A sample-to-detector distance of 5340 mm is chosen, giving access to a range of scattering vectors q of 0.11-0.89 nm^{-1}. The temperatures of the specimens are monitored by using a Linkam thermal stage THMS600 (Linkam Scientific Instruments). One-dimensional (1D) integrated intensity curves are obtained from the 2D SAXS patterns by employing the Fit2D software. The PS-b-PAAs (PS : PAA = 3000 : 5000) is purchased from

Sigma-Aldrich Inc and used directly (without any treatment prior to experiment). The PS-b-PAA is dissolved in solvents of N, N-Dimethylformamide and H_2O with various proportions. The concentration of solution of PS-b-PAA is 10 mg/mL. The experiments show that the sizes of micelle particles in PS3000-b-PAA(5000) solution are grown with water content increasing, and double scattering peaks (q_{peak1} = 0.418 nm^{-1}, q_{peak1}= 0.456 nm^{-1}) appear for the solution with 10% water. A temperature-dependent change of SAXS intensity is demonstrated by in-situ SAXS. The intensities of peak 1 and peak 2 vary in a contrary waywith the sample's warming up, but the positions of the peaks are independent of temperature. The double peaks in SAXS profiles suggest that the size of micelle particles in the solution is not homogeneous but the micelles with two close sizes coexist. It is interesting that the number of two-sized particles changes at the same rate in the heating process although there is a significant difference between the initial number and the final number of micelles.

ACTA Physica Sinica, 2018, 67(4): 048301

Electromagnetic fields in small systems from a multiphase transport model

Zhao Xinli Ma Yugang Ma Guoliang

We calculate the electromagnetic fields generated in small systems by using a multiphase transport (AMPT) model. Compared to *A+A* collisions, we find that the absolute electric and magnetic fields are not small in *p+Au* and *d+Au* collisions at energies available at the BNL Relativistic Heavy Ion Collider and in *p+Pb* collisions at energies available at the CERN Large Hadron Collider. We study the centrality dependencies and the spatial distributions of electromagnetic fields. We further investigate the azimuthal fluctuations of the magnetic field and its correlation with the fluctuating geometry using event-by-event simulations. We find that the azimuthal correlation $\langle \cos2(\Psi_B-\Psi_2)\rangle$ between the magnetic field direction and the second harmonic participant plane is almost zero in small systems with high multiplicities, but not in those with low multiplicities. This indicates that the charge azimuthal correlation, $\langle cos(\phi_\alpha+\phi_\beta-2\Psi_{RP})\rangle$, is not a valid probe to study the chiral magnetic effect (CME) in small systems with high multiplicities. However, we suggest searching for possible CME effects in small systems with low multiplicities.

Physical Review C, 2018, 97(2): 024910

Experimental investigation and thermodynamic modeling of an innovative molten salt for thermal energy storage (TES)

Li Xiang Wu Shuang Wang Yang Xie Leidong

Key words Computational thermodynamic approach, Molten salts, Thermal energy storage

A novel computational thermodynamic approach based on thermodynamic principles was applied to design and develop innovative molten salt mixtures for thermal energy storage. In this work, the eutectic composition of the NaCl-NaF-Na_2CO_3 ternary system was predicted based on experimental data via computational thermodynamic approach. Substitutional solution model (SSM) was used to describe the Gibbs energies for all liquid phases. Thus, a set of self-consistent thermodynamic model parameters was obtained for three subsystems and the parameters were used to predict the eutectic composition of the NaF-NaCl-Na_2CO_3 ternary system. Results manifested that the predicted eutectic point of the ternary system were located at $T = 849\ K$ and $X_{NaF} = 21.66$ mol%, $X_{NaCl} = 41.87$ mol% and $X_{Na2CO3} = 36.47$ mol%. By means of Differential Scanning Calorimetry method, the predicted results were verified experimentally and the agreement between the measured and predicted values was satisfactory. Thermal-physical properties for eutectic salt mixtures, such as enthalpies of fusion, heat capacity, density and thermal stability, were also determined experimentally via thermal analysis methods in this work. Through computational thermodynamics approach, an innovative eutectic salt was designed and developed as thermal energy storage (TES) materials at high temperatures, especially it can be serve as candidate thermal energy storage materials for next generation concentrated solar power (CSP) plants.

Applied Energy, 2018, 212: 516

Optimizing the Crystallinity and Phase Separation of PTB7: PC71BM Films by Modified Graphene Oxide

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Ghiggino Kenneth P. Hao Xiaotao

A facile method is proposed to obtain modified shorn graphene oxide (DDAB-sGO) with improved dispersion in organic solvents. Didodecyl dimethylammonium bromide (DDAB)-sGO, which exhibits good dispersibility in the nonpolar solvent *o*-dichlorobenzene, was obtained *via* the sono-Fenton reaction and DDAB ionic functionalization. DDAB-sGO was used in the preparation

of conjugated polymer: fullerene blend composites. UV–visible absorption spectra, steady-state photoluminescence spectra, fluorescence decay, and grazing incidence X-ray scattering measurements were applied to characterize morphologies, structural features, and charge-transport characteristics of the composites. Doped into poly[[4,8-bis[(2-ethylhexyl)oxy]benzo[1,2-*b*: 4,5-*b*′]dithiophene-2,6-diyl][3-fluoro-2-[(2-ethylhexyl)carbonyl]thieno[3,4-*b*]thiophenediyl]] (PTB7): [6,6]-phenyl C_{71} butyric acid methyl ester ($PC_{71}BM$) conjugated polymer blends, DDAB-sGO is shown to facilitate increased crystallinity and phase separation of PTB7 and $PC_{71}BM$ to achieve a more optimal morphology for bulk heterojunction solar cells, resulting in a ~12% enhancement in power conversion efficiency over the undoped PTB7: $PC_{71}BM$ blend.

Journal of Physical Chemistry, 2018, 122(5): 2572

Identifying the Genotypes of Hepatitis B Virus (HBV) with DNA Origami Label

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Key words atomic force microscope (AFM), DNA origami, genotype, HBV

The hepatitis B virus (HBV) genotyping may profoundly affect the accurate diagnosis and antiviral treatment of viral hepatitis. Existing genotyping methods such as serological, immunological, or molecular testing are still suffered from substandard specificity and low sensitivity in laboratory or clinical application. In a previous study, a set of high-efficiency hybridizable DNA origami-based shape ID probes to target the templates through which genetic variation could be determined in an ultrahigh resolution of atomic force microscopy (AFM) nanomechanical imaging are established. Here, as a further confirmatory research to explore the sensitivity and applicability of this assay, differentially predesigned DNA origami shape ID probes are also developed for precisely HBV genotyping. Through the specific identification of visualized DNA origami nanostructure with clinical HBV DNA samples, the genetic variation information of genotypes can be directly identified under AFM. As a proof-of-concept, five genotype B and six genotype C are detected in 11 HBV-infected patients' blood DNA samples of Han Chinese population in the single-blinded test. The AFM image-based DNA origami shape ID genotyping approach shows high specificity and sensitivity, which could be promising for virus infection diagnosis and precision medicine in the future.

Small, 2018, 14(6): 1701718

Merits of the Addition of PTFE Micropowder in Supercritical Carbon Dioxide Foaming of Polypropylene: Ultrahigh Cell Density, High Tensile Strength, and Good Sound Insulation

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Zhao Quan Wu Guozhong

Ultrahigh-cell-density polypropylene (PP) foam was prepared by supercritical carbon dioxide ($scCO_2$) foaming in the presence of porous polytetrafluoroethylene (PTFE) micropowder. The voids of PTFE microparticles were filled with supercritical CO_2, causing them to split into multiple granules due to the force of its expansion during the pressure release, resulting in the formation of a large number of nucleation sites. The cell density of this foam reached 10^{10}–10^{11} cells/cm^3, which was 2–5 orders of magnitude higher than pristine PP foam. We proposed that the nanoscale granules resulting from the splitting of PTFE microparticles, and the growth of nucleated small cells that generated the local strain field variation in the multiple-phase system, were responsible for the considerably increased nucleation number of PP foaming. Additionally, the tensile strength and sound absorption property of PP/PTFE foam were largely enhanced and the preparation of ultrahigh-cell-density PP/PTFE foam was easily controlled over a wider foaming temperature window.

Industrial & Engineering Chemistry Research, 2018, 57(5): 1498

A Large Family of Centrosymmetric and Chiral f-Element-Bearing Iodate Selenates Exhibiting Coordination Number and Dimensional Reductions

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The exploration of phase formation in the f-element-bearing iodate selenate system has resulted in 14 novel rare-earth-containing iodate selenates, $Ln(IO_3)(SeO_4)$ (Ln = La, Ce, Pr, Nd, LnISeO-1), $Ln(IO_3)(SeO_4)(H_2O)$ (Ln = Sm, Eu, LnISeO-2), and $Ln(IO_3)(SeO_4)(H_2O)_2{\cdot}H_2O$ (Ln = Gd, Dy, Ho, Er, Tm, Yb, Lu, Y, LnISeO-3), as well as two new thorium iodate selenates,

$Th(OH)(IO_3)(SeO_4)(H_2O)$ (ThISeO-1) and $Th(IO_3)_2(SeO_4)$ (ThISeO-2). LnISeO-3 and ThISeO-2 crystallize in the chiral space group $P2_12_12_1$, while LnISeO-1, LnISeO-2, and ThISeO-1 crystallize in the centrosymmetric space group $P2_1/c$. The numbers of both coordinating and hydrating water molecules crystallized in LnISeO-1, LnISeO-2, and LnISeO-3 increase along these three series, in line with the increasingly negative values of hydration enthalpies of heavier trivalent lanthanide ions. Such a systematic change in compositions, especially the first coordination sphere of Ln, further induces structural rearrangements, including coordination number and dimensional reductions. More specifically, the structures of LnISeO-1, LnISeO-2, and LnISeO-3 have undergone transitions from 2D Ln–oxo layers with 10-coordinate Ln centers to 1D Ln–oxo chains with 9-coordinate Ln centers and then to 0D Ln–oxo monomers with 8-coordinate Ln centers, respectively. The formation and characterization of this large family of Ln/Th iodate selenates suggest that such a mixed-anion system not only exhibits richer structural chemistry but also can be capable of generating intriguing properties, such as the second-harmonic generation (SHG) effect.

Inorganic Chemistry, 2018, 57(4): 1676

Design of wide-range energy material beamline at the Shanghai Synchrotron Radiation Facility

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Jiang Zheng Wang Yong Tai Renzhong

Key words Synchrotron radiation, Beamline, Wide energy range, E-line, Shanghai Synchrotron Radiation Facility

We report the design of a wide-range energy material beamline (E-line) with multiple experimental techniques at the Shanghai Synchrotron Radiation Facility. The undulators consisted of an elliptically polarizing undulator and in-vacuum undulator that generate the soft and hard X-rays, respectively. The beamline covered a wide energy range from 130 to 18 keV with both a high photon flux (> 10^{12} phs/s with exit silt 30 μm in soft X-ray and > 5×10^{12} phs/s in hard X-ray within 0.1%BW bandwidth) and promising resolving power (maximum $E/\Delta E$ > 15,000 in soft X-ray with exit silt 30 μm and > 6000 in hard X-ray). Moreover, the beam spots from the soft and hard X-rays were focused to the same sample position with a high overlap ratio, so that the surfaces, interfaces, and bulk properties were characterized in situ by changing the probing depth.

Nuclear Science and Techniques, 2018, 29(2): 26

New design for multi-crystal data collection at SSRF

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Key words Kapton membrane, Microcrystals, Multi-crystal data collection, Protein structure

Data collection with microcrystals at synchrotron radiation facilities is challenging because it is difficult to harvest and locate microcrystals. Moreover, microcrystals are sensitive to radiation damage, thus, typically, a complete data set cannot be obtained with a single microcrystal. Herein, we report a new method for data collection with multiple microcrystals having a crystal size ranging from 1 to 30 μm. This method is suitable for not only low-temperature (100 K) data collection but also room-temperature data collection. Thin Kapton membranes were used to capture multiple crystals simultaneously. The microcrystals were visible under an optical microscope and easily located because the membrane was transparent and sufficiently thin. The film was fixed to a bracket that was prepared using a three-dimensional printer. The bracket was fixed on a magnetic base via screwing and employed by the goniometer system for data collection. Multiple data sets of fatty acid-binding protein 4 (FABP4) and lysozyme microcrystals were collected using this novel designed device. Finally, the structures of protein FABP4 and lysozyme were obtained from these data via the molecule replacement method. The data statistics reveal that this method provides a comparable result to traditional methods such as a nylon loop.

Nuclear Science and Techniques, 2018, 29(2): 21

Wetting behaviors of methanol, ethanol, and propanol on hydroxylated SiO_2 substrate

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Key words Wetting behavior, Alcohol, SiO_2, Molecular dynamics simulation

Water molecules could form a liquid droplet on the water monolayer on a specific solid surface, which has been referred to as ‘‘ordered water monolayer that does not completely wet water’’ at room temperature. In contrast to the water molecules, the family of alcohol molecules has the same OH polar head and various lengths of their hydrophobic nonpolar tail, the length of the hydrophobic tail can affect the hydrophobic effect. In this study, using molecular dynamics simulations, we investigated the wetting behaviors of methanol, ethanol, and propanol molecules adsorbed on a SiO_2 surface. The results showed that the methanol, ethanol, and propanol molecules could form an ordered monolayer on the SiO_2 surface and a droplet on top of this monolayer, with

different contact angles. The differences in the contact angles were attributed to the differences in the interactions between the alcohol monolayer and droplet.

Nuclear Science and Techniques, 2018, 29(2): 18

Spectroscopic study of *β*-delayed particle emission from proton-rich nucleus ^{23}Si

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Lin C. J. Ma J. B. Ma P. Ma W. H. Nie M. W. Shi C. Z.
Wang H. W. Wang J. G. Wang J. S. Yang L. Yang Y. Y.
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Key words β-delayed particle emission, exotic nucleus, Si-23

The β-delayed particle emission from the exotic nucleus ^{23}Si has been studied using a detection system with silicon array and clover-type high-purity germanium (HPGe) detectors. The β-delayed charged-particle spectrum and γ-ray spectrum were identified. The half-life of ^{23}Si has been determined. A new β-delayed proton branch with an energy of 3811keV was observed. The β-delayed two-proton emission was confirmed.

International Journal of Modern Physics E, 2018, 27(2): 1850014

Anomalous compression behaviour in Nd_2O_3 studied by x-ray diffraction and Raman spectroscopy

Jiang Sheng Liu Jing Bai Ligang Li Xiaodong Li Yanchun
He Shangming Yan Shuai Liang Dongxu

The structural stability of hexagonal Nd_2O_3 under pressure has been investigated by *in situ* synchrotron angle dispersive x-ray diffraction and Raman spectroscopy up to 53.1 GPa and 37.0 GPa, respectively. Rietveld analysis of the x-ray diffraction data indicate that the hexagonal Nd_2O_3 undergoes an isostructural phase transition in the pressure range from 10.2 to 20.3 GPa, accompanied by anomalous lattice compressibility and pressure-volume curve. A third-order Birch-Murnaghan fit based on the observed Pressure-Volume data yields zero pressure bulk moduli (B_0) of 142(4) and 183(6) GPa for the low and high pressure hexagonal phases, respectively. Raman spectroscopy confirms this isostructural transition, the pressure dependence of the Raman modes display noticeable breaks in the pressure range of 9.7-20.9 GPa, which is consistent with the change of Nd-O bond length. The pressure coefficients of Raman peaks and the mode Grüneisen parameters of different Raman modes were also determined.

AIP Advances, 2018, 8(2): 025019

Protection-against-water-attack determined difference between strengths of backbone hydrogen bonds in kinesin's neck zipper region

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Key words kinesin, neck linker, water

Docking of the kinesin's neck linker (NL) to the motor domain is the key force-generation process of the kinesin. In this process, NL's β10 portion forms four backbone hydrogen bonds (HBs) with the motor domain. These backbone hydrogen bonds show big differences in their effective strength. The origins of these strength differences are still unclear. Using molecular dynamics method, we investigate the stability of the backbone HBs in explicit water environment. We find that the strength differences of these backbone HBs mainly arise from their relationships with water molecules which are controlled by arranging the surrounding residue sidechains. The arrangement of the residues in the C-terminal part of β10 results in the existence of the water-attack channels around the backbone HBs in this region. Along these channels the water molecules can directly attack the backbone HBs and make these HBs relatively weak. In contrast, the backbone HB at the N-terminus of β10 is protected by the surrounding hydrophobic and hydrophilic residues which cooperate positively with the central backbone HB and make this HB highly strong. The intimate relationship between the effective strength of protein backbone HB and water revealed here should be considered when performing mechanical analysis for protein conformational changes.

Chinese Physics B, 2018, 27(2): 028704

Microstructural evolution and hardening of GH3535 alloy under energetic Xe ion irradiation at room temperature and 650 °C

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Li Jianjian Lei Guanhong Huang Qing Liu Min Xie Ruobing

Key words GH3535 alloy, Xe ion irradiation, Microstructural evolution, Irradiation hardening, Temperature effect

The GH3535 alloy was irradiated with 7 MeV Xe^{26+} ions to a dose of 10 dpa at room temperature (RT) and 650 °C, and subsequently examined using Transmission Electron Microscopy (TEM) and nanoindentation. High numbers of nano-sized black dots, identified as dislocation loops were observed in both irradiated samples. The dislocation loops detected at the high temperature irradiated sample (size/number density: 9.5 nm/1.9 × 10^{21} m^{-3}) were found to be

larger in size but less in amount as compared to that of the case of RT irradiation (6.9 nm/18.7 × 10^{21} m^{-3}). In addition, the large-sized Mo-Cr rich precipitates (16.4 nm/3.7 × 10^{21} m^{-3}) were observed in the sample irradiated at 650 °C. Moreover, the Xe bubbles, with smaller size (2.9 nm) but higher number density (77.8 × 10^{21} m^{-3}) among the irradiated induced defects, were also detected in the case of high temperature irradiated sample via the diffusion and aggregation of Xe atoms. Nanoindentaion measurements showed a hardening phenomenon for the irradiated sample, and the hardness increment is higher in the case of high temperature irradiated sample. Dispersed barrier-hardening (DBH) model was applied to predict the hardening produced from the irradiation induced defects. The yield strength increment calculated based on TEM observations and the nanohardness increment measured using nanoindentation are in excellent agreement.

Journal of Nuclear Materials, 2018, 499: 431

Scalar field coupling to Einstein tensor in regular black hole spacetime

Zhang Chi Wu Chen

Key words Quasinormal modes, Scalar field coupling to Einstein's tensor, Regular black hole

In this paper, we study the perturbation property of a scalar field coupling to Einstein's tensor in the background of the regular black hole spacetimes. Our calculations show that the the coupling constant. imprints in the wave equation of a scalar perturbation. We calculated the quasinormal modes of scalar field coupling to Einstein's tensor in the regular black hole spacetimes by the 3rd order WKB method.

General Relativity and Gravitation, 2018, 50(2): 18

Study on the microstructure evolution of TiO_2-reinforced HDPE nanocomposites by synchrotron small angle X-ray scattering

Li Xiaoyun Liu Guoming Tang Zhongfeng Zhang Xiuqin
Zhou Ping Wang Jie Li Xiuhong Li Liangbin

This work studies the effect of titanium dioxide (TiO_2) nanoparticles on mechanical properties, thermal behavior and microstructures of high-density polyethylene (HDPE). Differential scanning calorimetry (DSC) results showed that melting temperature and crystallinity of the nanocomposites

are affected by incorporating TiO_2, the crystallinity reaches maximum at low TiO_2 loading following with a significant reduction when the content of TiO_2 higher than 2 wt%. To deeply understand structure–property relationship, SAXS experiments were carried out. The results indicated that the nanoparticles were homogeneously distributed in the HDPE matrix. The TiO_2 nanoparticles exhibit surface-fractal characteristic at small scale. At large scale, with TiO_2 content increasing, TiO_2 clusters grow gradually until 2 wt%. The optimum microstructures and mechanical properties of HDPE/TiO_2 nanocomposites were achieved at about 2 wt% loading.

Polymer Composites, 2018, 39(2): 580

Effect of CrF_3 on the corrosion behaviour of Hastelloy-N and 316L stainless steel alloys in FLiNaK molten salt

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Fei Zejie Zhao Sufang An Xuehui Cheng Jinhui Chen Tao
Zhang Peng Yu Guojun Xie Leidong

Key words CrF_3, FLiNaK, 316L stainless steel, Hastelloy-N, Corrosion

The effect of CrF_3 on the corrosion behaviour of Hastelloy-N and 316L austenitic stainless steel alloys in FLiNaK at 700 °C was investigated using synchrotron radiation and other characterisation techniques. The results showed that CrF_3 considerably accelerated the corrosion of both tested alloys by promoting the dissolution of Cr, Fe, and Mn from alloy matrices into molten salt. The 316L stainless steel alloys mainly exhibited intergranular corrosion, whereas the Hastelloy-N alloys tended to exhibit intergranular and pitting corrosion. After corrosion, the lattice parameter of both alloys decreased and $Cr_{1.07}Fe_{18.93}$ was formed on the surface of the 316L stainless steel alloys.

Corrosion Science, 2018, 131: 355

A study on $K^*(892)^0$ and Φ(1020) production in p-Pb and Pb-Pb collisions at the LHC from a multiphase transport model

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Key words rescattering, regeneration, transverse momentum distribution, elliptic flow

Using a multiphase transport (AMPT) model that includes both initial partonic and final

hadronic interactions, we study {K}* {(892)}^{0} and φ (1020) production at the Large Hadron Collider (LHC). It is found that a hadronic cascade time of {t}≥slant 10 fm c $^{-1}$ describes the strong suppression of the {K}^{*0}/{K}$^{-}$ ratio in central Pb-Pb collisions at \sqrt{{s}$_{\{NN\}}$}} = 2.76 TeV, while for the p-Pb collisions at \sqrt{{s}$_{\{NN\}}$}} = 5.02 TeV, a lower limit of hadronic interaction {t}≥slant 4 fm c $^{-1}$ is derived by comparison with the collision system dependence of the {K}^{*0}/{K}$^{-}$ and φ /{K}$^{-}$ ratios. Detailed studies on the transverse momentum dependence of the {K}^{*0}/{K}$^{-}$,φ /{K}$^{-}$ and {K}^{*0}/π ,φ /π ratios, and the elliptic flow of {K}^{*0} and ϕ show clear evidence of the dominance of rescattering over regeneration of {K}^{*0} in heavy-ion collisions at LHC energies. Our calculation describes the flat {{p}}/φ ratio well in central Pb-Pb collisions at 0< {p}$_{\{T\}}$}< 5 {GeV} c $^{-1}$, indicating fluid-like dynamics in the AMPT model.

Journal of Physics G-Nuclear and Particle Physics, 2018, 45(2): 025102

Targeted Imaging of Brain Tumors with a Framework Nucleic Acid Probe

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Liu Xinyi Xia Jiaoyun Shi Jiye Wang Lihua Lu Weiyue
Fan Chunhai

Key words blood-brain barrier, DNA tetrahedron, angiopep-2, glioma, imaging

Development of agents for delivering drugs and imaging probes across the blood-brain barrier (BBB) remains a major challenge. In this study, we designed a biocompatible framework nucleic acid (FNA)-based imaging probe for brain tumor-targeting. We employed a typical type of FNAs, tetrahedral DNA nanostructures (TDNs), as the building block, which were modified with angiopep-2 (ANG), a 19-mer peptide derived from human Kunitz domain of aprotinin. This probe exhibited high binding efficiency with low-density lipoprotein receptor-related protein-1 (LRP-1) of BBB and glioma. We found that ANG-functionalized TDNs (ANG-TDNs) stayed intact for at least 12 h in serum, and that ANG modification effectively enhanced cellular uptake of TDNs in brain capillary endothelial cells and Uppsala 87 malignant glioma (U87MG) cells. Remarkably, studies in both in vitro and in vivo models revealed that ANG-TDNs could cross the BBB. Especially, in vivo imaging showed strong fluorescent signals in U87MG human glioblastoma xenograft in nude mice. This study establishes that the FNA-based platform provides a new theranostic tool for the study and therapy of brain tumors.

ACS Applied Materials & Interfaces, 2018, 10(4): 3414

Microstructural characterization of Ni-201 weld cladding onto 304 stainless steel

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Li Zhijun Zhou Xingtai

Key words Gas Tungsten Arc Welding (GTAW), Microstructure, Interface, Precipitates, delta-Ferrite, Hardness, Corrosion resistance

Ni-201(ERNi-1), a cladding layer which is resistant to the corrosion of molten salts, was deposited on 304SS substrate by Gas Tungsten Arc Welding (GTAW). Microstructure characterization showed that the cladding interface was obviously divided into three zones from microstructures along depth, weld metal (WM), unmixed zone (UZ) and heat affected zone (HAZ). Element distribution presented that elements Ti, N, Si were segregated into interdendritic region of WM and formed the TiN precipitates during the solidification. The element distribution of UZ was similar to that of HAZ. A large quantity of vermicular δ-ferrite phases were precipitated in laminar UZ. Grain coarsening in HAZ was evident compared with the grains in base metal, and no precipitates were found in HAZ. The hardness of cladding layers was decreased from interface to surface. The cladding layer exhibited excellent corrosion resistance to molten FLiNaK salts.

Surface & Coatings Technology, 2018, 334: 19

In Situ Probing of the Particle-Mediated Mechanism of WO_3-Networked Structures Grown inside Confined Mesoporous Channels

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Wu Zhenduo Zeng Jianrong Tian Feng Fang Jixiang

Key words confined spaces, in situ transmission electron microscopy, oriented attachment, particle-mediated mechanisms, small-angle X-ray scattering spectroscopy

Nanocasting, using ordered mesoporous silica or carbon as a hard template, has enormous potential for preparing novel mesoporous materials with new structures and compositions. Although a variety of mesoporous materials have been synthesized in recent years, the growth mechanism of nanostructures in a confined space, such as mesoporous channels, is not well understood, which hampers the controlled synthesis and further application of mesoporous materials. Here, the nucleation and growth of WO_3 -networked mesostructures within an ordered

mesoporous matrix, using an in situ transmission electron microscopy heating technique and in situ synchrotron small-angle X-ray scattering spectroscopy, are probed. It is found that the formation of WO_3 mesostructures involves a particle-mediated transformation and coalescence mechanism. The liquid-like particle-mediated aggregation and mesoscale transformation process can occur in ≈10 nm confined mesoporous channels, which is completely unexpected. The detailed mechanistic study will be of great help for experimental design and to exploit a variety of mesoporous materials for diverse applications, such as catalysis, absorption, separation, energy storage, biomedicine, and nanooptics.

Small, 2018, 14(4): 1702565

In Situ Spatial Complementation of Aptamer-Mediated Recognition Enables Live-Cell Imaging of Native RNA Transcripts in Real Time

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Zhao Yun Shi Jiye Wang Lihua Glinsky Gennadi Chen Nan
Lal Ratnesh Fan Chunhai

Key words bioanalysis, cellular imaging, fluorescence, mRNA, split aptamers

Direct cellular imaging of the localization and dynamics of biomolecules helps to understand their function and reveals novel mechanisms at the single-cell resolution. In contrast to routine fluorescent-protein-based protein imaging, technology for RNA imaging remains less well explored because of the lack of enabling technology. Herein, we report the development of an aptamer-initiated fluorescence complementation (AiFC) method for RNA imaging by engineering a green fluorescence protein (GFP)-mimicking turn-on RNA aptamer, Broccoli, into two split fragments that could tandemly bind to target mRNA. When genetically encoded in cells, endogenous mRNA molecules recruited Split-Broccoli and brought the two fragments into spatial proximity, which formed a fluorophore-binding site in situ and turned on fluorescence. Significantly, we demonstrated the use of AiFC for high-contrast and real-time imaging of endogenous RNA molecules in living mammalian cells. We envision wide application and practical utility of this enabling technology to in vivo single-cell visualization and mechanistic analysis of macromolecular interactions.

Angewandte Chemie International Edition, 2018, 57(4): 972

Electrochemical deposition of neodymium in $LiF-CaF_2$ from Nd_2O_3 assisted by AlF_3

Chen Zi She Changfeng Zheng Haiyang Huang Wei
Zhu Tiejian Jiang Feng Gong Yu Li Qingnuan

Key words $LiF-CaF_2$, Nd_2O_3, AlF_3, Al-Nd alloys, Electrochemical deposition

This paper investigated the co-reduction process of Al-Nd alloys and the electrochemical extraction of neodymium from neodymium oxide in $LiF-CaF_2$ melt. Nd(III) at a tungsten electrode was reduced to Nd(0) through a one-step process involving the exchange of three electrons: $Nd(III) + 3e^- = Nd(0)$. The fluorination of Nd_2O_3 by AlF_3 produced Nd(III) ions in the $LiF-CaF_2$ molten salts. The co-reduction behavior of Nd(III) and Al(III) ions was studied on a W electrode in the $LiF-CaF_2-AlF_3-Nd_2O_3$ system. Four types of intermetallic Al-Nd compound were detected through cyclic voltammetry and open circuit chronopotentiometry. The Nd_3Al and NdAl phases were identified through X-ray diffraction, and the $NdAl_3$ and Nd_3Al_{11} phases were characterized by a scanning electron microscope equipped with an energy dispersive spectrometer.

Electrochimica Acta, 2018, 261: 289

Nanomanipulation of Individual DNA Molecules Covered by Single-Layered Reduced Graphene Oxide Sheets on a Solid Substrate

Wang Ying Shen Yue Li Bin Wang Shuo Zhang Jinjin
Zhang Yi Hu Jun

Nanomanipulation of single DNA molecules has great potential in fundamental genetic research and clinical analysis, and is a good model system for studying the interfacial effects on physiochemical processes, which occur when manipulating the linear DNA molecules with an atomic force microscope (AFM) tip. Here, we demonstrate that AFM nanomanipulation can be carried out on DNA molecules covered by a single-layered reduced graphene oxide sheet. Nanomanipulation, which includes cutting, pushing, and sweeping operations, specific to the covered DNA molecules can be achieved in a well-controlled manner using AFM in the PeakForce Quantitative Nano-Mechanics mode. It was found that the normal force required to cut covered DNA strands is over five times greater than that required for naked strands. This technique provides a distinctive method for the construction of graphene architecture by tailoring the underlying artificial DNA nanostructures.

Journal of Physical Chemistry B, 2018, 122(2): 612

Elliptic flow coefficients from transverse momentum conservation

Bzdak Adam Ma Guoliang

We calculate the k-particle (k=2,4,6,8) azimuthal cumulants resulting from the conservation of transverse momentum. We find that $c_2\{k\}>0$ and depending on the transverse momenta, $c_2\{k\}$ can reach substantial values even for a relatively large number of particles. The impact of our results on the understanding of the onset of collectivity in small systems is emphasized.

Physical Review C, 2018, 97(1): 014903

Epitope Binning Assay Using an Electron Transfer-Modulated Aptamer Sensor

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Song Hongbin Aldalbahi Ali Ge Zhilei Li Jiang Li Qian
Song Shiping Li Shaohua Shao Ningsheng Fan Chunhai
Wang Lihua

Key words binding affinity, conformation alteration, epitope binning, interfacial electron transfer, pairwise selection

Surface plasmon resonance and quartz crystal microbalance are workhorses of protein-DNA interaction research for over 20 years, providing ways to quantitatively determine the protein-DNA binding. However, the cost, necessary technical expertise, and severe nonspecific adsorption poses barriers to their use. Convenient and effective techniques for the measurement of protein-DNA binding affinity and the epitope binning between DNA and proteins for developing highly sensitive detection platform remain challenging. Here, we develop a binding-induced alteration in electron transfer kinetics of the redox reporter labeled (methylene blue) on DNA aptamer to measure the binding affinity between prostate-specific antigen (PSA) and aptamer. We demonstrate that the binding of PSA to aptamer decreases the electron transfer rate of methylene blue for ~45%. Further, we identify the best pairwise selection of aptamers for developing sandwich assay by sorting from 10 pairwise modes with the PSA detection limit of 500 ng/mL. Our study provides promising ways to analyze the binding affinity between ligand and receptor and to sort pairwise between aptamers or antibodies for the development of highly sensitive sandwich immunoassays.

ACS Applied Materials & Interfaces, 2018, 10(1): 341

Carboxylic Acid Group-Induced Oxygen Vacancy Migration on an Anatase (101) Surface

Li Yadong Gao Yi

Dye-sensitized solar cells (DSSCs) have aroused intensive interest for the replacement of conventional crystalline silicon solar cells. Through carboxylic acid groups, the dyes attach to the TiO_2 anatase (101) surface, on which the subsurface oxygen vacancies ($Vo^{sub}s$) are predominant. The performance of DSSCs can be affected by the presence and positions of oxygen vacancies (Vos). By applying density functional theory calculations, we found that the adsorption of a carboxylic acid group-decorated dye molecule reverses the relative stability between the surface oxygen vacancy (Vo^{surf}) and Vo^{sub} on the anatase (101) surface, which facilitates the migration of the Vo from the subsurface to the surface by overcoming an energy barrier of less than 0.16 eV, which is significantly lower than the 1.01 eV energy barrier on the clean surface. Further, ab initio molecular dynamics simulations indicate that the Vo^{sub} can easily migrate to the surface at room temperature. This dynamic interplay between the Vo of the anatase (101) surface and the carboxylic acid group would be important for future studies concerning the stability and photovoltaic efficiency of the solar cells.

Langmuir, 2018, 34(1): 546

Unveiling the Atomic Structures of the Minority Surfaces of TiO_2 Nanocrystals

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Determining the atomic structures of minority surfaces of TiO_2 is of critical importance in terms of accurately interpreting their demonstrated properties. Unlike well-studied majority surfaces [such as anatase TiO_2 (101)], the structures of the more attractive minority surfaces and edges are poorly known, which hampers the further understanding of their unique behaviors. Herein, through the aberration-corrected scanning transmission electron microscope, the atomic structures of the five minority surfaces [(100), (001), (102), (103), and (301)] and edges between six facets are experimentally determined. Several unique configurations are unveiled on the (301) and (102) surfaces. Intriguingly, the defective (103) and (102) surfaces are identified as distinct structures, completely different from the early predictions of stoichiometric surfaces, which are further confirmed by first-principles calculations. With the calculations based on density functional

theory, the intrinsic electronic properties of the minority surfaces are also revealed. This work provides new information on minority surfaces and edges, which contributes to advancing our knowledge in surfaces and better understanding their versatile performances.

Chemistry of Materials, 2018, 10(1): 288

Effect of proton irradiation on microstructure evolution of permanent magnet

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Xia Xiaobin Shen Weizu

Key words proton irradiation, $Nd_2Fe_{14}B$ rare permanent magnet, Sm_2Co_{17} type permanent magnet, microstructure

The effects of proton irradiation on the structure of NdFeB permanent magnet were investigated by X-ray diffraction and X-ray absorption fine structure (XAFS). The results reveal that proton irradiation has no effect on the long-range structure, but significantly affects the atomic local structure of the NdFeB magnet. The alignment degree of the magnet decreases and the internal stress of the lattice increases after proton irradiation. XAFS results show that the coordination number of Fe–Nd in the first neighboring coordination shell of the Fe atoms decreases and the disorder degree increases.

Acta Physica Sinica, 2018, 67(1): 016104

Criticality Properties and Control Rod Worth of the Critical Experiment Device for MSR Research

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Zhou Bo Yu Shihe

Key words Molten salt reactor, device, criticality properties, k_{eff}, control rod worth

Zero-power experiments are very important parts in design verification for all reactor types. In the 1970s, in China, at the Shanghai Institute of Applied Physics (then, Shanghai Institute of Nuclear Research), a Critical Experiment Device (cold) was established for research on the physics characteristics of the molten salt reactor (MSR), and a series of zero-power experiments was successfully performed, related experimental results were obtained later. The device consisted mainly of graphite moderator and powdered $BeF_2 – UF_4$ / ThF_4 fuel and could achieve a maximum power of 200 W. The current work is focused on criticality properties with various core

configurations and fuel arrangements of this device and the worths of the cadmium rods used in the device. Evaluations on the agreement of calculation results with experimental data showed good results. Discrepancies between the calculation results and the experimental data might be primarily caused by the simulated outermost fuel element positions not being exactly the same as the experimental arrangements and the unmodeled instruments used in the experiments. The findings in this work can be considered a step of verification of simulation methods and calculations for a cold MSR.

Nuclear Technology, 2018, 204(2): 203

Uranium thermochemical cycle: hydrogen production demonstration

Chen Aimei Zheng Xiaobei Liu Chunxia Liu Yuxia Zhang Lan

Key words Energy, hydrogen production, sodium diuranate, thermochemical cycle, uranium

In hydrogen production industry, thermochemical cycle technology for converting thermal energy into chemical storage energy of hydrogen owns absolute advantages. Compared with other thermochemical cycles, thermochemical cycle technology based on uranium (UTC) is safer and more efficient. This technology consists of three steps, where only the hydrogen production step is unique. In this paper, the verification has been done for this step. Solid products were characterized by XRD and Raman spectroscopy, which were confirmed to be -$Na_2U_2O_7$. Gas chromatographic analyses were performed for gas samples, in which hydrogen output was obtained using an internal standard method.

Energy Sources Part A-Recovery Utilization and Environmental Effects, 2018, 40(21): 2542

Enhanced removal of heavy metals by zerovalent iron in designed magnetic reactors

Fan Peng Jiang Xiao Qiao Junlian Li Lina

Key words Zerovalent iron, weak magnetic field, reactor electroplating wastewater, metal pollution

A magnetic propeller agitator and a magnetic reactor were designed to enhance the removal of heavy metals by zerovalent iron (ZVI) in comparison with the non-magnetic reactor. The weak magnetic field (WMF) applied significantly improved the CuII-EDTA removal by ZVI from 10%

without WMF to 98% with WMF within 2.5 h at pHini 6.0. The pseudo-first-order rate constants of Cu(II) and As(V) removal by ZVI in the magnetic reactor were increased by 1.51–5.17 and 2.97–5.91 fold, respectively, compared to those obtained in the non-magnetic reactor. The performance of ZVI for treating practical industrial wastewater in the designed magnetic reactor was tested, and the removal of total Cu, P and Zn by ZVI was greatly accelerated. After precipitation of the practical wastewater samples, the concentrations of total Cu, P, Zn decreased to the industrial drainage standard values in 20, 3, 25 min, respectively, in the magnetic reactor, whereas the reaction time needed to eliminate total P and Zn was 10 and 60 min, and the residual total Cu still exceeded the drainage standard values in 2 h in the non-magnetic reactor. The application of magnetic reactor for industrial wastewater treatment is expected to improve the sustainability of ZVI technology.

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environmental technology, 2018, 39(19): 2542

Coherent nanoscale cobalt/cobalt oxide heterostructures embedded in porous carbon for the oxygen reduction reaction

Li Xuecheng She Fashuang Shen Dong Liu Chaoping Chen Lihua Li Yu Deng Zhao Chen Zhenhua Wang Hongen

Cost-effective and efficient electrocatalysts for the oxygen reduction reaction (ORR) are crucial for fuel cells and metal–air batteries. Herein, we report the facile synthesis of a Co/CoO/Co_3O_4 heterostructure embedded in a porous carbon matrix by refluxing and annealing. This composite exhibits several structural merits for catalyzing the ORR: (1) the existence of metallic Co and graphitic carbon enhanced the electrical conduction, (2) the porous, loose carbon network facilitated the electrolyte permeation and mass transport, (3) more importantly, the nanosized coherent CoO/Co_3O_4 heterojunctions with structural defects and oxygen vacancies enhanced the charge transport/separation at the interface and adsorption affinity to O_2, thus promoting the ORR kinetics and lowering the reaction barrier. Consequently, the composite electrode manifests high electrocatalytic activity, attaining a current density of 6.7 mA cm^{-2} at −0.8 V (*vs.* Ag/AgCl), which is superior to pure CoO nanoparticles (4.7 mA cm^{-2}), and has good methanol tolerance. The present strategy based on heterostructure and vacancy engineering may pave the way for the exploration of more advanced, low-cost electrocatalysts for electrochemical reduction and evolution processes.

RSC Advances, 2018, 8(50): 28625

Study on the Electrochemical Co-Reduction of Gd(III) and Al(III) in LiF-CaF2 Melt

Chen Zi She Changfeng Zheng Haiyang Huang Wei
Zhu Tiejian Jiang Feng Gong Yu Li Qingnuan

This paper describes the co-reduction process of Gd-Al alloys and the electrochemical extraction of gadolinium from gadolinium oxide in LiF-CaF_2 melt. Gd_2O_3 was fluorinated by adding AlF_3, and dissolved into the melt as Gd(III). The electrochemical behaviors and alloy forming mechanisms of Gd(III) and Al(III) were analyzed through cyclic voltammetry, square wave voltammetry, chronopotentiometry, and open circuit chronopotentiometry. Potentiostatic electrolyses in the LiF-CaF_2-Gd_2O_3-AlF_3 system were conducted for three hours under -1.60 V and -2.20 V, respectively, and at least three kinds of Gd-Al alloys were obtained. The $GdAl_3$ phase was identified through a scanning electron microscope equipped with an energy dispersive spectrometer (SEM-EDS) and X-ray diffraction analysis, and GdAl2 and GdAl were characterized by SEM-EDS.

Journal of the Electrochemical Society, 2018, 165(9): D411

Electrochemical Behavior of UO_2F_2 and Its Electrodeposition from UO_2F_2-FLiNaK Melt

Han Dong She ChangFeng Peng Jia Jiang Feng Yang Xu
Peng Hao Yang Yang Zheng Haiyang Wang Xianbin
Xu Qianhui Wang Chenyang Zhu Tiejian Luo Yan Huang Wei
Gong Yu Li Qingnuan

he electrochemical behavior of UO_2F_2 in LiF-NaF-KF (46.5-11.5-42 mol%, FLiNaK) melt on Pt electrode was investigated at 550°C by cyclic voltammetry (CV) and square wave voltammetry (SWV). UO_2F_2 was prepared by the reaction of UF_4 powder and oxygen at 650°C, and ascertained by X-ray diffraction (XRD) and Raman spectroscopy. It was found that the reduction of UO_2^{2+} in FLiNaK exhibited two steps both with one exchanged electron: $UO_2^{2+} + e^- \rightarrow UO_2^+$ and $UO_2^+ + e^- \rightarrow UO_2$, with the CV reduction peak at about 2.02 V and 1.49 V (vs. K^+/K), respectively. Both of them were reversible and diffusion-controlled. By means of potentiostatic electrolysis, the product of UO_2 was obtained and the separation ratio of uranium from UO_2F_2-FLiNaK melt was approximately 54.5% at 550°C, which were characterized by XRD and the inductively coupled plasma atomic emission spectrometer (ICP-AES).

Journal of the Electrochemical Society, 2018, 165(7): D301

Development of a Coupled Code for Steady-State Analysis of the Graphite-Moderated Channel Type Molten Salt Reactor

He Long Yu Chenggang Guo Wei Dai Ye Wang Hailing
Cai Xiangzhou

The molten salt reactor (MSR) is one of the six advanced reactor concepts selected by Generation IV International Forum (GIF) because of its inherent safety and the promising capabilities of TRU transmutation and Th-U breeding. In this study, a three-dimensional thermal-hydraulic model (3DTH) is developed for evaluating the steady-state performance of the graphite-moderated channel type MSR. The coupled code is developed by exchanging the power distribution, temperature, and fuel density distribution between SCALE and 3DTH. Firstly, the thermal-hydraulic model of the coupled code is validated by RELAP5 code. Then, the mass flow distribution, temperature field, keff, and power density distribution for a conceptual design of the 2MWt experimental molten salt reactor are calculated and analyzed by the coupled code under both normal operating situation and the central fuel assembly partly blocked situation. The simulated results are conductive to facilitate the understanding of the steady behavior of the graphite-moderated channel type MSR.

Science and Technology of Nuclear Installations, 2018: 4053254

Development of the Tritium Transport Analysis Code for the Thorium-Based Molten Salt Reactor

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Qian Nan Wu Xiaoling Liu Wenguan Huang Yu Qian Yuan

Key words Thorium-based molten salt reactor, tritium transport, tritium distribution

The Thorium-Based Molten Salt Reactor (TMSR) has been highlighted for its safety, economy, and nuclear nonproliferation. A program for developing the TMSR system has been launched in Shanghai Institute of Applied Physics, Chinese Academy of Sciences. In the TMSR system, mixtures of LiF and BeF_2, termed FLiBe, are proposed and used as the primary coolant salt, in which tritium is produced mainly by the neutron reactions of lithium. In the TMSR system, at high temperatures, tritium can permeate through metal walls to the surroundings, leading to a potential radiological hazard. Thus, tritium control becomes a major problem hindering the development of the TMSR system. Evaluation of the tritium distribution is necessary for tritium control in the TMSR system. In this study, the Tritium Transport Analysis Code (TTAC) has been developed for

simulating the tritium behaviors in the TMSR system (hence, the code TMSR-TTAC), such as tritium chemical forms in coolant salts, tritium transport behaviors, and tritium distribution in the system. The model code is developed by the MATLAB/SIMULINK package, and it is based on the mass balance equations of the tritium-containing species and hydrogen. TMSR-TTAC is benchmarked with the molten salt reactor model, which is based on Molten Salt Reactor Experiment designs. The results show that TMSR-TTAC has the ability to calculate the tritium distribution in the TMSR system.

Nuclear Technology, 2018, 203(1): 48

A new promising nucleating agent for polymer foaming: effects of hollow molecular-sieve particles on polypropylene supercritical CO_2 microcellular foaming

Yang Chenguang Wang Mouhua Xing Zhe Zhao Quan
Wang Minglei Wu Guozhong

Because polypropylene (PP) foam normally exhibits nonuniform cell size and cracked cellular structure, a narrow cell-size distribution and a well-defined morphology are always the focus of PP foaming technology. In this work, hollow molecular-sieve (MS) particles were applied as a potential nucleating agent in supercritical carbon dioxide ($scCO_2$) foaming of PP. It was observed that the addition of MS particles largely narrowed the cell-size distribution. The resultant PP/MS foams exhibited significant concurrent enhancement in their cell density and mechanical properties: the cell density increased remarkably, by approximately 10 times, and the tensile strength increased from 6.1 MPa to 12.6 MPa. The hollow-structure MS particles resulted in a higher heterogeneous nucleation efficiency in the PP foaming process. We believe that the trapping of CO_2 in the hollow holes of MS particles largely increased the solubility CO_2 in PP and a number of gas cavities were formed. The existence of gas cavities reduced the energy barrier of heterogeneous nucleation, favoring the formation of a well-defined cellular structure. Additionally, the regular-hexagon shape of the cells might endow the PP foam with better mechanical properties compared with a circular cell shape.

RSC Advances, 2018, 8(36): 20061

The preparation of a three dimensional terbium doped reduced graphene oxide aerogel with photoluminescence and paramagnetic properties

Chen Keqin Gao Hui Wang Dongdong Li Xiaolong
Wang Deying Khan Waheed Ullah

A 3D reduced graphene oxide (rGO) material with good photoluminescence (PL) and magnetism properties was self-assembled using the hydrothermal method. The resultant material possessed a flower-like structure, which leads to a high surface area. To dehydrate the hydrogel for conservation, the sublimation process we use can effectively maintain the porosity as it uses the freeze drying method. Then, rGO was endowed with paramagnetism and green photoluminescence properties *via* the introduction of Tb ions, which also reinforces the significance of the building block. Finally, the coordination between Tb ions and the carbonyl was proven with photoluminescence excitation (PLE) spectra and the UV-vis absorption spectra, which are likely to offer an effective way to study the carbonyl compound.

RSC Advances, 2018, 8(17): 9287

Determination of the Mercury Isotopic Ratio by Cold Vapor Generation Sector Field-Inductively Coupled Plasma-Mass Spectrometry Using Lead as the Internal Standard

Tang Xiaoxing Qian Yuan Li Yulan Fei Zejie Yao Jian
Ma Jifei Liu Wei

Key words Cold vapor generation, inductively coupled plasma-mass spectrometry (ICP-MS), isotopic ratios, lead, mercury

Lead was applied as an internal standard for the determination of Hg isotopic ratios. Cold vapor generation (CV) coupled with sector field–inductively coupled plasma–mass spectrometry (CV-SF-ICP-MS) was used for determination of Hg. It was effective to avoid interferences of Pb from samples while improving the sensitivity of Hg isotopic analysis by an approximate factor of 45 times higher than the aerosol mode. CV-SF-ICP-MS system was constructed and operational parameters were optimized. Research showed that the long stability of the system was limited by SF-ICP-MS and had no relationship with CV under the optimized conditions. The optimized precision of Hg isotopic ratio analysis was approximately 0.1% during 4 h. Five models were

applied for the mass bias correction and the Baxter model obtained the smallest relative difference, 0.52‰. The results showed that the mean value of NIST SRM 3133 Hg isotopic ratios obtained by Pb internal standard was nearly identical with the value for Tl. The same performance was also obtained in two environmental reference materials. The results show that Pb may be used as the internal standard for determination of Hg isotopic ratio instead of Tl.

Analytical Letters, 2018, 51(12): 1944

Surrogate Fluid Experimental Study and CFD Simulation on the Hydraulic Characteristics of Vortex Diode

Qu Shixiang Wu Yanhua He Zhaozhong Chen Kun

Key words Vortex diode, scaling experiment, computational fluid dynamics

The vortex diode is a key candidate for the equipment of the passive safety system of the molten salt reactor. Experimental studies to determine the diodicity (ratio of reverse flow Euler number to the forward flow Euler number at the same Reynolds number) using high-temperature molten salt are strongly limited because of the huge technical effort and financial requirements for such studies, moreover, possible solutions that involve a scaling method that uses surrogate fluid to obtain the diodicity must be validated. To determine the diodicity and verify the scaling method, an experiment using one kind of heat transfer oil (Dowtherm-a) as the surrogate fluid was carried out. In addition, a computational fluid dynamics (CFD) simulation method was also adopted to study the flow characteristics in the vortex diode using three different fluids. The results show the following: it is feasible to study the diodicity of a vortex diode by a scaling experimental method using surrogate fluid, the CFD simulation method established in this paper can be applied to study the diodicity of the vortex diode, and the structure of the flow field and velocity distribution in the vortex chamber for reverse flow are independent of fluids and only related to the Reynolds number.

Nuclear Science and Engineering, 2018, 189(3): 282

Thiolate-Protected Hollow Gold Nanospheres

Xu Wenwu Gao Yi

Key words Thiolate-protected hollow Au nanosphere, Density-functional theory, Grand unified model, "Divide and protect" rule, Nucleus-independent chemical shift

We present the atomic structure of thiolate-protected hollow Au nanosphere (HAuNS), $Au_{60}(SR)_{20}$, with high symmetry and stability based on the grand unified model (GUM, *Nat. Commun*. 2016, *7*, 13574) and density-functional theory (DFT) calculations. Using C_{20} fullerene

(with I_h symmetry) as a template, 20 tetrahedral Au_4 units were used to replace the C atoms of C_{20}, and three Au atoms of each Au_4 were fused with three neighboring Au_4 units by sharing one Au atom to form an icosahedral Au_{50} fullerene cage as the inner core. Subsequently, the unfused Au atom in each Au_4 was bonded with the [—RS—Au—SR—] staple to form the completely hollow $Au_{60}(SR)_{20}$ nanosphere. Therefore, the $Au_{60}(SR)_{20}$ is composed of an icosahedral Au_{50} fullerene hollow cage (constructed by fusing 20 tetrahedral Au_4 units) with 10 [—RS—Au—SR—] staples, obeying the "divide and protect" rule. Each Au_4 unit has 2*e* valence electrons, namely, the tetrahedral $Au_4(2e)$ elementary block in the grand unified model. The DFT calculations showed that this hollow $Au_{60}(SR)_{20}$ nanosphere had a large HOMO–LUMO (HOMO: the highest occupied molecular orbital, LUMO: the lowest unoccupied molecular orbital) gap (1.3 eV) and a negative nucleus-independent chemical shift (NICS) value (−5) at the center of the hollow cage, indicating its high chemical stability. Furthermore, the NICS values in the center of the tetrahedral Au_4 units were much more negative than that in the center of the hollow cage, revealing that the overall stability of $Au_{60}(SR)_{20}$ likely stemmed from the local stability of each tetrahedral Au_4 unit. The harmonic vibrational frequencies were all positive, suggesting that the HAuNS corresponded to the local minimum of the potential energy surface. In addition, the bilayer HAuNS was designed by fusing the tetrahedral Au_4 layers, indicating the feasibility of tuning the thickness of the shell of HAuNS. In bilayer HAuNS, each tetrahedral Au_4 unit in the first layer shared four Au atoms, while those in the second layer shared one Au atom. The other three Au atoms of each tetrahedral unit bonded with the SR groups, demonstrating that each tetrahedral Au_4 unit has 2*e* valence electrons (namely the tetrahedral $Au_4(2e)$ elementary block in GUM). The HOMO-LUMO gap of the bilayer $Au_{140}(SH)_{60}$ nanosphere is 1.5 eV, indicating its chemical stability. The thicknesses of the shells in monolayer and bilayer HAuNS are about 0.2 and 0.4 nm, respectively. This process could be easily understood in terms of the local stabilities of the tetrahedral $Au_4(2e)$ elementary block in GUM. Finally, the design of larger HAuNS, $Au_{180}(SR)_{60}$, has also been presented. The HOMO-LUMO gap of $Au_{180}(SH)_{60}$ was 0.9 eV, which showed that it was also a stable HAuNS. This work provides a new strategy to controllably design the HAuNS.

Acta Physico-Chimica Sinica, 2018, 34(7): 770

Study on the performance of a large-size CsI detector for high energy γ-rays

Dong He Fang De-Qing Li Chen

Key words CsI: Tl, Scintillation detector, Full absorption efficiency, Energy resolution, GEANT4 simulation

The measurement of high-energy γ-rays is an important experimental method to study the giant resonance in a nucleus, γ reaction in nuclear astrophysics, and so on. The performance of a

large-size CsI detector for γ-rays detection is studied by comparison between the experimental measurements and GEANT4 simulation. The reliability of the simulated efficiency for low-energy γ-rays is verified by comparing with the experimental data. The efficiency of the CsI detector for high-energy γ-rays was obtained by the GEANT4 simulation. The simulation shows that the detection efficiency of 20 MeV γ-rays can reach 3.8%.

Nuclear Science and Techniques, 2018, 29(1): 7

Transverse phase space reconstruction study in Shanghai soft X-ray FEL facility

Yu Qinglin Gu Duan Zhang Meng Zhao Minghua

Key words Emittance, Phase space reconstruction, MENT algorithm, SXFEL

Phase space is one of the most important parameters used to describe beam properties. Computer tomography, as a method for reconstructing phase space and measuring beam emittance, has been used in many accelerators over the past few decades. In this paper, we demonstrate a transverse phase space reconstruction study in the Shanghai soft X-ray free electron laser facility. First, we discuss the basic principles of phase space reconstruction and the advantage of reconstructing beam distribution in normalized phase space. Then, the phase space reconstruction results by different computer tomography methods based on the maximum entropy (MENT) algorithm and the filtered back projection algorithm in normalized phase space are presented. The simulation results indicate that, with proper configuration of the phase advance between adjacent screens, the MENT algorithm is feasible and has good efficiency. The beam emittance and Twiss parameters are also calculated using the reconstructed phase space.

Nuclear Science and Techniques, 2018, **29**(1): 9

Protein-mimicking nanoparticle (Protmin)-based nanosensor for intracellular analysis of metal ions

Zhu Dan Zhao Dongxia Huang Jiaxuan Li Jiang Zuo Xiaolei
Wang Lihua Fan Chunhai

Key words Protmin, Nanosensor, Poly-adenine, Lead ion, Intracellular detection

In this study, we designed and applied protein-mimicking nanoparticles (Protmin) as an intracellular nanosensor for in vivo detection of lead ions (Pb^{2+}). Monodispersed gold nanoparticles (AuNPs) of 13 nm in diameter were modified using poly-adenine-tailed Pb2+ specific 8-17 DNAzyme to form a spherical and functional Protmin. Substrate strands modified with a

fluorophore at the 5' end and a quencher at the 3' end were bound to DNAzyme. Pb^{2+} facilitated cleavage of DNAzyme to release the fluorophore-modified short strands to generate fluorescence. We observed rapid kinetics of the Protmin nanosensor, for which the typical assay time was 10 min. Further, we demonstrated the Protmin nanosensor could readily enter living cells and respond to Pb^{2+} in the intracellular environment. The broad of range of Protmin designs will be useful for advancing biological and medical applications..

Nuclear Science and Techniques, 2018, **29**(1): 5

Fabrication of polyacrylamide-carbon nanotubes by One-Step Radiation-Induced Graft Polymerization

Fan Kai Li Jihao Li Linfan Li Jingye

Key words Gamma ray, Carbon nanotubes, Functionalization, acryl amide

A facile strategy for the preparation of organic nitrogen functional multi-walled carbon nanotubes (MWCNTs) in aqueous solution is proposed, where MWCNTs were functionalized by simultaneous radiation-induced graft polymerization of acrylamide under the g-ray. The structure of the poly(acryl amide) grafted MWCNTs (denoted as MWCNT-g-PAM) is characterized by means of FT-IR, XPS spectroscopies, TGA analysis and TEM imaging. The degree of grafting dependent on the reaction conditions such as the monomer concentration was also discussed in this paper.

Fullerenes Nanotubes and Carbon Nanostructures, 2018, **26**(1): 12

A facile approach to fabricate few-layer chemically modified and reduced graphene oxide sheets: Combination of stitching, reduction and functionaliztion

Fan Kai Li Jihao Li Linfan Li Jingye

Key words graphene oxide, linear diaminoalkane, reduction and functionalization, few-layer

A facile strategy for the preparation of few-layer chemically stitched and reduced graphene oxide (FL-CMRG) in water using various linear diaminoalkanes with the general formula $H_2N(CH_2)_nNH_2$ (n = 4, 6, 8) is proposed, and the resulting FL-CMRG was characterized by means of AFM, TEM, XPS, UV-*vis*, TGA and XRD. Interlayer spacing between bridged FL-CMRG sheets can reach 1.038 nm when the size of the intercalant to (n = 6) $H_2N\ (CH_2)_6\ NH_2$.

A mechanism for forming the FL-CMRG via removal of epoxide and hydroxyl groups from GO and stitching of the GO sheets by various linear diaminoalkanes in water solution has been proposed.

Fullerenes Nanotubes and Carbon Nanostructures, 2018, **26**(1): 30

Electric field distribution and initial jet motion induced by spinneret configuration for molecular orientation in electrospun fibers

Li Xiang Lin Jinyou Zeng Yongchun

Key words Molecular orientation, Electric field distribution, Jet motion, Electrospinning, Spinneret configuration

Understanding the molecular orientation of electrospun fibers is a key challenge for tailoring fiber properties. The studies of electric field distribution, and the motion of the initial portion of the polymer jet, are of interest for clarifying molecular orientation in fibers during electrospinning. In this work, we study the impact of electric field distribution and the initial jet motion induced by two kinds of spinneret configurations, referred to as a needle configuration and a hole configuration, on molecular orientation in electrospun PEO fibers. Using FE-SEM, FTIR and WAXD techniques, the fiber diameter and molecular orientation of the fibers prepared with the needle electrospinning system and the hole electrospinning system are characterized. To explore jet stretching and chain orientation during the spinning process, electric field simulation and high-speed photography are performed to obtain the electric field characteristics and to measure the initial jet velocities for the needle and the hole systems. Our results reveal the higher electric field strength around the spinneret and the larger initial jet velocities, which depend on the spinneret configuration, result in the higher degree of molecular orientation in fibers.

European Polymer Journal, 2018, **98**: 330

Structure and performances changes during tensile of aromatic copolysulfonamide fibers under different thermal temperatures *via* in-situ synchrotron SAXS/WAXS

Li Xiaoyun Yu Jinchao Wang Jianning Chen Kang Li Xiuhong
Zhang Yumei Bian Fenggang Wang Jie

Key words Aromatic copolysulfonamide fiber, Mechanical property, Small angle X-ray scattering, Wide angle X-ray scattering

In *situ* studies of structure and performance changes in aromatic copolysulfonamide (*co*-PSA) fibers during stretching at different thermal exposure temperature range from room temperature to 300 °C were carried out using synchrotron small angle X-ray scattering and wide angle X-ray scattering techniques. Results showed that the optimum microstructure and mechanical property of *co*-PSA fibers were achieved when stretched at 200 °C, the fibril length, fibril misorientation, crystal sizes L_{002} reached minimum, the long period became maximum at the same strain indicating that lamella and fibrils aligned perfectly, fiber structure compactness at 200 °C. During stretching at RT to 200 °C, at low strain, fibril length, crystal size L_{002} increased, fibrils oriented along stretching direction, the long period was enlarged; the opposite trend evolution of structure appeared under high strain. But stretching at 300 °C, L_{002} increased, fibril orientation became poor, the lamellae destroyed easily resulting in the decreasing strength. It can be concluded that *co*-PSA fibers remain good property under thermal at 200 °C, external force use environment..

European Polymer Journal, 2018, **98**: 354

Optimization of pencil beam f-theta lens for high-accuracy metrology

Peng Chuanqian He Yumei Wang Jie

Key words deflectometric profiler, Fourier transform lens, Least squares fitting, X-ray mirror, Metrology, Synchrotron radiation

Pencil beam deflectometric profilers are common instruments for high-accuracy surface slope metrology of x-ray mirrors in synchrotron facilities. An f-theta optical system is a key optical component of the deflectometric profilers and is used to perform the linear angle-to-position conversion. Traditional optimization procedures of the f-theta systems are not directly related to the angle-to-position conversion relation and are performed with stops of large size and a fixed working distance, which means they may not be suitable for the design of f-theta systems working with a small-sized pencil beam within a working distance range for ultra-high-accuracy metrology. If an f-theta system is not well-designed, aberrations of the f-theta system will introduce many systematic errors into the measurement. A least-squares' fitting procedure was used to optimize the configuration parameters of an f-theta system. Simulations using ZEMAX software showed that the optimized f-theta system significantly suppressed the angle-to-position conversion errors caused by aberrations. Any pencil-beam f-theta optical system can be optimized with the help of this optimization method.

Optical Engineering, 2018, **57**(1): 15101

The role of EDTA on rutile flotation using Al^{3+} ions as an activator

Xiao Wei Fang Chaojun Wang Jun Liang Qiannan CaoPan Wang Xingxing Zhang Lijuan Qiu Guanzhou Hu Jun

Rutile is a relatively stable mineral, due to its weakly specific adsorption to collectors. The development and application of a high efficiency and low-toxicity activator is the main challenge in rutile flotation. In this study, Al^{3+} ions and EDTA (ethylene diamine tetraacetic acid) as mixed activators were investigated using micro-flotation tests. The results of the micro-flotation tests showed that the flotation recovery was slightly increased (from 65.8% to 69.7%) using single Al^{3+} ions as the activator and surprisingly, the activating effect was sharply improved (from 69.7% to 80.6%) after adding EDTA. The activating mechanism of Al^{3+} ions and EDTA was revealed by adsorption capacity measurements, zeta potential measurements, FT-IR spectroscopy analysis and XPS analysis. Al^{3+} ions were adsorbed on the rutile surface in the form of $Al(OH)_n^{3-n}$ (n = 0, 1, 2), which increased the zeta potential and the activating sites for anionic collector adsorption. The addition of EDTA removed the surplus Al^{3+} ions, and prevented the generation of hydrophilic colloidal $Al(OH)_3$ over the pH range of optimum flotation..

Ras Advances, 2018, **8**(9): 4872

Evolution of carbide precipitates in Hastelloy N joints during welding and post weld heat treatment

Wang Wanxia Li Chaowen Jiang Li Ye Xiangxi Yu Kun Chen Shuangjian Li Zhijun Zhou Xingtai

Key words Hastelloy N alloy, Welding, Post-weld heat treatment, M_6C carbide, Diffusion

The effects of welding and post weld heat treatment (PWHT) on the morphology, composition and lattice parameter of the precipitates in the welding joints of Hastelloy N alloy have been investigated. Joint samples were prepared using a gas tungsten arc welding process with ERNiMo-2 fillers, and then solid-solution treated at 1100 degrees C for 20 min. After welding, eutectic M6C carbides can be observed in the heat affected zones (HAZ) and weld zones (WZ). These eutectic M_6C carbides become spheroidized during the following PWHT. The concentration of Si decreases during the transformation from the primary ones to eutectic ones, and then increases during the spheroidizing process. The total concentration of Si + Cr in M_6C carbides remains stable during welding and PWHT. At the same time, the heat leads to the outward diffusion of Mo from the M_6C carbides, which results in a decrease of the lattice parameter.

Materials Characterization, 2018, **135**: 311

Insight into the Formation of Co@Co_2C Catalysts for Direct Synthesis of Higher Alcohols and Olefins from Syngas

Zhao Ziang Lu Wei Yang Ruoou Zhu Hejun Dong Wenda
Sun Fanfei Jiang Zheng Lyu Yuan Liu Tao
Du Hong Ding Yunjie

Key words Higher alcohols, Olefins, Fischer-Tropsch synthesis, Mn promoter, Cobalt carbide

Cobalt carbide (Co_2C) has recently been reported to efficient for the conversion of syngas ($CO+H_2$) to lower olefins (C_2−C_4)and higher alcohols (C_{2+}alcohols); however, its properties and formation conditions remain ambiguous. On the basis of our previous investigation sconcerning the formation of Co_2C, the work herein was aimed at defining the mechanism by which the manganese promoter functions in the Co-based catalysts supported on activated carbon (CoxMn/AC). Exper-imental studies validated that Mn facilitates the dissociation and disproportionation of CO on the surface of catalyst and prohibits H2adsorption to some extent, creating a relative C-rich and H-lean surface chemical environment. We advocate that the surface conditions result in the transformation from metallic Co to Co_2C phase under realistic reaction conditions to form Co@Co_2C nanoparticles, in which residual small Co0ensembles (<6 nm) distribute on the surface of Co_2C nanoparticles (~20 nm). Compared with the Co/AC catalyst, where the active site is composed of Co_2C phase on the surface of Co0nanoparticles (Co_2C@Co), the Mn-promoted catalysts (Co@Co_2C) displayed much higher olefin selectivity (10% versus 40%), while the selectivity to alcohols over the two catalysts are similar (~20%). The rationale behind the strong structure−performance relationship is twofold. On the one hand, Co−Co_2C interfaces exist universally in the catalysts, where synergistic effects between metallic Co and Co_2C phase occur and are responsible for the formation of alcohols. On the other hand, the relative C-rich and H-lean surface chemical environment created by Mn on the Co@Co_2C catalysts facilitates the formation of olefins.

Acs Catalysis, 2018, **8**(1): 228

Graphene oxide as an additive to improve perovskite film crystallization and morphology for high-efficiency solar cells

Zhang Xiaonan Ji Gengwu Xiong Dongbin Su Zhenhuang Zhao Bin
Shen Kongchao Yang Yingguo Gao Xingyu

The quality of a perovskite film has a great impact on its light absorption and carrier transport, which is vital to improve high-efficiency perovskite solar cells (PSCs). Herein, it is demonstrated

that graphene oxide (GO) can be used as an effective additive in the precursor solution for the preparation of high-quality solution-processed $CH_3NH_3PbI_3$ ($MAIPbI_3$) films. It is evidenced by scanning electron microscopy that the size of the grains inside these films not only increases but also becomes more uniform after the introduction of an optimized amount of 1 vol% GO. Moreover, 1 vol% GO also enhances the crystallization of perovskite film with intact preferential out-of-plane orientation as proven by 2-dimensional grazing-incidence X-ray diffraction. As a consequence of the improved film quality, enhanced charge extraction efficiency and optical absorption are demonstrated by photoluminescence (PL) spectroscopy and UV-visible absorption spectroscopy, respectively. Using 1 vol% GO, the fabricated champion heterojunction PSC with a structure of ITO/SnO_2/perovskite/spiro-OMeTAD/Au shows a significant power conversion efficiency increase to 17.59% with reduced hysteresis from 16.10% for the champion device based on pristine perovskite. The present study thus proposes a simple approach to make use of GO as an effective and cheap addictive for high-performance PSCs with large-scale production capability.

Ras Advances, 2018, **8**(2): 987

Synergistic effects of different co-monomers on the uranium adsorption performance of amidoximated polyethylene nonwoven fabric in natural seawater

Li Rong Ma Hongjuan Xing Zhe Wu Guozhong

Key words Polyethylene nonwoven fabric, Amidoxime, Co-monomer, Seawater, Uranium recovery

Several co-monomers were co-grafted with acrylonitrile onto polyethylene nonwoven fabric to prepare amidoximated sorbents. The grafted co-monomer was found to play an important role in the uranium adsorption capacity and sorption selectivity of amidoximated sorbent in natural seawater in the following order: acrylamide (AAm) < acrylic acid (AA) < itaconic acid (ITA) < methacrylic acid (MAA), which agreed well with the result in U-spike brine. The amidoximated sorbent co-grafted with MAA exhibited the highest uranium adsorption capacity (1.05 mg/g) and the best uranium/vanadium sorption selectivity (U/V mass ratio: ~ 0.95) after 56 days of immersion in natural seawater.

Journal of Radioanalytical and Nuclear Chemistry, 2018, **315** (1): 111

Characterization of organic matter pores in typical marine and terrestrial shales, China

Wang Yu Wang Lihua Wang Jianqiang Jiang Zheng
Jin Chan Wang Yanfei

Key words Organic matter pores, Mineralogy, Marine and terrestrial shale, Burial-diagenesis history

Organic matter (OM) is a significant component in shale and controls gas storage and transportation. Typical marine (JLD sample, NTT sample, WF sample and LMX sample) and terrestrial (C7 sample) OM-rich shale samples from the Sichuan Basin and Erdos Basin in China were investigated using X-ray diffraction and scanning electron microscopy (SEM) to study their mineralogy and OM pore network properties. The X-ray diffraction results indicated that the content of brittle minerals (quartz, plagioclase, calcareous dolomite, dolomite and pyrite) in each shale sample was higher than 60%, providing material in which original matrix pores and microfractures formed during an early stage of diagenesis. The types and contents of clay minerals vary among the shale samples. The main clay mineral in most of the marine shale samples is illite, but the primary clay in the terrestrial shale is an illite-smectite mixed layer. The maturity data of the OM in the marine shale samples suggested a moderate to high stage of maturity, while the terrestrial shale was collected at a relatively low stage of thermal evolution. The SEM observations suggested that the OM was either tight or porous, and the former was the dominant state. The OM pores preserved in the shale consisted of pores within, between and at the interfaces of the OM particles. For the OM pores within the OM particles, the most dominant pore type, type I, exhibits honeycomb-like pores formed by hydrocarbon generation; this type of pore is most developed in the marine LMX shale and NTT shale. Pore type II is related to biogenic residue and is more developed in the JLD shale and LMX shale. Pore type. includes mainly elliptical pores or microcracks related to the volume loss of bitumen. The OM pores between the OM particles are narrow and laminar; these structures were inherited from the previous clay mineral structures. The OM pores at the interfaces of the OM particles and the mineral grains are usually observed as microfractures and are more developed in the C7 shale. The lack of pores within the OM in the terrestrial C7 shale was due to low maturity. A combination of SEM results, mineral compositions and carbon analyses indicated a positive correlation between the development of OM pores and the organic carbon content, as well as the thermal maturity. With increasing burial and maturity, migrated OM was squeezed into mineral matrix pores and appears to be continuous, especially along the bedding planes, forming an effective network due to the interconnectivity of the OM.

Journal of Natural Gas Science and Engineering, 2018, **49**: 56

Transverse momentum spectra and nuclear modification factors of charged particles in pp, p-Pb and Pb-Pb collisions at the LHC

STAR Collaboration

Key words Heavy Ion Experiments, Heavy-ion collision

We report the measured transverse momentum (p_T) spectra of primary charged particles from pp, p-Pb and Pb-Pb collisions at a center-of-mass energy $\sqrt{S_{NN}}$ = 5.02TeV in the kinematic range of 0.15 < p_T < 50 GeV/c and |η| <0.8. A significant improvement of systematic uncertainties motivated the reanalysis of data in pp and Pb-Pb collisions at $\sqrt{S_{NN}}$ = 2.76TeV, as well as in p-Pb collisions at $\sqrt{S_{NN}}$= 5.02TeV, which is also presented. Spectra from Pb-Pb collisions are presented in nine centrality intervals and are compared to a reference spectrum from pp collisions scaled by the number of binary nucleon-nucleon collisions. For central collisions, the P_T spectra are suppressed by more than a factor of 7 around 6-7 GeV/c with a significant reduction in suppression towards higher momenta up to 30 GeV/c. The nuclear modification factor RpP_b, constructed from the pp and p-Pb spectra measured at the same collision energy, is consistent with unity above 8 GeV/c. While the spectra in both pp and Pb-Pb collisions are substantially harder at $\sqrt{S_{NN}}$ = 5.02TeV compared to 2.76TeV, the nuclear modification factors show no significant collision energy dependence. The obtained results should provide further constraints on the parton energy loss calculations to determine the transport properties of the hot and dense QCD matter.

Journal of High Energy Physics, 2018, (11): 13

Measurement of D^0, D^+, D^{*+} and Ds^+ production inPb-Pb collisions at $\sqrt{S_{NN}}$ =5.02 TeV

STAR Collaboration

Key words Heavy Ion Experiments

We report measurements of the production of prompt D^0, D^+, D^{*+} and D^+_s mesons in Pb–Pb collisions at the centre-of-mass energy per nucleon-nucleon pair $\sqrt{S_{NN}}$=5.02 TeV, in the centrality classes 0–10%, 30–50% and 60–80%. The D-meson production yields are measured at mid-rapidity (|y|<0.5) as a function of transverse momentum (p_T). The p_T intervals covered in central collisions are: 1 <p_T< 50GeV/c for D^0, 2 <p_T< 50GeV/c for D^+, 3 <p_T< 50GeV/c for D^{*+}, and 4 < p_T< 16GeV/c for D^+_s mesons. The nuclear modification factors (R_{AA}) for non-strange

D mesons (D^0, D^+, D^{*+}) show minimum values of about 0.2 for p_T=6–10 GeV/c in the most central collisions and are compatible within uncertainties with those measured at $\sqrt{S_{NN}}$=2.76 TeV. For D_s^+ mesons, the values of R_{AA} are larger than those of non-strange D mesons, but compatible within uncertainties. In central collisions the average R_{AA} of non-strange D mesons is compatible with that of charged particles for p_T> 8 GeV/c, while it is larger at lower p_T. The nuclear modification factors for strange and non-strange D mesons are also compared to theoretical models with different implementations of in-medium energy loss.

Journal of High Energy Physics, 2018, (10): 174

Medium modification of the shape of small-radius jets in central Pb-Pb collisions at $\sqrt{S_{NN}}$ =2.76 TeV

STAR Collaboration

Key words Heavy Ion Experiments

We present the measurement of a new set of jet shape observables for track-based jets in central Pb-Pb collisions at $\sqrt{S_{NN}}$=2.76 TeV. The set of jet shapes includes the first radial moment or angularity, g; the momentum dispersion, $_{PT}$D; and the difference between the leading and sub-leading constituent track transverse momentum, *LeSub*. These observables provide complementary information on the jet fragmentation and can constrain different aspects of the theoretical description of jet-medium interactions. The jet shapes were measured for a small resolution parameter R=0.2 and were fully corrected to particle level. The observed jet shape modifications indicate that in-medium fragmentation is harder and more collimated than vacuum fragmentation as obtained by PYTHIA calculations, which were validated with the measurements of the jet shapes in proton-proton collisions at $\sqrt{S}$ = 7 TeV. The comparison of the measured distributions to templates for quark and gluon-initiated jets indicates that in-medium fragmentation resembles that of quark jets in vacuum. We further argue that the observed modifications are not consistent with a totally coherent energy loss picture where the jet loses energy as a single colour charge, suggesting that the medium resolves the jet structure at the angular scales probed by our measurements (R = 0.2). Furthermore, we observe that small-*R* jets can help to isolate purely energy loss effects from other effects that contribute to the modifications of the jet shower in medium such as the correlated background or medium response.

Journal of High Energy Physics, 2018, (10): 139

Azimuthally-differential pion femtoscopy relative to the third harmonic event plane in Pb-Pbcollisions at $\sqrt{S_{NN}}$ =2.76 TeV

STAR Collaboration

Azimuthally-differential femtoscopic measurements, being sensitive to spatio-temporal characteristics of the source as well as to the collective velocity fields at freeze out, provide very important information on the nature and dynamics of the system evolution. While the HBT radii oscillations relative to the second harmonic event plane measured recently reflect mostly the spatial geometry of the source, model studies have shown that the HBT radii oscillations relative to the third harmonic event plane are predominantly defined by the velocity fields. In this Letter, we present the first results on azimuthally-differential pion femtoscopy relative to the third harmonic event plane as a function of the pion pair transverse momentum $k(T)$ for different collision centralities in Pb-Pb collisions at $\sqrt{S_{\rm NN}}$ = 2.76TeV. We find that the $R_{\rm side}$ and $R_{\rm out}$ radii, which characterize the pion source size in the directions perpendicular and parallel to the pion transverse momentum, oscillate in phase relative to the third harmonic event plane, similar to the results from 3+1D hydrodynamical calculations. The observed radii oscillations unambiguously signal a collective expansion and anisotropy in the velocity fields. A comparison of the measured radii oscillations with the Blast-Wave model calculations indicate that the initial state triangularity is washed out at freeze out.

Physics Letters B, 2018, **785**: 320

Inclusive J/ψ production in Xe–Xe collisions at $\sqrt{S_{NN}}$=5.44 TeV

STAR Collaboration

Inclusive J/ψ production is studied in Xe-Xe interactions at a centre-of-mass energy per nucleon pair of $\sqrt{S_{\rm NN}}$= 5.44 TeV, using the ALICE detector at the CERN LHC. The J/ψ meson is reconstructed via its decay into a muon pair, in the centre-of-mass rapidity interval $2.5 < y < 4$ and down to zero transverse momentum. In this Letter, the nuclear modification factors R_{AA} for inclusive J/ψ, measured in the centrality range 0-90% as well as in the centrality intervals 0-20% and 20-90% are presented. The R_{AA} values are compared to previously published results for Pb-Pb

collisions at $\sqrt{S_{\mathrm{NN}}}$= 5.02 TeV and to the calculation of a transport model. A good agreement is found between Xe-Xe and Pb-Pb results as well as between data and the model.

Physics Letters B, 2018, **785**: 419

Measurements of low-p_{T} electrons from semileptonic heavy-flavour hadron decays at mid-rapidity in pp and Pb-Pb collisions at $\sqrt{S_{NN}}$=2. 76 TeV

STAR Collaboration

Key words Heavy Ion Experiments

Transverse-momentum (p_{T}) differential yields of electrons from semileptonic heavy-flavour hadron decays have been measured in the most central (0–10%) and in semi-central (20–40%) Pb–Pb collisions at $\sqrt{S_{\mathrm{NN}}}$ =2.76 TeV. The corresponding production cross section in pp collisions has been measured at the same energy with substantially reduced systematic uncertainties with respect to previously published results. The modification of the yield in Pb–Pb collisions with respect to the expectation from an incoherent superposition of nucleon-nucleon collisions is quantified at mid-rapidity ($|y| < 0.8$) in the p_{T} interval 0.5–3 GeV/c via the nuclear modification factor, R_{AA}. This paper extends the p_{T} reach of the R_{AA} measurement towards significantly lower values with respect to a previous publication. In Pb–Pb collisions the p_{T}-differential measurements of yields at low p_{T} are essential to investigate the scaling of heavy-flavour production with the number of binary nucleon-nucleon collisions. Heavy-quark hadronization, a collective expansion and even initial-state effects, such as the nuclear modification of the Parton Distribution Function, are also expected to have a significant effect on the measured distribution.

Journal of High Energy Physics, 2018, (10): 61

Searching for states analogous to the ^{12}C Hoyle state in heavier nuclei using the thick target inverse kinematics technique

STAR Collaboration

Identification of α-cluster states analogous to the ^{12}C Hoyle state in heavier α-conjugate nuclei can provide tests of the existence of α condensates in nuclei. Such states are predicted

for ^{16}O, ^{20}Ne, ^{24}Mg, ^{28}Si, etc., at excitation energies slightly above the multi- α-particle decay threshold but have not yet been experimentally identified. The thick target inverse kinematics (TTIK) technique can be used to study the breakup of excited self-conjugate nuclei into many α particles. The reaction ^{20}Ne+α was studied using a ^{20}Ne beam at 12 MeV/nucleon from the K150 cyclotron at Texas A&M University. The TTIK method was used to study both single α-particle emission and multiple α-particle decays. Events with α multiplicity up to four were analyzed. The analysis of the three α-particle emission data allowed the identification of the Hoyle state and other ^{12}C excited states decaying into three α particles. The results are shown and compared with other data available in the literature. Although the statistics for events with α-multiplicity four is low, the data show a structure at about 15.2 MeV that could indicate the existence in ^{16}O of a state analogous to the ^{12}C Hoyle state. Moreover, the reconstructed excitation energy of ^{24}Mg for these events peaks at around 34 MeV, very close to the predicted excitation energy for an excited state analogous to the ^{12}C Hoyle state in ^{24}Mg. The structure is further confirmed by the reanalysis of α-multiplicity-four events from a previous experiment performed at 9.7 MeV/nucleon with a similar, but lower granularity, experimental setup.

Physical Review C, 2018, **98**(4): 44601

Harmonic decomposition of three-particle azimuthal correlations at energies available at the BNL Relativistic Heavy Ion Collider

STAR Collaboration

We present measurements of three-particle correlations for various harmonics in Au+Au collisions at energies ranging from $\sqrt{S_{NN}}$=7.7 to 200 GeV using the STAR detector. The quantity $\langle\cos(m\phi_1+n\phi_2-(m+n)\phi_3)\rangle$, with ϕ being the azimuthal angles of the particles is evaluated as a function of $\sqrt{S_{NN}}$, collision centrality, transverse momentum, p_T, pseudorapidity difference, $\Delta\eta$, and harmonics (m and n). These data provide detailed information on global event properties such as the three-dimensional structure of the initial overlap region, the expansion dynamics of the matter produced in the collisions, and the transport properties of the medium. A strong dependence on $\Delta\eta$ is observed for most harmonic combinations, which is consistent with breaking of longitudinal boost invariance. An interesting energy dependence is observed when one of the harmonics m,n, or m+n is equal to two, for which the correlators are dominated by the two-particle correlations relative to the second-harmonic event plane. These measurements can be

used to constrain models of heavy-ion collisions over a wide range of temperature and baryon chemical potential.

Physical Review C, 2018, **98**(3): 34918

Low-p_T e^+e^- Pair Production in Au + Au Collisions at $\sqrt{S_{NN}}$=200 GeV and U + U Collisions at $\sqrt{S_{NN}}$=193 GeV at STAR

STAR Collaboration

We report first measurements of e^+e^- pair production at low transverse momentum (p_T < 0.15 GeV/c) in non-central Au+Au collisions at $\sqrt{S_{NN}}$ = 200 GeV and U+U collisions at $\sqrt{S_{NN}}$= 193 GeV. Significant enhancement factors, expressed as ratios of data over known hadronic contributions, are observed in the 40-80% centrality of these collisions. The excess yields peak distinctly at low- p_T with a width ($\sqrt{\langle P_T^2 \rangle}$) between 40 to 60 MeV/c. The absolute cross section of the excess 3 depends weakly on centrality while those from a theoretical model calculation incorporating inmedium broadened ρ spectral function and radiation from a Quark Gluon Plasma or hadronic cocktail contributions increase dramatically with increasing number of participant nucleons (N_{part}). Model calculations of photon-photon interactions generated by the initial projectile and target nuclei describe the observed excess yields but fail to reproduce the P_T^2 distributions.

Physical Review Letters, 2018, **121**(13): 132301

Two-particle angular correlations in *pp* and *p*-Pb collisions at energies available at the CERN Large Hadron Collider from a multiphase transport model

STAR Collaboration

We apply a multiphase transport (AMPT) model to study two-particle angular correlations in pp collisions at $\sqrt{S}$=7 TeV. In addition to being able to describe the angular correlation functions of meson-meson pairs, a large improvement for the angular correlations of baryon-baryon and antibaryon-antibaryon is achieved. We further find that the AMPT model with new quark coalescence provides an even better description on the anticorrelation feature of baryon-baryon

correlations observed in the experiments. We also extend the study to *p*-Pb collisions at $\sqrt{S}$=5.02 TeV and obtained similar results. These results help us better understand the particle production mechanism in pp and *p*-Pb collisions at Large Hadron Collider energies.

Physical Review C, 2018, **98**(3): 34912

Anisotropic flow in Xe-Xe collisions at $\sqrt{S_{NN}}$=5.44 TeV

STAR Collaboration

The first measurements of anisotropic flow coefficients for mid-rapidity charged particles in Xe–Xe collisions at $\sqrt{S_{NN}} = 5.44$TeV are presented. Comparing these measurements to those from Pb–Pb collisions at $\sqrt{S_{NN}} = 5.02$TeV, v_2 is found to be suppressed for mid-central collisions at the same centrality, and enhanced for central collisions. The values of v_3 are generally larger in Xe–Xe than in Pb–Pb at a given centrality. These observations are consistent with expectations from hydrodynamic predictions. When both v_2 and v_3 are divided by their corresponding eccentricities for a variety of initial state models, they generally scale with transverse density when comparing Xe–Xe and Pb–Pb, with some deviations observed in central Xe–Xe and Pb–Pb collisions. These results assist in placing strong constraints on both the initial state geometry and medium response for relativistic heavy-ion collisions.

Physics Letters B, 2018, **784**: 82

Anisotropic flow of identified particles in Pb-Pb collisions at root $\sqrt{S_{NN}}$=5.02 TeV

STAR Collaboration

Key words Heavy Ion Experiments

The elliptic (v_2), triangular (v_3), and quadrangular (v_4) flow coefficients of $\pi^{\pm}$, $K^{\pm}$, $p+\bar{p}$, $\Lambda+\bar{\Lambda}$ K^0_S, and the ϕ-meson are measured in Pb-Pb collisions at $\sqrt{S_{NN}}$=5.02 TeV. Results obtained with the scalar product method are reported for the rapidity range $|y| < 0.5$ as a function of transverse momentum, p_T, at different collision centrality intervals between 0–70%, including ultra-central (0–1%) collisions for $\pi^{\pm}$, $K^{\pm}$, and $p+\bar{p}$. For $p_T < 3$ GeV/c, the flow coefficients exhibit a particle mass dependence. At intermediate transverse momenta ($3 < p_T <$ 8–10 GeV/c), particles show an approximate grouping according to their type (i.e., mesons and baryons). The ϕ-meson v_2, which tests both particle mass dependence and type scaling, follows $p+\bar{p}$ v_2 at low p_T and $\pi^{\pm}$ v_2 at

intermediate p_T. The evolution of the shape of $v_n(p_T)$ as a function of centrality and harmonic number n is studied for the various particle species. Flow coefficients of $\pi^{\pm}$, $K^{\pm}$, and $p+\bar{p}$ for $p_T < 3$ GeV/c are compared to iEBE-VISHNU and MUSIC hydrodynamical calculations coupled to a hadronic cascade model (UrQMD). The iEBE-VISHNU calculations describe the results fairly well for $p_T < 2.5$ GeV/c, while MUSIC calculations reproduce the measurements for $p_T < 1$ GeV/c. A comparison to v_n coefficients measured in Pb-Pb collisions at $\sqrt{S_{NN}}$=2.76 TeV is also provided.

Journal of High Energy Physics, 2018, (9): 6

Longitudinal Double-Spin Asymmetries for π^0s in the Forward Direction for 510 GeV Polarized *pp* Collisions

STAR Collaboration

The STAR Collaboration reports measurements of the longitudinal double-spin asymmetry, A_{LL}, forneutral pions produced at forward directions in polarized proton-proton collisions, at a center-of-massenergy of 510 GeV. Results are given for transverse momenta in the range2< p_T <10GeV/c within two regions of pseudorapidity that span 2.65<η<3.9. These results are sensitive to the polarized gluon parton distribution function, Δg(x), down to the region of Bjorken x~10^{-3}. The asymmetries observed are less than5×10^{-3} in magnitude and will help constrain the contribution to the spin of the proton from polarized gluons at low x, when combined with other measurements as part of a global analysis.

Physical Review D, 2018, **98**(3): 32013

Longitudinal double-spin asymmetries for dijet production at intermediate pseudorapidity in polarized pp collisions at $\sqrt{s}$=200 GeV

STAR Collaboration

We present the first measurements of the longitudinal double-spin asymmetry A_{LL} for dijets with at least one jet reconstructed within the pseudorapidity range 0.8<η<1.8. The dijets were measured in polarized *pp* collisions at a center-of-mass energy $\sqrt{S}$=200 GeV. Values for ALL are determined for several distinct event topologies, defined by the jet pseudorapidities, and span a range of parton momentum fraction x down to x~0.01. The measured asymmetries are found to be

consistent with the predictions of global analyses that incorporate the results of previous RHIC measurements. They will provide new constraints on $\Delta g(x)$ in this poorly constrained region when included in future global analyses.

Physical Review D, 2018, **98**(3): 32011

Azimuthal anisotropy in Cu + Au collisions at $\sqrt{S_{NN}}$=200 GeV

STAR Collaboration

The azimuthal anisotropic flow of identified and unidentified charged particles has been systemat-ically studied in Cu+Au collisions at $\sqrt{S_{NN}}$ = 200 GeV for harmonicsn= 1–4 in the pseudorapidityrange|η|<1. The directed flow in Cu+Au collisions is compared with the rapidity-odd and, forthe first time, the rapidity-even components of charged particle directed flow in Au+Au collisions at $\sqrt{S_{NN}}$= 200 GeV. The slope of the directed flow pseudorapidity dependence in Cu+Au colli-sions is found to be similar to that in Au+Au collisions, withthe intercept shifted toward positive pseudo rapidity values, i.e., the Cu-going direction. The mean transverse momentum projected onto the spectator plane, 〈px〉 , in Cu+Au collision also exhibits approximately linear dependence on pseudo rapidity with the intercept at about η≈ −0.4 (shifted from zero in the Au-going direction),

3closer to the rapidity of the Cu+Au system center-of-mass. The observed dependencies find natural explanation in a picture of the directed flow originating partly due the “tilted source” and partly due to the asymmetry in the initial density distribution. A charge-dependence of〈px〉was also observed in Cu+Au collisions, consistent with an effect of the initial electric field created by charge difference of the spectator protons in two colliding nuclei. The rapidity-even component of directed flow in Au+Au collisions is close to that in Pb+Pb collisions at $\sqrt{S_{NN}}$= 2.76 TeV, indicating a similarmagnitude of dipole-like fluctuations in the initial-state density distribution. Higher harmonic flow in Cu+Au collisions exhibits similar trends to those observed in Au+Au and Pb+Pb collisions and is qualitatively reproduced by a viscous hydrodynamic model and a multi-phase transport model. For all harmonics with n≥2 we observe an approximate scaling of v_n with the number of constituent quarks; this scaling works as well in Cu+Au collisions as it does in Au+Au collisions.

Physical Review C, 2018, **98**(1): 14915

Inclusive J/ψ production at forward and backward rapidity in p-Pb collisions at $\sqrt{S_{NN}}$=8.16 TeV

STAR Collaboration

Key words

Inclusive J/ψproduction is studied in p-Pb interactions at a centre-of-massenergy per nucleon-nucleon collision $\sqrt{S_{NN}}$ = 8.16 TeV, using the ALICE detector at theCERN LHC. The J/ψis reconstructed, via its decay to a muon pair, in the centre-of-mass rapidity intervals 2.03< y_{cms}<3.53 and 4.46< y_{cms}<2.96, where positive and negative y_{cms} refer to the p-going and Pb-going direction, respectively. The trans-verse momentum coverage is p_T <20 GeV/c. In this paper, y_{cms}-and p_T -dierential crosssections for inclusive J/production are presented, and the corresponding nuclear modification factors R_pP_b are shown. Forward results show a suppression of the J/ψ withrespect to pp collisions, concentrated in the region $p_T \lesssim$ 5 GeV/c. At backward rapidity no signi ficant suppression is observed. The results are compared to previous measurements by ALICE in p-Pb collisions at $\sqrt{S_{NN}}$= 5.02 TeV and to theoretical calculations. Finally, the ratios R_{FB} between forward- and backward-y_{cms} R_pP_b values are shown and discussed.

Journal of High Energy Physics, 2018, (7): 160

Global polarization of Lambda hyperons in Au + Au collisions at $\sqrt{S_{NN}}$=200 GeV

STAR Collaboration

Key words

Global polarization of Lambda hyperons has been measured to be of the order of a few tenths of a percentage in Au+Au collisions at $\sqrt{S_{NN}}$ = 200 GeV, with no significant difference between Lambda and (Lambda) over bar. These new results reveal the collision energy dependence of the global polarization together with the results previously observed at $\sqrt{S_{NN}}$ = 7.7-62.4 GeV and indicate noticeable vorticity of the medium created in noncentral heavy-ion collisions at the highest Relativistic Heavy Ion Collider collision energy. The signal is in rough quantitative agreement with the theoretical predictions from a hydrodynamic model and from a multi-phase transport model. The polarization is larger in more peripheral collisions, and depends weakly on the hyperon's transverse momentum and pseudorapidity eta(H) within vertical bar eta(H)vertical bar<1. An indication of the polarization dependence on the event-by-event charge asymmetry is observed at

the 2 sigma level, suggesting a possible contribution to the polarization from the axial current induced by the initial magnetic field.

Physical Review C, 2018, **98**(1): 14910

Beam Energy Dependence of Jet-Quenching Effects in Au plus Au Collisions at $\sqrt{S_{NN}}$=7.7, 11.5, 14.5, 19.6, 27, 39, and 62.4 GeV

STAR Collaboration

We report measurements of the nuclear modification factor RCP for charged hadrons as well as identified $\pi^{+(-)}$, $K^{+(-)}$, and $p(\bar{p})$ for Au+Au collision energies of $\sqrt{S_{NN}}$ =7.7, 11.5, 14.5, 19.6, 27, 39, and 62.4 GeV. We observe a clear high-*pt* net suppression in central collisions at 62.4 GeV for charged hadrons which evolves smoothly to a large net enhancement at lower energies. This trend is driven by the evolution of the pion spectra but is also very similar for the kaon spectra. While the magnitude of the proton R_{CP} at high *pt* does depend on the collision energy, neither the proton nor the antiproton R_{CP} at high p_T exhibit net suppression at any energy. A study of how the binary collision scaled high-p_T yield evolves with centrality reveals a nonmonotonic shape that is consistent with the idea that jet quenching is increasing faster than the combined phenomena that lead to enhancement.

Physical Review Letters, 2018, **121**(3): 32301

Energy dependence and fluctuations of anisotropic fow in Pb-Pb collisions at $\sqrt{S_{NN}}$=5.02 and 2.76 TeV

STAR Collaboration

Measurements of anisotropic flow coefficients with two- and multi-particle cumulants for inclusive charged particles in Pb-Pb collisions at $\sqrt{S_{NN}}$ =5.02 and 2.76 TeV are reported in the pseudorapidity range $|\eta| < 0.8$ and transverse momentum $0.2 < p_T < 50$ GeV/*c*. The full data sample collected by the ALICE detector in 2015 (2010), corresponding to an integrated luminosity of 12.7 (2.0) μb^{-1} in the centrality range 0-80%, is analysed. Flow coefficients up to the sixth flow harmonic (v_6) are reported and a detailed comparison among results at the two energies is carried out. The p_T dependence of anisotropic flow coefficients and its evolution with respect to centrality and harmonic number *n* are investigated. An approximate power-law scaling of the

form $v_n(p_T) \sim p^{n/3}{}_T$ is observed for all flow harmonics at low p_T ($0.2 < p_T < 3$ GeV/c). At the same time, the ratios $v_n/v^{n/m}{}_m$ are observed to be essentially independent of p_T for most centralities up to about $p_T = 10$ GeV/c. Analysing the differences among higher-order cumulants of elliptic flow (v_2), which have different sensitivities to flow fluctuations, a measurement of the standardised skewness of the event-by-event v_2 distribution $P(v_2)$ is reported and constraints on its higher moments are provided. The Elliptic Power distribution is used to parametrise $P(v_2)$, extracting its parameters from fits to cumulants. The measurements are compared to different model predictions in order to discriminate among initial-state models and to constrain the temperature dependence of the shear viscosity to entropy-density ratio.

Journal of High Energy Physics, 2018, (7): 103

Measurement of the inclusive J/ψ polarization at forward rapidity in pp collisions at $\sqrt{S}$= 8 TeV

STAR Collaboration

We report on the measurement of the inclusive J/ψ polarization parameters in pp collisions at a center of mass energy $\sqrt{S}$= 8 TeV with the ALICE detector at the LHC. The analysis is based on a data sample corresponding to an integrated luminosity of 1.23 pb−1. J/ψ resonances are reconstructed in their di-muon decay channel in the rapidity interval $2.5 < y < 4.0$ and over the transverse-momentum interval $2 < p_T < 15$ GeV/c. The three polarization parameters (λ_θ , λ_ϕ, $\lambda_{\theta\phi}$) are measured as a function of P_T both in the helicity and Collins-Soper reference frames. The measured J/ψ polarization parameters are found to be compatible with zero within uncertainties, contrary to expectations from all available predictions. The results are compared with the measurement in pp collisions at $\sqrt{S}$= 7 TeV.

European Physical Journal C, 2018, **78**(7): 562

Prompt and non-prompt J/ψ production and nuclear modification at mid-rapidity in p-Pb collisions at $\sqrt{S_{NN}}$=5.02 TeV

STAR Collaboration

A measurement of beauty hadron production at mid-rapidity in proton-lead collisions at a nucleon-nucleon centre-of-mass energy $\sqrt{S_{NN}}$ =5.02 TeV is presented. The semi-inclusive decay channel of beauty hadrons into J/ψ is considered, where the J/ψ mesons are reconstructed in the

dielectron decay channel at mid-rapidity down to transverse momenta of 1.3 GeV/c. The $b\bar{b}$ production cross section at mid-rapidity, $d\sigma_{b\bar{b}}/dy$, and the total cross section extrapolated over full phase space, $\sigma_{b\bar{b}}$, are obtained. This measurement is combined with results on inclusive J/ψ production to determine the prompt J/ψ cross sections. The results in p-Pb collisions are then scaled to expectations from pp collisions at the same centre-of-mass energy to derive the nuclear modification factor R_pP_b, and compared to models to study possible nuclear modifications of the production induced by cold nuclear matter effects. R_pP_b is found to be smaller than unity at low P_T for both J/ψ coming from beauty hadron decays and prompt J/ψ.

European Physical Journal C, 2018, **78**(6): 466

Measurement of the ${}^{3}_{\Lambda}H$ lifetime in Au+Au collisions at the BNL Relativistic Heavy Ion Collider

STAR Collaboration

An improved measurement of the ${}^{3}_{\Lambda}H$ lifetime is presented. In this paper, the mesonic decay modes ${}^{3}_{\Lambda}H \rightarrow {}^{3}\mathrm{He} + \pi^-$ and ${}^{3}_{\Lambda}H \rightarrow \mathrm{d+p+}\pi^-$ are used to reconstruct the ${}^{3}_{\Lambda}H$ from Au+Au collision data collected by the STAR collaboration at Relativistic Heavy Ion Collider (RHIC). A minimum χ^2 estimation is used to determine the lifetime of $\tau=142\,^{+24}_{-21}(\mathrm{stat.})\pm29(\mathrm{syst.})$ ps. This lifetime is about 50% shorter than the lifetime $\tau=263\pm2$ ps of a free Λ, indicating strong hyperon-nucleon interaction in the hypernucleus system. The branching ratios of the mesonic decay channels are also determined to satisfy $\mathrm{B.R._{(^3He+\pi^-)}}/(\mathrm{B.R._{(^3He+\pi^-)}}+\mathrm{B.R._{(d+p+\pi^-)}})=0.32\pm0.05(\mathrm{stat.})\pm0.08(\mathrm{syst.})$. Our ratio result favors the assignment $J({}^{3}_{\Lambda}H)=\frac{1}{2}$ over $J({}^{3}_{\Lambda}H)=\frac{3}{2}$. These measurements will help to constrain models of hyperon-baryon interactions.t.

Physical Review C, 2018, **97**(5): 54909

Search for neutrinoless β^+EC decay of ^{120}Te with CUORE-0

STAR Collaboration

We have performed a search for neutrinoless β^+EC decay of ^{120}Te using the final CUORE-0 data release. We describe a new analysis method for the simultaneous fit of signatures with

different event topology, and of data subsets with different signal efficiency, obtaining a limit on the half-life of the decay of $T_{1/2}>1.6\cdot10^{21}$ yr at 90% credibility interval (CI). Combining this with results from Cuoricino, a predecessor experiment, we obtain the strongest limit to date, corresponding to $T_{1/2}>2.7\cdot10^{21}$ yr at 90% CI.

Physical Review C, 2018, **97**(5): 55502

First Results from CUORE: A Search for Lepton Number Violation via $0\nu\beta\beta$ Decay of ^{130}Te

STAR Collaboration

The CUORE experiment, a ton-scale cryogenic bolometer array, recently began operation at the Laboratori Nazionali del Gran Sasso in Italy. The array represents a significant advancement in this technology, and in this work we apply it for the first time to a high-sensitivity search for a lepton-number-violating process: ^{130}Te neutrinoless double-beta decay. Examining a total TeO_2 exposure of 86.3 kg yr, characterized by an effective energy resolution of (7.7±0.5) keV FWHM and a background in the region of interest of (0.014±0.002) counts/(keV kg yr), we find no evidence for neutrinoless double-beta decay. Including systematic uncertainties, we place a lower limit on the decay half-life of $T^{0V}_{1/2}(^{130}Te)>1.3\times10^{25}$ yr (90% C.L.); the median statistical sensitivity of this search is 7.0×10^{24} yr. Combining this result with those of two earlier experiments, Cuoricino and CUORE-0, we find $T^{0V}_{1/2}(130Te)>1.5\times10^{25}$ yr (90% C.L.), which is the most stringent limit to date on this decay. Interpreting this result as a limit on the effective Majorana neutrino mass, we find $m_{\beta\beta}<(110-520)$ meV, where the range reflects the nuclear matrix element estimates employed.

Physical Review Letters, 2018, **120**(13): 132501

Beam-Energy Dependence of Directed Flow of Λ, $\bar{\Lambda}$, $K^{\pm}$, K^0_S and ϕ in Au+Au Collisions

STAR Collaboration

Rapidity-odd directed flow measurements at midrapidity are presented for Λ, $\bar{\Lambda}$, $K^{\pm}$, K^0_S and ϕ at $\sqrt{S_{\rm NN}}$ = 7.7, 11.5, 14.5, 19.6, 27, 39, 62.4 and 200 GeV in Au+Au

collisions recorded by the STAR detector at the Relativistic Heavy Ion Collider. These measurements greatly expand the scope of data available to constrain models with differing prescriptions for the equation of state of quantum chromodynamics. Results show good sensitivity for testing a picture where flow is assumed to be imposed before hadron formation and the observed particles are assumed to form *via* coalescence of constituent quarks. The pattern of departure from a coalescence-inspired sum-rule can be a valuable new tool for probing the collision dynamics.

Physical Review Letters, 2018, **120**(6): 62301

Azimuthal transverse single-spin asymmetries of inclusive jets and charged pions within jets from polarized-proton collisions at $\sqrt{S_{NN}}$=500 GeV

STAR Collaboration

We report the first measurements of transverse single-spin asymmetries for inclusive jet and jet+$\pi^{\pm}$ production at midrapidity from transversely polarized proton-proton collisions at s=500 GeV. The data were collected in 2011 with the STAR detector sampled from 23 pb^{-1} integrated luminosity with an average beam polarization of 53%. Asymmetries are reported for jets with transverse momenta $6 < p_T < 55$ GeV/c and pseudorapidity $|\eta| < 1$. Presented are measurements of the inclusive-jet azimuthal transverse single-spin asymmetry, sensitive to twist-3 initial-state quark-gluon correlators; the Collins asymmetry, sensitive to quark transversity coupled to the polarized Collins fragmentation function; and the first measurement of the "Collins-like" asymmetry, sensitive to linearly polarized gluons. Within the present statistical precision, inclusive-jet and Collins-like asymmetries are small, with the latter allowing the first experimental constraints on gluon linear polarization in a polarized proton. At higher values of jet transverse momenta, we observe the first nonzero Collins asymmetries in polarized-proton collisions, with a statistical significance of greater than 5σ. The results span a range of x similar to results from semi-inclusive deep-inelastic scattering but at much higher Q^2. The Collins results enable tests of universality and factorization breaking in the transverse momentum-dependent formulation of perturbative quantum chromodynamics.

Physical Review D, 2018, **97**(3): 32004

The Magnetic Field Measurement Systems for a Cryogenic Undulator and a Superconducting Undulator at SSRF

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Two cryogenic permanent magnet undulators (CPMU) have been developed and assembled into storage ring at Shanghai Synchrotron Radiation Facility (SSRF) in order to produce higher brilliance in the hard X rays domain. At low temperatures, permanent magnet materials can provide both higher magnetic field and higher resistance to radiation induced demagnetization of the magnet compared to room temperature operation. Test results indicate that lowering the temperature of permanent magnets (Nd2Fe14B) increases the magnetic field strength about by 11%. The magnetic field distribution of the CPMU must be measured after the magnetic arrays are installed into the vacuum chamber and cooled to cryogenic temperature. We have finished a magnetic measurement bench based on a Hall probe to perform cryogenic temperature measurement. In this paper, the details of the magnetic field measurement system and some test results of a CPMU20 with 20mm period and Nd2Fe14B type are described. In addition, two superconducting planar undulator (SCU) prototypes with period 16 mm are also under development at SSRF to research some key technologies.

Journal of Physics: Conference Series, 2018, **1067**(8): 3881

Elastic, mechanical, electronic, and defective properties of Zr–Al–C nanolaminates from first principles

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Key words Elastic constants, Electrical properties, First principles theory, MAX phases

By means of first principles calculations, Zr–Al–C nanolaminates have been studied in the aspects of chemical bonding, elastic properties, mechanical properties, electronic structures, and vacancy stabilities. Although the investigated Zr–Al–C nanolaminates show crystallographic similarities, their predicated properties are very different. For $(ZrC)_nAl_3C_2$ (n = 2, 3, 4), the Zr–C bond adjacent to the Al–C slab with the C atom intercalated in the Zr layers is the strongest, but the one with the C atom intercalated between the Zr layer and Al layer is the weakest. In contrast, the situation for $(ZrC)_nAl_4C_3$ (n = 2, 3) is just the opposite. For Zr–Al–C nanolaminates, the calculated bulk, shear and Young's modulus increase in the sequence of

Zr_2AlC < Zr_3AlC_2 < $Zr_2Al_4C_5$ < $Zr_3Al_4C_6$ < $Zr_2Al_3C_4$ < $Zr_3Al_3C_5$ < $Zr_4Al_3C_6$. The $(ZrC)_nAl_3C_2$ (n = 2, 3, 4) series exhibit the most outstanding elastic properties. In the presence of the external pressure, the bulk and shear moduli exhibit a linear response to the pressure, except for Zr_2AlC and Zr_3AlC_2, both of which belong to the so-called MAX phases. The two materials also exhibit very distinct properties in the strain-stress relationship, electronic structures and vacancy stabilities. As the intercalated Al layers increase, the formation energy of V_{Zr} and V_{Al} increases, while the formation energy of V_C decreases.

Journal of the American Ceramic Society, 2018, **101**(2): 756

A strategy for the preparation of closed-cell and crosslinked polypropylene foam by supercritical CO_2 foaming

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Wu Guozhong

Key words Applications, Crosslinking, Foams, Irradiation, Morphology

We report the preparation of a closed-cell polypropylene (PP) foam material by supercritical carbon dioxide foaming with the assistance of γ-ray radiation crosslinking. Styrene–ethylene–butadiene–styrene (SEBS) copolymer was added to PP to enhance radiation crosslinking and nucleation. Radiation effects on the foaming of the PP/SEBS blend with different ratios were investigated. A significant improvement in the foaming of the crosslinked PP/SEBS blend was achieved as compared to pristine PP. The cell density of the crosslinked PP/SEBS foam greatly increased at a dose of 10 kGy and a high closed-cell ratio was obtained. The tensile strength of the crosslinked PP/SEBS foams (10 kGy) was improved from 14 to 20.7 MPa compared to pristine PP foam (0 kGy). In addition, the crosslinked PP/SEBS blend exhibited a wider foaming temperature window (10 °C) as compared to the non-crosslinked ones (4 °C).

Journal of Applied Polymer Science, 2018, **135**(6)

An Efficient Family of Misfit-Layered Calcium Cobalt Oxide Catalyst for Oxygen Evolution Reaction

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Key words Electrocatalysts, Misfit-layered calcium cobaltite, Oxygen evolution reaction, Surface valence states

The oxygen evolution reaction's (OER) poor kinetics is a considerable obstacle to overcome in the development of water-derived hydrogen fuel. Research into OER catalysts using earth abundant elements is required to achieve desirable catalytic efficiency. Herein, a selection of misfit-layered calcium cobaltite and transition metal (Mn, Fe, and Cu)-doped compounds are synthesized and investigated in order to evaluate their potential as OER catalysts in an alkaline environment. It is discovered that $Ca_3Co_4O_9$ OER activity may be substantially improved through incorporation of Fe, exhibiting low overpotential (331 mV) at 10 mA cm^{-2} current density, small Tafel slope of 52 mV dec^{-1}, and an exceptional long-term stability of electrolysis in 1 m KOH alkaline solution >100 h. Moreover, all materials used are systematically studied using a variety of characterization techniques, resulting in enhanced activity, which is attributed to the enhanced electrical conductivity, and optimized proportion of Co (III) and Co (IV), as well as the synergistic effect between Fe with Co.

Advanced Materials Interfaces, 2018, **5**(23)

Application of surface plasmon polaritons on charged particle beam diagnostics

Jiang Zenggong　Gu Duan　Zhao Minghua　Gu Qiang

In Recent years, the Cherenkov light radiation transformed from surface plasmon polaritons has been found and proposed for a compact and adjustable light source. As the process is motivated by charged particle beam, the characteristics of the light are not only related with the device but can also reflect certain characteristics of the beam. In this paper, a beam position and energy measurement method has been proposed based on the Cherenkov light radiation transformed from surface plasmon polaritons. Early-stage numerical and analytical investigations are also presented for a planar structure device.

Journal of Physics:　Conference Series, 2018, **1067**(7)

Influence of carboxyl and amide groups on *in vitro* hemocompatibility of sulfonated polypropylene non-woven fabric

Li Rong　Cai XiMing　Ye Yin　Wu GuoZhong

Key words　Biomaterials, Biomimetic, Grafting, Irradiation

The sulfonated polypropylene non-woven fabric (PP_{NWF}) was successfully fabricated *via* γ-ray simultaneous radiation-induced graft polymerization of acrylic acid (AA)/sodium styrenesulfonate

(NaSS) and acrylamide (AAm)/NaSS. The existence of graft chains in both PP-*g*-P(AA-*co*-NaSS) and PP-*g*-P(AAm-*co*-NaSS) was proved by attenuated total reflection Fourier transform infrared spectroscopy and X-ray photoelectron spectroscopy. Water contact angle measurement illustrated the sulfonated PP_{NWF} owning good hydrophilicity. The *in vitro* hemocompatibility evaluation showed that both PP-*g*-P(AA-*co*-NaSS) and PP-*g*-P(AAm-*co*-NaSS) inhibited effectively the adhesion of platelets and were significantly compatible with erythrocytes. Moreover, no obvious difference was confirmed in the prevention of platelet adhesion and hemolysis ratio between carboxyl and amide groups. However, as compared with that of PP-*g*-P(AAm-*co*-NaSS), PP-*g*-P(AA-*co*-NaSS) exhibited outstanding anticoagulant activity via increased activated partial thromboplastin time and thrombin time. This result indicated that the carboxyl group but not amide group featured strong synergistic effect on the anticoagulant activity of sulfonated PP_{NWF}.

Journal of Applied Polymer Science, 2018, **135**(9)

Corrosion behavior of 316SS and Ni-based alloys in a ternary NaCl-KCl-$MgCl_2$ molten salt

Sun Hua Wang Jianqiang Li Zhijun Zhang Peng Su Xingzhi

Key words Alloy, Molten chloride salt, Corrosion, Alloying element

This paper mainly investigated the corrosion of Fe-based 316SS and seven Ni-based alloys in molten NaCl-KCl-$MgCl_2$ under N_2 at 700 °C using static immersion experiment and microstructure observation. All alloys suffered the selective dissolution of Cr, resulting in the formation of subsurface voids. 316SS exhibited worse corrosion resistance than that of Ni-based alloys. Among Ni-based alloy, the corrosion resistance of alloys increased in the following order of Ni-Fe-Cr < Ni-W-Cr < Ni-Mo-Cr. The minor alloying elements such as Fe, Mo and W have also an obvious effect on the corrosion of alloys. Furthermore, Mo plays a better role in improving the corrosion resistance of Ni-based alloys than W due to the beneficial influence of Mo on preventing the outward diffusion of Cr from the alloys, in contrast to their calculated thermodynamical similarity. Otherwise, the morphology and composition of carbides on the alloy matrix have also an influence on corrosion of the alloys. The small continuous Mo-rich carbides on the grain boundaries tend to mitigate corrosion, while the large isolated W-rich carbides have no similar role.

Solar Energy, 2018, **171**: 320

Thermodynamic assessment of the SrBr2-MBr (M: alkali metal) binary systems

Li Xiang Xie Leidong

Key words Strontium bromide, Thermodynamics modeling, Phase equilibria

The phase diagrams of the $SrBr_2$-MBr (M: alkali metal) binary systems based on phase equilibria and thermochemical data were evaluated and optimized using the CALPHAD method. The substitutional solution model was used to describe the Gibbs energies of all liquid phases. All intermediate compounds were handled to be stoichiometric of which the Gibbs energies comply with the Neumann-Kopp rule. Self-consistent datasets with all model parameters were developed, and thermodynamic properties of liquid phase (mixing enthalpy and activity) were also calculated for the whole range of compositions. Meanwhile, the empirical method based on ionic parameter function was successfully used to validate the mixing enthalpies calculated. Results manifest that the calculated results were in excellent agreement with the experimental values reported in the present work. By means of thermodynamic calculation, this database of strontium bromide system was used to predict the $SrBr_2$-based multicomponent system with low melting points, which will design and prepare composite materials for low temperature thermal energy storage (TES).

Calphad: Computer Coupling of Phase Diagrams and Thermochemistry, 2018, **63**: 116

Enhancing decontamination of zirconium and ruthenium in the Thorex process using acetohydroxamic acid

Li Zheng Zhao Haogui Chen Mumei Li Qingnuan Zhang Lan

Key words Acetohydroxamic acid, Thorex process, Decontamination, Centrifugal extractors

The decontamination of some extractable fission products, such as Zr and Ru, is an important issue in the Thorex process. Acetohydroxamic acid (AHA) is an organic ligand composed of only C, H, N and O atoms. It can be used as complexing and reducing agent to inhibit the extraction of Zr and Ru. In this paper, the effect of AHA and preheating on the extraction of Th, U, Zr and Ru was studied. It is found the extraction of Zr and Ru would be inhibited in the presence of AHA and preheating, meanwhile there was no obvious effect on the extraction of Th and U. Afterwards, the countercurrent extraction using centrifugal extractors was performed to further test and verify the effect of AHA in a typical Thorex process. The results indicate that the

decontamination of Zr and Ru could be enhanced evidently due to the effect of AHA, and the corresponding decontamination factor would be improved from 27.0 to 3.3×10^3 and 111.0 to 1.5×10^3, respectively. Thus, the use of AHA would be an efficient means for enhancing the decontamination of Zr and Ru in Thorex process.

Hydrometallurgy, 2018, **182**: 1

Significantly reduced pre-oxidation period of PAN fibers by continuous electron beam irradiation: Optimization by monitoring radical variation

Zhang Wenli Wang Mouhua Zhang Wenfa Liu Weihua Yang Chenguang Shen Rongfang Wu Guozhong

Key words PAN fibers, Pre-oxidation, Irradiation, ESRRadical concentration, Optimization

A self-shielded electron beam (EB) accelerator was connected to the front of a pre-oxidation furnace to evaluate the effect of radiation on the pre-oxidation of polyacrylonitrile (PAN) fibers; with this setup, PAN fibers could be irradiated and pre-oxidized in sequence to obtain stabilized fibers. Radiation effects during different temperature stages of the pre-oxidation process were analyzed by differential scanning calorimetry, Fourier-transform infrared spectroscopy, and electron spin resonance spectroscopy. The results indicated that radiation exerted significant but different effects at various stages of the pre-oxidation process. The alkane radicals induced by radiation are rapidly transformed into polyene structures and produced polyenyl radicals after a short heat treatment period. The polyenyl radicals promoted dehydrogenation and cyclization reactions and polyene structures improved the thermal stability of the PAN fibers. Therefore, radiation can greatly shorten the time required for the stabilization of PAN fibers, owing to which the time needed for each temperature stage can be reduced by a large extent. The effects of radiation on various temperature stages of the pre-oxidation process were analyzed accurately by studying the changes in the concentration of polyenyl radicals. An optimized pre-oxidation process for irradiated PAN fibers was designed, which reduced the time period required for stabilization by 75%. The optimized pre-oxidation plus continuous EB irradiation process induced good properties in the stabilized PAN fibers, in terms of fiber density, oxygen content, and degree of cyclization. Radical concentration was found to be an appropriate indicator to express the degree of pre-oxidation.

Polymer Degradation and Stability, 2018, **158:** 72

Design a high power pulse transformer for c-band klystron modulator

Liu, Y. Gu, M. Yuan, Q.

Shanghai soft X-ray Free Electron Lasers (SXFEL) used C-band accelerator structure to accelerate electrons at SINAP (Shanghai Institute of Applied Physics). 50MW C-band klystron and 110MW modulator are used to provide power supply for accelerator structure. In order to meet the modulator-klystron demands, a reliable and stable high power pulse transformer is indispensable. In this paper, the key design points for the high voltage pulse transformer are presented. The methods of shortening rise time and diminishing flattop droop are highlighted.

Journal of Physics: Conference Series, 2018, **1067**(8): 082020

工程索引

Engineering Index

In Situ Investigations of Structures Evolution of Mg Doped Zn_4Sb_3

Wang Yu Li Hong Yang Yingguo Ji Gengwu Shen Kongchao
Sun Haoliang Li Jiong Jiang Zheng Song Fei

The beta-phase of Zn_4Sb_3 has been regarded as a very promising thermoelectric material since middle nineties, owing to its unique merit: intermediate temperature region (200-400 °C), made of cheap, non-toxic and abundant elements and high thermoelectric property. However, the thermal stability of Zn_4Sb_3 seems to be an inherent obstacle for the practical application during the working temperatures. Herein, magnesium doped Zn-Sb semiconductor ($Mg_{0.04}Zn_{3.96}Sb_3$) was investigated thoroughly in-situ during thermal annealing up to 600 K, whilst both microstructure and electronic structures were recorded via the combination of synchrotron-based two dimensional X-ray diffraction techniques and the X-ray photoemission spectroscopy. While the time-resolved grazing incidence XRD reveals the preserved crystal structures during thermal annealing to 600 K, XPS measurement demonstrate the robustness of electronic structures. On basis of these findings, it was concluded in the end that the doping of magnesium significantly improves the thermal stability of zinc-antimonite compounds and introduces minor influence on the electronic structure of Zn-Sb alloy. Our study may propose an effective approach towards the wild application of Zn_4Sb_3related thermoelectric materials.

Key Engineering Materials, 2017, 727: 178.

Thorium molten salt reactor nuclear energy system (TMSR)

Dai zhimin

Keywords Molten salt reactor, thorium, hybrid nuclear energy application

The thorium molten salt reactor nuclear energy system (TMSR) is designed for thorium-based nuclear energy utilization and hybrid nuclear energy application, based on a liquid-fueled thorium molten salt reactor (TMSR-LF) and a solid-fueled thorium molten salt reactor (TMSR-SF).

Key Engineering Materials, 2017, 727: 178.

附录 1

2017–2018 年博士、硕士学位授予一览表

PhD and MD Programs Completed at SINAP IN 2017-2018

2017

No.	学位	姓名	专业	论文题目	研究方向	导师
1	博士	王春鹏	光学	软 X 射线扫描相干衍射成像方法学研究	X 射线显微成像	郜仁忠
2	博士	王耿	光学	同步辐射 X 射线小角散射与数值模拟研究 纳米材料的结构与光学特性	同步辐射和光学	郜仁忠
3	博士	朱亮	粒子物理与原子核物理	核反应系统的多层网络结构特征研究	核物理与计算物理	马余刚
4	博士	赵颖	核技术及应用	智能球流运动探测系统的开发及初步应用	反应堆安全分析	陈堃
5	博士	孙雪平	无机化学	碳氧化物加氢催化的原位 XAFS 方法研究	碳氧化物加氢催化的原位 XAFS 方法研究	黄宇营
6	博士	朱智	粒子物理与原子核物理	水中热噪声的自相关和频谱特性的研究	纳米科学与单分子生物物理	方海平
7	博士	高乾宏	无机化学	超高分子量聚乙烯纤维及织物的辐射接枝改性与功能化研究	高分子辐射化学	吴国忠
8	博士	段佩权	核技术及应用	同步辐射 X 射线高分辨吸收谱和发射谱及其在核能材料中的应用	同步辐射 X 射线吸收谱及发射谱	黄宇营
9	博士	许良	光学	基于单色光的 X 射线动态显微 CT 研究	X 射线光学与同步辐射相关物理	肖体乔
10	博士	魏泉	核能科学与工程	液态熔盐堆物理热工研究与安全特性初步分析	反应堆物理	蔡翔舟
11	博士	汪启胜	核技术及应用	SSRF 生物大分子光束线站自动化集成及实验技术发展	加速器与束线技术及应用	何建华
12	博士	马龙	粒子物理与原子核物理	RHIC 能区 D 介子触发方位角关联的实验测量及各向异性流涨落的唯象研究	高能核物理	马余刚
13	博士	徐亦飞	粒子物理与原子核物理	相对论重离子碰撞中超氚的实验研究	粒子物理与原子核物理	马余刚
14	博士	黄勃松	粒子物理与原子核物理	基于原子核反应输运模型对光核反应的研究	光核反应	马余刚
15	博士	杨金荣	粒子物理与原子核物理	水分子诱导氢终止硅的老化及荧光光谱红移的理论研究	硅团簇的荧光性质研究	方海平
16	博士	杨一鸣	粒子物理与原子核物理	X 射线衍射层析成像及其合金晶粒三维定量研究	X 射线衍射层析成像	肖体乔
17	博士	秦威	核技术及应用	氟盐冷却高温球床堆组件均匀化方法研究	反应堆物理	蔡翔舟

18	博士	戴明	核技术及应用	球床氟盐冷却高温堆堆芯燃料管理研究	反应堆物理	余笑寒
19	博士	王健	核技术及应用	低温永磁波荡器冷却关键技术的研究	加速器技术及应用	王莉
20	博士	李光超	核能科学与工程	基于能谱分区的熔盐堆 Th-U 燃料增殖性能研究	熔盐堆中子物理设计和钍铀燃料增殖	徐洪杰
21	博士	刘峰瑞	核能科学与工程	氟盐冷却球床堆堆芯燃料球离散模拟	核能科学与工程	黎忠
22	博士	张正桥	粒子物理与原子核物理	反质子间相互作用的测量	重离子物理	马余刚
23	博士	彭川黔	核技术及应用	扫描型表面斜率测量的方法研究	面形检测	王劼
24	博士	王建榜	无机化学	基于 DNA 分子的微纳米材料的构建和应用	DNA 纳米反应器	樊春海
25	博士	刘知晓	无机化学	人间充质干细胞物理生物学标记的开发及应用	物理生物	胡钧
26	博士	许杭华	粒子物理与原子核物理	能量连续可调激光康普顿散射光源的研制和相关应用研究	粒子物理与原子核物理	王东
27	博士	雷豪志	无机化学	纳米尺度上多肽与磷脂膜相互作用的研究	纳米生物学	张益
28	博士	方维娜	无机化学	以 DNA 折纸为模板构建具有表面等离子体性质的金属纳米结构	DNA 纳米技术	樊春海
29	博士	施承斌	核能科学与工程	液态燃料熔盐堆系统分析程序及安全特性研究	反应堆热工水力	刘桂民
30	博士	戚威	核能科学与工程	基于钍基熔盐堆环境的核石墨研究	基于钍基熔盐堆环境的核石墨研究	怀平,夏汇浩
31	博士	蒋力	核能科学与工程	Si 含量对 GH3535 合金中碳化物形成和转变行为的影响	反应堆结构材料	闫隆
32	博士	刘星	光学	周期性纳米金属粒子表面等离子体共振的调控及应用	X 射线干涉光刻	邰仁忠
33	博士	崔德阳	核能科学与工程	熔盐堆利用富集铀/钚燃料启动建立钍铀循环运行模式的研究	熔盐堆钍铀燃料循环物理	蔡翔舟
34	博士	杨超	核技术及应用	纳米碳化硅弥散强化镍基合金的制备及显微结构与性能研究	核技术及应用	周兴泰
35	博士	王洪龙	无机化学	超高分子量聚乙烯辐射效应与改性研究	高分子辐射效应与改性研究	吴国忠
36	博士	赵彦	无机化学	DNA 纳米结构的功能化及其生物学应用	DNA 纳米技术	宋世平
37	博士	张祎男	无机化学	基于 DNA 折纸的纳米排布及其在信息加密中的应用	DNA 纳米技术	王丽华

38	博士	赵剑锋	无机化学	氟喹诺酮类抗生素的光敏毒性及其抑制机理研究	快速反应动力学	王文锋
39	博士	蒋芳玲	无机化学	利用同步辐射 XAFS 方法研究离子液体的微观结构及金属离子的还原过程	离子液体微观结构及金属离子还原的同步辐射研究	吴国忠
40	博士	杜培培	无机化学	氧化铈负载型纳米催化材料的可控合成和“构效关系”研究	负载型催化剂“构效关系”研究	黄宇营
41	博士	季庚午	光学	钙钛矿太阳能电池中界面电子结构的研究	钙钛矿太阳能电池界面电子结构	高兴宇
42	博士	孔海云	粒子物理与原子核物理	中质子有效质量劈裂和对称能效应研究	中低能核物理	马余刚
43	博士	彭天欢	无机化学	贵金属局域表面等离子体材料在成像、检测及催化领域的应用研究	贵金属纳米材料	李迪
44	博士	段立武	核技术及应用	双频法束长测量关键技术研究	加速器束流诊断	冷用斌
45	博士	胡兴杰	无机化学	纳米材料细胞摄取和胞内运输的成像学研究	DNA 纳米技术	李迪
46	博士	马付银	无机化学	氧化石墨烯薄膜在放射化学分离中的应用研究	乏燃料后处理	张岚
47	博士	赵斌清	核技术及应用	质子治疗束配系统电离室电子学研究	核电子学与探测技术	赵明华
48	博士	孔华庭	无机化学	纳米碳黑-金属复合物的联合呼吸毒性研究	纳米生物学	李迪
49	博士	陈双建	核能科学与工程	GH3535 合金焊接热影响区组织演变及性能研究	镍基高温合金焊接	黎忠
50	博士	苏静	无机化学	SERS 纳米探针和电化学纳米界面用于生物诊断的新方法	生物传感和疾病早期诊断	宋世平
51	博士	彭浩	无机化学	氟熔盐体系腐蚀杂质及氧化物溶解行为的研究	熔盐电化学	谢雷东
52	博士	鄂彦志	核能科学与工程	GPU 加速的氟盐冷却球床堆堆芯瞬态分析方法研究	反应堆物理与热工水力	徐洪杰
53	博士	薛春	核能科学与工程	组件型熔盐堆的设计与研究	反应堆设计	朱智勇
54	博士	陈怀灿	核能科学与工程	镍及镍基合金的离子辐照效应研究	反应堆材料与工程	周兴泰
55	博士	诸兵	无机化学	自组装 DNA 纳米材料结构与功能的研究	DNA 纳米材料生物学效应	陈楠
56	博士	夏银	粒子物理与原子核物理	基于 IBUU 输运模型研究中能重离子碰撞中的自旋轨道耦合作用	中低能核物理	徐骏
57	博士	徐博	核技术及应用	小型模块化固态燃料熔盐堆 TMSR-SF2 的热工水力设计与安全事故分析	反应堆物理	余笑寒

58	博士	高兆帅	无机化学	受激辐射损耗超分辨显微术的研究与应用	超分辨成像	王丽华
59	硕士	姜淑颖	核技术及应用	RELAP5 程序流动熔盐与不凝气体接触问题的扩展、验证及应用	反应堆热工水力	戴志敏
60	硕士	李洋	核能科学与工程	CR-39 固体核径迹探测器应用于中子探测的实验研究	辐射防护、环境监测	夏晓彬
61	硕士	胡修源	生物物理学	氧化石墨烯与基底表面人工磷脂双分子层的相互作用探究	单分子探测与操纵	张益
62	硕士	王中庆	核技术及应用	碘化钆闪烁体的辐射探测性能与中子探测的γ抑制研究	辐射探测与测量	李勇平
63	硕士	刘莉军	核技术及应用	低温永磁波荡器过冷液氮冷却系统及其关键设备的计算分析和控压关键技术的实验研究	低温工程 核技术	王莉
64	硕士	邓明君	核技术及应用	双光束单脉冲三维成像装置离线对准系统研究	同步辐射技术及其应用	邰仁忠
65	硕士	王京华	核技术及应用	TMSR-SF1 自适应功率控制器的设计与分析	反应堆控制系统	戴志敏
66	硕士	陈家豪	核技术及应用	10MW 固态燃料钍基熔盐堆稳态中子物理-热工耦合研究	核燃料设计与研究	朱智勇
67	硕士	谢雪松	核技术及应用	一体化小型氟盐冷却高温堆自然循环研究	反应堆热工水力	戴志敏
68	硕士	冯权胜	粒子物理与原子核物理	小型固态燃料球床熔盐堆堆芯入口流场优化设计	熔盐堆流场设计	徐洪杰
69	硕士	张海云	核技术及应用	高能劳厄单色器晶体压弯机构的优化设计	精密机械	薛松
70	硕士	颜锋	高分子化学与物理	氧化石墨烯基正渗透膜的制备及其分离性能的研究	氧化石墨烯基功能滤膜材料	李景烨
71	硕士	徐翔宇	核技术及应用	电纺聚丙烯腈纳米纤维的辐照效应及对预氧化的影响	高分子材料改性	吴国忠
72	硕士	胡传伟	核技术及应用	基于开源热工水力程序的 GPU 并行化实现与应用	反应堆热工水力数值计算	徐洪杰
73	硕士	樊奇伟	核技术及应用	熔盐管内强化传热实验研究	核反应堆热工水力	朱志远
74	硕士	贾亚军	核技术及应用	质子治疗中扫描照射的模拟计算及并行加速	质子治疗中的扫描照射	蒲越虎
75	硕士	刘舒婷	无机化学	吸收光谱法研究三元硝酸/亚硝酸熔盐的吸光率和分解机理	熔盐光谱学	刘洪涛
76	硕士	张明星	无机化学	尼龙 66 纤维辐射接枝改性及在铀废水处理和抗菌方面的应用	高分子材料辐射接枝改性	吴国忠
77	硕士	王建军	电磁场与微波技术	SXFEL 装置中纯永磁移相器积分场优化方法的研究	移相器的研究	周巧根

78	硕士	黄益琪	电磁场与微波技术	个性化人眼模型及精准角膜手术研究	眼视光学	李宾
79	硕士	孙宝星	核能科学与工程	同步辐射小角散射研究碳化硅纤维中的晶体颗粒结构	材料科学	徐洪杰
80	硕士	杨雨晖	信号与信息处理	上海质子治疗示范装置慢引出模拟研究	加速器技术应用	李德明
81	硕士	陈建樵	核技术及应用	基于同步辐射的串行晶体学实验技术研究	同步辐射晶体学	何建华
82	硕士	丰丙刚	光学	毛细管聚焦特性及其 X 射线荧光与纳米全场成像应用研究	X 射线光学与同步辐射相关物理	肖体乔
83	硕士	张露灏	生物物理学	配体介导的 DNA 纳米颗粒与细胞之间的相互作用研究	纳米材料的细胞摄取	樊春海
84	硕士	邱杰	核技术及应用	体相纳米气泡产生及其稳定性研究	纳米气泡	胡钧
85	硕士	乔延凯	核技术及应用	高温剪断式触发吸收球非能动停堆装置断裂模拟研究	反应堆结构设计	戴志敏
86	硕士	顾晨光	核能科学与工程	熔盐堆核石墨断裂模拟与研究	固体力学	曾广礼
87	硕士	王雷	核能与核技术工程	熔盐自然循环实验回路热损失研究	核反应堆热工水力与安全分析	陈堃
88	硕士	杨硕	核能与核技术工程	石墨烯精细结构及其性质的研究	石墨烯的结构与性质	胡钧
89	硕士	李威	核能与核技术工程	锡锌氧化物负载的金催化剂在一氧化碳氧化反应中的“构效”关系研究	纳米材料“构效”关系研究	司锐
90	硕士	潘要霖	核能与核技术工程	亚微米聚焦高稳定柔性铰链压弯机构的模拟分析	同步辐射微纳聚焦技术	李爱国
91	硕士	程振东	光学工程	有机配体包裹金纳米颗粒薄膜制备及其表征	纳米金颗粒薄膜	高兴宇
92	硕士	孙思思	电子与通信工程	SXFEL 装置上基于 LLRF 控制系统的速调管输入输出特性曲线的线性化	电子与通信工程	赵明华
93	硕士	张月月	生物工程	纳米电极的制备及细胞间神经递质的实时监测	细胞间神经递质的电化学监测	左小磊
94	硕士	宋明豪	核能与核技术工程	自由电子激光中的尾波场效应研究	自由电子激光物理技术	邓海啸
95	硕士	沈志伟	生物工程	硅油对晶状体蛋白体外积聚性影响研究	生物纳米医药	张益
96	硕士	王亚迪	生物工程	基于同步辐射红外显微光谱技术的微生物组方法学初步研究	单分子探测与操纵	吕军鸿

2018

No.	学位	姓名	专业	论文题目	研究方向	导师
1	博士	THANAPONG PHIMSEN	粒子物理与原子核物理	电子储存环中高次谐波腔束流动力学研究	加速器物理	赵振堂
2	博士	于清林	核技术及应用	束团横向相空间重建技术研究	加速器物理	赵明华
3	博士	邵宽	核能科学与工程	核燃料中裂变产物行为的理论研究	核燃料中的裂变产物	怀平
4	博士	边宇	核技术及应用	基于相干渡越辐射的亚皮秒级电子束长测量研究	自由电子激光	王东
5	博士	郑官豪杰	无机化学	钙钛矿太阳能电池微观结构调控和性能研究	薄膜太阳能电池制备、表征和性能测试	高兴宇
6	博士	张洵	粒子物理与原子核物理	镍基合金中微结构优化材料抗辐照性能的理论研究	镍基合金抗辐照性能	朱志远
7	博士	彭玉	核能科学与工程	固态燃料熔盐冷却快堆的钍铀增殖特性研究	反应堆物理和热工水力	徐洪杰
8	博士	李健健	核能科学与工程	熔盐堆中辐照损伤对 SiC 力学性能和熔盐腐蚀性能影响的研究	核材料的辐照效应	闫隆
9	博士	李亚东	粒子物理与原子核物理	二氧化钛表面及界面性质的第一性原理研究	计算材料学	高嶷
10	博士	刘涛	粒子物理与原子核物理	基于横向梯度波荡器的束流物理和自由电子激光物理的相关研究	束流物理和自由电子激光物理	王东
11	博士	黄晓霞	核技术及应用	X 波段高梯度加速结构及尾场效应研究	加速器物理及微波技术	赵振堂
12	博士	陈家华	核技术及应用	超高能量分辨软 X 射线光栅单色器与光束线的设计优化	同步辐射光学与技术	薛松
13	博士	刘以勇	核技术及应用	超导波荡器冷却和冷质量支撑系统的研究	低温工程	王莉
14	博士	王东兴	核技术及应用	超大电流磁铁电源并联实现及电流检测技术研究	电力电子及自动控制技术	李德明
15	博士	聂雪川	粒子物理与原子核物理	SiO2 表面上醇类分子的浸润行为的分子动力学模拟研究	纳米科学和单分子生物物理	方海平
16	博士	陈姆妹	无机化学	基于石墨烯气凝胶溶剂浸渍材料的放化分离方法研究	钍基核燃料水法后处理	张岚
17	博士	冀锐敏	核能科学与工程	FLiBe 熔盐堆中光激中子的影响研究	反应堆物理	刘桂民
18	博士	唐辉	核能科学与工程	基于熔盐堆环境的核石墨熔盐浸渗特性及力学性能研究	核材料	夏汇浩

19	博士	王先彬	无机化学	Th4+在 ThF4-LiCl-KCl 熔盐中的电化学行为与电解分离	乏燃料干法后处理	李晴暖
20	博士	王硕	无机化学	对纳米气泡的稳定性及其内部密度的研究	界面物理	胡钧
21	博士	刘畅	核技术及应用	高温熔盐蓄热风电系统设计及研究	高温熔盐蓄热风电系统设计及研究	戴志敏
22	博士	苗春晖	核技术及应用	点扫描束配系统的扫描算法研究	加速器技术	赵振堂
23	博士	聂茂武	粒子物理与原子核物理	相对论重离子碰撞中各向异性流的研究	相对论重离子碰撞	马国亮
24	博士	金鑫	核技术及应用	基于同步辐射 X 射线小角散射的嵌段共聚物自组装原位研究	高分子材料表征	王劼
25	博士	夏凯	无机化学	纳米颗粒-蛋白复合物对细胞自噬调控的研究	纳米材料的生物效应	李宾
26	博士	彭佳	无机化学	加速剂在钍基熔盐堆氟化物高温水解转化中的应用	钍基核燃料水法后处理方法研究	张岚
27	博士	张晓楠	光学	钙钛矿太阳能电池活性层结晶性与界面研究	同步辐射光学	高兴宇
28	博士	荣丽媛	光学	拓扑材料 SrSn2As2, EuCd2As2 和铁基超导材料 Ba2Ti2Fe2As4O 的 ARPES 研究	同步辐射应用	邰仁忠
29	博士	王兴亚	光学	利用先进纳米探测技术对纳米气泡特性的研究	界面物理	高兴宇
30	博士	庞利娟	无机化学	聚乙烯纤维（无纺布）辐射改性及其对金属离子的吸附研究	高分子辐射改性	吴国忠
31	博士	胡涛	光学	X 射线小角散射 CT 方法及其应用研究	光学（同步辐射相关物理）	肖体乔
32	博士	陈汉骄	核技术及应用	逐束团截面尺寸测量技术研究	加速器技术及应用	冷用斌
33	博士	韩仲康	粒子物理与原子核物理	二氧化铈表面物理化学性质的第一性原理研究	计算化学	高嶷
34	博士	管纪鹏	无机化学	辐射接枝聚偏氟乙烯及其共聚物的结构与性能研究	辐射接枝	李景烨
35	博士	周开尚	粒子物理与原子核物理	超高亮度 X 射线自由电子激光物理研究	自由电子激光	王东
36	博士	王则君	无机化学	核酸纳米技术在活细胞成像和癌症免疫治疗中的应用	纳米生物	王丽华
37	博士	孙乐乐	无机化学	基于功能 DNA 的单分子水平蛋白动态及活细胞蛋白递送研究	酶学研究	李宾
38	博士	秦来来	核技术及应用	核设施周围大气中多形态氚监测方法研究	氚科学与技术	刘桂民

39	博士	刘星	粒子物理与原子核物理	界面水诱导的分子筛和仿生物膜表面结构的理论研究	纳米科学和单分子生物物理	方海平
40	博士	解春雨	核技术及应用	功能性材料对铀的吸附行为及机制研究	功能材料在钍铀化学中的应用	王建强
41	博士	李敏	无机化学	纳米生物传感界面的功能调控及其在生物检测中的应用	纳米电化学生物传感	宋世平
42	博士	王皓	粒子物理与原子核物理	高温陶瓷材料热输运和微观结构的理论研究	高温陶瓷材料物理性质的理论研究	怀平
43	博士	王亨缇	无机化学	聚烯烃的辐射效应及其流变行为研究	高分子辐射原理	李景烨
44	博士	赵炳晨	核技术及应用	熔盐单罐填充床蓄热系统性能分析及优化设计研究	高温蓄热技术	戴志敏
45	博士	高波	核技术及应用	上海光源诊断线站升级中的若干关键技术研究	加速器技术及应用	冷用斌
46	博士	崔之芬	无机化学	三氧化二砷叠加纳米金刚石的抗实体瘤效应研究	纳米生物	李宾
47	博士	阮见	核能科学与工程	熔盐堆系统瞬态分析程序开发	反应堆热工水力	徐洪杰
48	博士	王旭	无机化学	氧化铈负载的双金属型小尺寸催化材料的合成、催化性能及其“构效关系”研究	纳米催化	司锐
49	博士	朱大明	光学	石墨烯原位同步辐射表征及应用	同步辐射技术及应用	邰仁忠
50	博士	孟祥雨	光学	部分相干光在同步辐射光束线中的传播及应用研究	同步辐射光学与技术	王勇
51	博士	玉昆	核能科学与工程	GH3535 合金激光焊接头组织性能演变及腐蚀行为研究	反应堆材料与工程	周兴泰
52	博士	王飞	无机化学	基于 DNA 的生物计算和超分辨成像	超分辨成像	王丽华
53	博士	樊凯	无机化学	基于均相共辐射法的 PES 接枝改性高分子超滤膜的制备及应用	均相溶液辐射接枝法制备超滤膜研究	胡钧
54	硕士	王菲	粒子物理与原子核物理	热处理对金纳米颗粒超薄膜结构和光电子发射影响的研究	烷基硫醇包裹金纳米粒子薄膜制备及其光电子发射的研究	高兴宇
55	硕士	张振方	粒子物理与原子核物理	激发态原子核的退激性质研究	放射性核束物理与重离子物理	方德清
56	硕士	徐秀清	核技术及应用	CR-39 探测器应用于带电粒子识别的实验研究	固体核径迹	夏晓彬
57	硕士	李明达	核技术及应用	RFQ 低电平算法设计与实现	加速器技术	赵振堂
58	硕士	黄文	粒子物理与原子核物理	兰州冷却储存环外靶时间投影室样机的研制和激光标度	中低能核物理	徐骏

59	硕士	高崚威	无机化学	磷酸盐玻璃固化放射性含氟废物 的分子动力学模拟研究	钍基熔盐堆放射性废物处理与处置	夏晓彬
60	硕士	邵任之	光学	基于超快动力学模型的阿秒脉冲复原方法	X 射线光学及超快电子谱学	李宾
61	硕士	李凯	核技术及应用	X 射线自由电子激光振荡器的理论研究	自由电子激光	邓海啸
62	硕士	薛韩	粒子物理与原子核物理	基于 TALYS 程序的中子俘获反应和光核反应研究	粒子物理与原子核物理	马余刚
63	硕士	林大富	核能科学与工程	基于折射率匹配方法的可视化球床三维重构研究	热工水力	邹杨
64	硕士	梁子薇	信号与信息处理	高温熔盐流量标定平台控制系统的研究与设计	自动控制	陈永忠
65	硕士	彭一鹏	核技术及应用	钍基氯盐快堆燃耗性能研究	钍基熔盐堆反应堆物理方向	蔡翔舟
66	硕士	于晓萌	粒子物理与原子核物理	有序水及其周围水分子自扩散行为的理论研究	纳米科学和单分子生物物理	方海平
67	硕士	郄美英	无机化学	钍、铀及其裂变产物配合物的 合成、结构及性质研究	配位化学	王建强
68	硕士	秦超	核技术及应用	同步辐射椭圆柱面压弯镜机构的研究	光学精密仪器	薛松
69	硕士	许六军	核技术及应用	燃料元件基体石墨的固相增密及其性能研究	核燃料科学与工程	朱智勇
70	硕士	徐千惠	无机化学	LiCl-KCl 熔盐体系中氟离子浓度对钍离子的电化学行为及电解提取的影响	无机化学（熔盐电化学）	李晴暖
71	硕士	代其隆	核能科学与工程	表面堆焊纯 Ni 的 800H 合金的组织与服役性能的研究	反应堆结构材料	周兴泰
72	硕士	姚超	核能科学与工程	基于近场外差散斑的自由电子激光横向相干性测量的研究	自由电子激光横向相干性测量研究	王东
73	硕士	何越	核技术及应用	基于云计算技术的 TMSR 仿真平台设计及性能分析	先进仿真技术	戴志敏
74	硕士	钟长游	粒子物理与原子核物理	高能 X 射线复合折射透镜设计和应用	同步辐射光束线技术	何建华
75	硕士	刘震	粒子物理与原子核物理	故宫南大库出土紫金釉和黄釉的微观结构研究	同步辐射应用	魏向军
76	硕士	俞成	光学	波荡器磁中心高精度标定的技术研究	精密测量	周巧根
77	硕士	侯祯	核技术及应用	熔盐-空气热交换器风冷通道内空气自然循环的流体力学分析	核安全	陈堃
78	硕士	陈涛	信号与信息处理	质子点扫描系统调试测量与分析	质子治疗设备调试	赵明华

79	硕士	董赫	粒子物理与原子核物理	碘化铯晶体测量高能伽马的实验和模拟研究	实验核物理	方德清
80	硕士	郭崇强	粒子物理与原子核物理	高能重离子碰撞直接流的研究	高能重离子碰撞	徐骏
81	硕士	黄山	电子与通信工程	加速器电源电流突变及纹波抑制技术研究	电力电子技术及其自动化	李瑞
82	硕士	赵晶	核能与核技术工程	氟盐冷却高温堆在主要事故工况下对RVACS散热能力的需求	反应堆安全分析	陈堃
83	硕士	张根灿	电子与通信工程	上海质子治疗装置注入器远程控制系统的构建	加速器控制	李德明
84	硕士	陶芬	电子与通信工程	X射线纳米成像椭球镜设计与检测	电子与通信工程	邓彪
85	硕士	石先武	核能与核技术工程	不锈钢表面堆焊纯镍的微观组织及高温时效组织的研究	反应堆材料	李志军
86	硕士	朱帆	核能与核技术工程	氢化锆慢化熔盐堆中子学性能研究	钍铀燃料循环物理	陈金根
87	硕士	梁兆峰	核能与核技术工程	低维薄膜材料的第一性原理研究	低维薄膜材料的第一性原理计算	宋飞
88	硕士	刘磊	光学工程	显微镜的多功能改造及其生物成像中的应用	超分辨技术	宋世平
89	硕士	赵玉平	光学工程	基于单模光纤光源的大口径细光束自准直技术的研究	光学元件加工与检测	王劼
90	硕士	刘佳煜	核能与核技术工程	固体聚合物氚电解浓缩系统的性能研究	氚科学与工程	刘卫
91	硕士	缪洪康	核能与核技术工程	熔盐-熔盐板(翅)式换热器数值模拟研究	反应堆热工水力	王纳秀

附录 2

2017-2018 年论文发表一览表

Papers Published in 2017-2018

2017

	论文名称	期刊名称	期	卷	页	作者
1	Development and Use of an Open-Source, User-Friendly Package To Simulate Voltammetry Experiments	JOURNAL OF CHEMICAL EDUCATION	94	10	1567	Wang, Shuo; Wang, Jing; Gao, Yanjing
2	Elliptic flow of electrons from heavy-flavor hadron decays in Au plus Au collisions at root s(NN)=200, 62.4, and 39 GeV	PHYSICAL REVIEW C	95	3	34907	Adamczyk, L.; Adkins, J. K.; Agakishiev, G.
3	Compact beam transport system for free-electron lasers driven by a laser plasma accelerator	PHYSICAL REVIEW ACCELERATORS AND BEAMS	20	2	20701	Liu, Tao; Zhang, Tong; Wang, Dong
4	Parameter optimization and start-to-end simulation for the phase-merging enhanced harmonic generation free electron laser	NUCLEAR INSTRUMENTS & METHODS IN PHYSICS RESEARCH SECTION A-ACCELERATORS SPECTROMETERS DETECTORS AND ASSOCIATED EQUIPMENT	875		119	Qi, Zheng; Feng, Chao; Deng, Haixiao
5	Precise magnetic field control of the scanning magnets for the APTRON beam delivery system	NUCLEAR SCIENCE AND TECHNIQUES	28	12	172	Miao, Chun-Hui; Liu, Ming; Yin, Chong-Xian
6	Gain cascading scheme of a free-electron-laser oscillator	PHYSICAL REVIEW ACCELERATORS AND BEAMS	20	11	110703	Li, Kai; Deng, Haixiao;
7	Design of a nondestructive two-in-one instrument for measuring the polarization and energy spectrum at an X-ray FEL facility	JOURNAL OF INSTRUMENTATION	12		T10003	Zhang, Qingmin; Deng, Bangjie; Chen, Yuanmiaoliang
8	A new consecutive energy calibration method for X/gamma detectors based on energy continuously tunable laser Compton scattering light source	NUCLEAR SCIENCE AND TECHNIQUES	28	9	121	Xu, Hang-Hua; Wu, Hai-Long; Fan, Gong-Tao
9	RF design of a C-band compact spherical RF pulse compressor for SXFEL	NUCLEAR INSTRUMENTS & METHODS IN PHYSICS RESEARCH SECTION A-ACCELERATORS SPECTROMETERS	863		7	Li, Zongbin; Fang, Wencheng; Gu, Qiang

		DETECTORS AND ASSOCIATED EQUIPMENT				
10	Improving Touschek lifetime and synchrotron frequency spread by passive harmonic cavity in the storage ring of SSRF	NUCLEAR SCIENCE AND TECHNIQUES	28	8	108	Phimsen, Thanapong; Jiang, Bo-Cheng; Hou, Hong-Tao
11	Two-stage EEHG for coherent hard X-ray generation based on a superconducting linac	NUCLEAR SCIENCE AND TECHNIQUES	28	8	117	Zhao, Zhen-Tang; Feng, Chao; Zhang, Kai-Qing
12	Using a Bessel light beam as an ultrashort period helical undulator	PHYSICAL REVIEW ACCELERATORS AND BEAMS	20	7	70701	Jiang, B. C.; Zhang, Q. L.; Chen, J. H.
13	A Storage Ring Based Free-Electron Laser for Generating Ultrashort Coherent EUV and X-ray Radiation	SCIENTIFIC REPORTS	7		4724	Feng, Chao; Zhao, Zhentang;
14	Wakefields studies for the SXFEL user facility	NUCLEAR SCIENCE AND TECHNIQUES	28	7	90	Song, Ming-Hao; Feng, Chao; Huang, Da-Zhang
15	Status of the SXFEL Facility	APPLIED SCIENCES-BASEL	7	6	607	Zhao, Zhentang; Wang, Dong; Gu, Qiang
16	The front-end electronics design of dose monitors for beam delivery system of Shanghai Advanced Proton Therapy Facility	NUCLEAR SCIENCE AND TECHNIQUES	28	6	83	Zhao, Bin-Qing; Zhao, Ming-Hua; Liu, Ming
17	Extending the photon energy coverage of an x-ray self-seeding FEL via the reverse taper enhanced harmonic generation technique	NUCLEAR INSTRUMENTS & METHODS IN PHYSICS RESEARCH SECTION A-ACCELERATORS SPECTROMETERS DETECTORS AND ASSOCIATED EQUIPMENT	854		3	Zhang, Kaiqing; Qi, Zheng; Feng, Chao
18	Design of an X-band accelerating structure using a newly developed structural optimization procedure	NUCLEAR INSTRUMENTS & METHODS IN PHYSICS RESEARCH SECTION A-ACCELERATORS SPECTROMETERS DETECTORS AND ASSOCIATED EQUIPMENT	854		45	Huang, Xiaoxia; Fang, Wencheng; Gu, Qiang
19	Simplified model for fast optimization of a free-electron laser oscillator	PHYSICAL REVIEW ACCELERATORS AND BEAMS	20	3	30702	Li, Kai; Song, Minghao; Deng, Haixiao

20	Generation of double pulses at the Shanghai soft X-ray free electron laser facility	NUCLEAR SCIENCE AND TECHNIQUES	28	3	28	Wang, Zhen; Feng, Chao; Gu, Qiang
21	Generating high-brightness and coherent soft x-ray pulses in the water window with a seeded free-electron laser	PHYSICAL REVIEW ACCELERATORS AND BEAMS	20	1	10702	Zhou, Kaishang; Feng, Chao; Deng, Haixiao
22	Chromatic effect in a novel THz generation scheme	NEW JOURNAL OF PHYSICS	19		113025	Li, Bin; Zhang, Wenyan; Liu, Xiaoqing
23	Vacancy-assisted oxygen reduction reaction on cobalt-based catalysts in direct borohydride fuel cell revealed by in-situ XAFS and XRD	ELECTROCHIMICA ACTA	254		72	Wang, Juan; Lin, Longxia; He, Yan
24	Speckle-tracking X-ray phase-contrast imaging for samples with obvious edge-enhancement effect	APPLIED PHYSICS LETTERS	111	17	174101	Wang, Feixiang; Wang, Yudan; Wei, Gongxiang
25	Characterization of heat treatment-induced pore structure changes in cold-sprayed titanium	MATERIALS CHARACTERIZATION	132		69	Ren, Y. Q.; King, P. C.; Yang, Y. S.
26	Temperature-dependent thermal properties of Ru/C multilayers	JOURNAL OF SYNCHROTRON RADIATION	24		975	Yan, Shuai; Jiang, Hui; Wang, Hua
27	Single bounce ellipsoidal glass monocapillary condenser for X-ray nano-imaging	OPTICS COMMUNICATIONS	398		91	Jiang, Bowen; Liu, Zhiguo; Sun, Xuepeng
28	Comparative study of the low-lying valence electronic states of carbon dioxide by high-resolution inelastic x-ray and electron scattering	PHYSICAL REVIEW A	96	1	12518	Ni, Dong-Dong; Xu, Long-Quan; Liu, Ya-Wei
29	Identification of ginseng root using quantitative X-ray microtomography	JOURNAL OF GINSENG RESEARCH	41	3	290	Ye, Linlin; Xue, Yanling; Wang, Yudan
30	3D investigation on polystyrene colloidal crystals by floatage self-assembly with mixed solvent via synchrotron radiation x-ray phase-contrast computed tomography	RADIATION PHYSICS AND CHEMISTRY	135		49	Fu, Yanan; Xie, Honglan; Deng, Biao
31	Scan system for arbitrary-shaped samples at the synchrotron radiation facility	NUCLEAR SCIENCE AND TECHNIQUES	28	5	60	Lan, Xu-Ying; Liang, Dong-Xu; Mao, Cheng-Wen
32	Compensation for gravitational sag of bent mirror	NUCLEAR INSTRUMENTS & METHODS IN PHYSICS RESEARCH SECTION	853		20	Mao, Chengwen; Jiang, Hui; He, Yan

		A-ACCELERATORS SPECTROMETERS DETECTORS AND ASSOCIATED EQUIPMENT				
33	Non-destructive identification of unknown minor phases in polycrystalline bulk alloys using three-dimensional X-ray diffraction	MATERIALS CHARACTERIZATION	124		206	Yang, Yiming; Xu, Liang; Wang, Yudan
34	Development of high-performance cathode catalyst of polypyrrole modified carbon supported CoOOH for direct borohydride fuel cell	JOURNAL OF POWER SOURCES	339		13	He, Yan; Zhu, Cai; Chen, Kaijian
35	Current Status of the Hard X-ray Nanoprobe Beamline at the SSRF	X-RAY NANOIMAGING: INSTRUMENTS AND METHODS III	10389		UNSP 103890J	Li, Aiguo; Jiang, Hui; Wang, Hua
36	X-ray multilayer mid-frequency characterizations using speckle scanning techniques	ADVANCES IN METROLOGY FOR X-RAY AND EUV OPTICS VII	10385		UNSP 103850Q	Jiang, Hui; Yan, Shuai; Liang, Dongxu
37	LOW DOSE AND IN-VIVO IMAGING SYSTEM BASED ON EQUALLY SLOPED TOMOGRAPHY	2017 IEEE 14TH INTERNATIONAL SYMPOSIUM ON BIOMEDICAL IMAGING (ISBI 2017)			60	Zhou, Guangzhao; Du, Guohao; Wang, Yudan
38	Monochromatic-beam-based dynamic X-ray microtomography based on OSEM-TV algorithm	JOURNAL OF X-RAY SCIENCE AND TECHNOLOGY	25	6	1007	Xu, Liang; Chen, Rongchang; Yang, Yiming
39	Surface States in Ternary CdSSe Quantum Dot Solar Cells	JOURNAL OF NANOSCIENCE AND NANOTECHNOLOGY	17	2	1373	Chen, Zhenhua; Li, Hui; Zhang, Xiangzhi
40	Fabrication of large-area high-aspect-ratio periodic nanostructures on various substrates by soft X-ray interference lithography	APPLIED SURFACE SCIENCE	425		553	Xue, Chaofan; Zhao, Jun; Wu, Yanqing
41	Interfacial nanobubbles produced by long-time preserved cold water	CHINESE PHYSICS B	26	10	106803	Zhou, Li-Min; Wang, Shuo; Qiu, Jie
42	Robust phase-retrieval-based X-ray tomography for morphological assessment of early hepatic echinococcosis infection in rats	PLOS ONE	12	9	e0183396	Liu, Huiqiang; Zhang, Chuanshan; Fan, Xiaoxi
43	Mutual optical intensity propagation through non-ideal mirrors	JOURNAL OF SYNCHROTRON RADIATION	24		954	Meng, Xiangyu; Shi, Xianbo; Wang, Yong
44	Monte Carlo simulation on a new artificial spin ice lattice consisting of hexagons and	AIP ADVANCES	7	8	85211	Yu, Liju; Wang, Yong; Li, Junqin

	three-moment vertices					
45	Independent control of the vortex chirality and polarity in a pair of magnetic nanodots	JOURNAL OF MAGNETISM AND MAGNETIC MATERIALS	435		167	Li, Junqin; Wang, Yong; Cao, Jiefeng
46	Electronic structure of SrSn2As2 near the topological critical point	SCIENTIFIC REPORTS	7		6133	Rong, L. -Y.; Ma, J. -Z.; Nie, S. -M.
47	Effects of temperature, mechanical motion and source positional jitter on the resolving power of beamline 02B at the SSRF	JOURNAL OF SYNCHROTRON RADIATION	24		877	Guo, Zhi; Meng, Xiangyu; Wang, Yong
48	Soft X-ray ptychography method at SSRF	NUCLEAR SCIENCE AND TECHNIQUES	28	6	74	Wang, Chun-Peng; Xu, Zi-Jian; Liu, Hai-Gang
49	Background noise removal in x-ray ptychography	APPLIED OPTICS	56	8	2099	Wang, Chunpeng; Xu, Zijian; Liu, Haigang
50	Influence of symmetry and duty cycles on the pattern generation in achromatic Talbot lithography	JOURNAL OF VACUUM SCIENCE & TECHNOLOGY B	35	2	21601	Yang, Shumin; Zhao, Jun; Wang, Liansheng
51	Fabrication of high aspect ratio nanoscale periodic structures by the soft X-ray interference lithography	MICROELECTRONIC ENGINEERING	170		49	Zhao, Jun; Wu, Yanqing; Xue, Chaofan
52	High sensitivity and homogeneity of surface enhanced Raman scattering on three-dimensional array-film hybrid platform	APPLIED PHYSICS LETTERS	110	8	81605	Liu, Xing; Yu, Liju; Yang, Shumin
53	Formation of surface nanobubbles on nanostructured substrates	NANOSCALE	9	3	1078	Wang, Lei; Wang, Xingya; Wang, Liansheng
54	Interfacial gas nanobubbles or oil nanodroplets?	PHYSICAL CHEMISTRY CHEMICAL PHYSICS	19	2	1108	Wang, Xingya; Zhao, Binyu; Hu, Jun
55	Low-dose, high-resolution and high-efficiency ptychography at STXM beamline of SSRF	X-RAY MICROSCOPY CONFERENCE 2016 (XRM 2016)	849		12033	Xu, Zijian; Wang, Chunpeng; Liu, Haigang
56	Real-Time Imaging of Single-Molecule Enzyme Cascade Using a DNA Origami Raft	JOURNAL OF THE AMERICAN CHEMICAL SOCIETY	139	48	17525	Sun, Lele; Gao, Yanjing; Xu, Yan
57	PCR-Free Colorimetric DNA Hybridization Detection Using a 3D DNA	ACS APPLIED MATERIALS & INTERFACES	9	44	38281	Yang, Xue; Wen, Yanli; Wang,

	Nanostructured Reporter Probe					Lele
58	Organelle-Specific Triggered Release of Immunostimulatory Oligonucleotides from Intrinsically Coordinated DNA-Metal-Organic Frameworks with Soluble Exoskeleton	JOURNAL OF THE AMERICAN CHEMICAL SOCIETY	139	44	15784	Wang, Zejun; Fu, Yao; Kang, Zhengzhong
59	Enzyme-Triggered Fluorescence Turn-on: A Probe for Specifically Imaging Ovarian-Cancer-Related gamma-Glutamyltranspeptidase	CHINESE JOURNAL OF CHEMISTRY	35	11	1711	Tian, Jie; Yan, Qinglong; Zhu, Ying
60	Computation in Chemistry: A Summary of the Development and Models of DNA Computing	PROGRESS IN CHEMISTRY	29	11	1297	Yin, Xiaoyao; Li, Fei; Bo, Xiaochen
61	Evolution of grain boundary carbides in thermal exposed Ti-modified alloy N	MATERIALS CHARACTERIZATION	133		54	Shen, Lin; Jiang, Li; Liu, Renduo
62	Engineering nucleic acid structures for programmable molecular circuitry and intracellular biocomputation	NATURE CHEMISTRY	9	11	1056	Li, Jiang; Green, Alexander A.; Yan, Hao
63	Recognizing single phospholipid vesicle collisions on carbon fiber nanoelectrode	SCIENCE CHINA-CHEMISTRY	60	11	1474	Zhang, Yueyue; Li, Min; Li, Zhenhua
64	Special topic for "single-molecule, single-particle and single-cell bioimaging"	SCIENCE CHINA-CHEMISTRY	60	10	1265	Fan, Chunhai; Fang, Xiaohong;
65	Sub-diffraction-limit cell imaging using a super-resolution microscope with simplified pulse synchronization	SCIENCE CHINA-CHEMISTRY	60	10	1305	Gao, Zhaoshuai; Deng, Suhui; Li, Jiang
66	Assembling and Powering Up Nanostructures!	CHEMNANOMAT	3	10	668	Nam, Jwa-Min; Fan, Chunhai; Gianneschi, Nathan
67	A Gold-Nanoparticle-Based SERS Reporter that Rolls on DNA Origami Templates	CHEMNANOMAT	3	10	760	Liu, Bing; Ren, Shaokang; Xing, Yikang
68	Humidity-Responsive Single-Nanoparticle-Layer Plasmonic Films	ADVANCED MATERIALS	29	35	1606796	Shen, Jianlei; Luan, Binquan; Pei, Hao
69	Multifunctional Yolk-Shell Nanostructure as a Superquencher for Fluorescent Analysis of Potassium Ion Using Guanine-Rich Oligonucleotides	ACS APPLIED MATERIALS & INTERFACES	9	36	30406	Lu, Na; Wen, Yanli; Liu, Gang
70	DNA Hydrogel with Aptamer-Toehold-Based Recognition, Cloaking, and Decloaking of Circulating Tumor Cells for Live Cell Analysis	NANO LETTERS	17	9	5193	Song, Ping; Ye, Dekai; Zuo, Xiaolei

71	Sequence-dependent interactions between model peptides and lipid bilayers	NUCLEAR SCIENCE AND TECHNIQUES	28	9	124	Lei, Hao-Zhi; Tian, Tian; Du, Qiqige
72	Dual-mode electrochemical analysis of microRNA-21 using gold nanoparticle-decorated MoS2 nanosheet	BIOSENSORS & BIOELECTRONICS	94		552	Su, Shao; Cao, Wenfang; Liu, Wei
73	Nuclease-free target recycling signal amplification for ultrasensitive multiplexing DNA biosensing	BIOSENSORS & BIOELECTRONICS	94		605	Zhao, Zhihan; Chen, Shixing; Wang, Jianbang
74	Enzymatic O-GlcNAcylation of alpha-synuclein reduces aggregation and increases SDS-resistant soluble oligomers	NEUROSCIENCE LETTERS	655		90	Zhang, Jiaming; Lei, Haozhi; Chen, Yubei
75	Programming Cell Adhesion for On-Chip Sequential Boolean Logic Functions	JOURNAL OF THE AMERICAN CHEMICAL SOCIETY	139	30	10176	Qu, Xiangmeng; Wang, Shaopeng; Ge, Zhilei
76	Synchrotron-based X-ray microscopy for sub-100 nm resolution cell imaging	CURRENT OPINION IN CHEMICAL BIOLOGY	39		11	Zhu, Ying; Zhang, Jichao; Li, Aiguo
77	In situ TEM studies of the shape evolution of Pd nanocrystals under oxygen and hydrogen environments at atmospheric pressure	CHEMICAL COMMUNICATIONS	53	99	13213	Zhang, Xun; Meng, Jun; Zhu, Beien
78	Effect of pH on the Stability of DNA Origami	ACTA POLYMERICA SINICA		12	1993	Fang, Wei-na; Fan, Chun-hai; Liu, Hua-jie
79	Application Progress of DNA Nanostructures in Drug Delivery and Smart Drug Carriers	CHINESE JOURNAL OF ANALYTICAL CHEMISTRY	45	7	1078	Zhao Yan; Guo Lin-Jie; Dai Jiang-Bing
80	Real-Time Imaging of Endocytosis and Intracellular Trafficking of Semiconducting Polymer Dots	ACS APPLIED MATERIALS & INTERFACES	9	25	21200	Han, Yuping; Li, Xiaoming; Chen, Haobin
81	Preservation of DNA Nanostructure Carriers: Effects of Freeze - Thawing and Ionic Strength during Lyophilization and Storage	ACS APPLIED MATERIALS & INTERFACES	9	22	18434	Zhu, Bing; Zhao, Yan; Dai, Jiangbing
82	Nanodiamonds Mediate Oral Delivery of Proteins for Stem Cell Activation and Intestinal Remodeling in Drosophila	ACS APPLIED MATERIALS & INTERFACES	9	22	18575	Hu, Xingjie; Li, Xiaojiao; Yin, Min
83	Size-Dependent Regulation of Intracellular Trafficking of Polystyrene Nanoparticle-Based Drug-Delivery Systems	ACS APPLIED MATERIALS & INTERFACES	9	22	18619	Wang, Ting; Wang, Lu; Li, Xiaoming
84	Study on physisorption between G-actin	LUMINESCENCE	32	4	618	Du, Qiqige; Li,

	and amphiphilic polymer-coated gold nanoparticles					Wanrong; Yuan, Ming
85	Real-time visualization of clustering and intracellular transport of gold nanoparticles by correlative imaging	NATURE COMMUNICATIONS	8		15646	Liu, Mengmeng; Li, Qian; Liang, Le
86	Graphene Nanoprobes for Real-Time Monitoring of Isothermal Nucleic Acid Amplification	ACS APPLIED MATERIALS & INTERFACES	9	18	15245	Li, Fan; Liu, Xiaoguo; Zhao, Bin
87	Carbides Evolution in a Ni-16Mo-7Cr Base Superalloy during Long-Term Thermal Exposure	MATERIALS	10	5	521	Han, Fenfen; Jiang, Li; Ye, Xiangxi
88	Synthesis and Applications of Triangular Gold Nanoplates	PROGRESS IN CHEMISTRY	29	5	459	Fang, Weina; Lu, Shuang; Wang, Lihua
89	Precisely Tailored DNA Nanostructures and their Theranostic Applications	CHEMICAL RECORD	17	12	1213	Zhu, Bing; Wang, Lihua; Li, Jiang
90	The Inhibition Effect of Graphene Oxide Nanosheets on the Development of Streptococcus mutans Biofilms	PARTICLE & PARTICLE SYSTEMS CHARACTERIZATION	34	5	1700001	He, Jianliang; Zhu, Xiaodan; Qi, Zhengnan
91	EDXRF and XAFS Analysis on the White Porcelains of Ding Kiln of Successive Dynasties	SPECTROSCOPY AND SPECTRAL ANALYSIS	37	5	1542	Zhang Mao-lin; Wang Li-hua; Li Qi-jiang
92	Yolk-shell nanostructured Fe3O4@C magnetic nanoparticles with enhanced peroxidase-like activity for label-free colorimetric detection of H2O2 and glucose	NANOSCALE	9	13	4508	Lu, Na; Zhang, Min; Ding, Lei
93	Discrimination of foodborne pathogenic bacteria using synchrotron FTIR microspectroscopy	NUCLEAR SCIENCE AND TECHNIQUES	28	4	49	Wang, Ya-Di; Li, Xue-Ling; Liu, Zhi-Xiao
94	The effect of aluminum ion on the aggregation of human islet amyloid polypeptide (11-28)	ACTA BIOCHIMICA ET BIOPHYSICA SINICA	49	4	355	Su, Lanlan; Lu, Cheng; Yan, Peng
95	Construction of DNA-based logic gates on nanostructured microelectrodes	NUCLEAR SCIENCE AND TECHNIQUES	28	3	35	Wei, Tao; Li, Min; Zhang, Yue-Yue
96	Multicolor Gold Silver Nano-Mushrooms as Ready-to-Use SERS Probes for Ultrasensitive and Multiplex DNA/miRNA Detection	ANALYTICAL CHEMISTRY	89	4	2531	Su, Jing; Wang, Dongfang; Noerbel, Lena
97	Clamped Hybridization Chain Reactions for the Self-Assembly of Patterned DNA Hydrogels	ANGEWANDTE CHEMIE-INTERNATIONAL EDITION	56	8	2171	Wang, Jianbang; Chao, Jie; Liu, Huajie

98	An Exonuclease III-Powered, On-Particle Stochastic DNA Walker	ANGEWANDTE CHEMIE-INTERNATIONAL EDITION	56	7	1855	Qu, Xiangmeng; Zhu, Dan; Yao, Guangbao
99	Catalysis-Driven Self-Thermophoresis of Janus Plasmonic Nanomotors	ANGEWANDTE CHEMIE-INTERNATIONAL EDITION	56	2	515	Qin, Weiwei; Peng, Tianhuan; Gao, Yanjing
100	Nanoplasmonic Biological Sensing and Imaging	ACTA CHIMICA SINICA	75	11	1036	Su Yingying; Peng Tianhuan; Xing Feifei
101	Self-Assembly of Amyloid-Like Peptides at Interfaces Investigated by Atomic Force Microscopy	SCIENCE OF ADVANCED MATERIALS	9	1	65	Lei, Haozhi; Zhang, Xueqiang; Hu, Jun
102	DNA Nanostructure-Based Engineering of the Biosensing Interface for Biomolecular Detection	PROGRESS IN CHEMISTRY	29	1	36	Ye, Dekai; Zuo, Xiaolei; Fan, Chunhai
103	BIOSENSING CRISPR-powered diagnostics	NATURE BIOMEDICAL ENGINEERING	1	6	UNSP 0091	Zuo, Xiaolei; Fan, Chunhai; Chen, Hong-Yuan
104	Nanodiamonds Interfere with Wnt-Regulated Cell Migration and Adipocyte Differentiation in Cells and Embryonic Development In Vivo	PARTICLE & PARTICLE SYSTEMS CHARACTERIZATION	34	1	1600208	Yi, Hongyang; Li, Xiaojiao; Wang, Zhuyao
105	Programming Cell Adhesion for On-Chip Sequential Boolean Logic Functions	JOURNAL OF THE AMERICAN CHEMICAL SOCIETY	139	30	10176	Qu, Xiangmeng; Wang, Shaopeng; Ge, Zhilei
106	Expression and radiolabeling of Cas9 protein	NUCLEAR SCIENCE AND TECHNIQUES	28	1	11	Yan, Qing-Long; Kong, Hua-Ting; Xia, Kai
107	Silicone oil promotes amyloid-like aggregation of alpha B-crystallin	RSC ADVANCES	7	10	6000	Shen, Zhiwei; Du, Qiqige; Lei, Haozhi
108	Autophagy and lysosomal dysfunction: A new insight into mechanism of synergistic pulmonary toxicity of carbon black-metal ions co-exposure	CARBON	111		322	Kong, Huating; Xia, Kai; Pan, Liang
109	pH and thermal-dependent ultrafiltration membranes prepared from poly (methacrylic acid) grafted onto polyethersulfone synthesized by simultaneous irradiation in homogenous phase	JOURNAL OF MEMBRANE SCIENCE	543		335	Fan, Kai; Huang, Jianxi; Yang, Haijun

110	An infrared spectroscopy study of PES PVP blend and PES-g-PVP copolymer	POLYMER TESTING	59		212	Huang, Jianxi; Yang, Haijun; Chen, Min
111	Magic compositions in Pd-Au nanoalloys	COMPUTATIONAL AND THEORETICAL CHEMISTRY	1107		49	Zhu, Beien; Front, Alexis; Guesmi, Hazar
112	S-shaped velocity deformation induced by ionic hydration in aqueous salt solution flow	PHYSICAL CHEMISTRY CHEMICAL PHYSICS	19	44	30055	Fan, Wen; Chen, Jige; Lei, Xiaoling
113	Reply to 'On the bonding in ligand-protected gold clusters'	NATURE COMMUNICATIONS	8		1351	Xu, Wen Wu; Zeng, Xiao Cheng; Gao, Yi
114	Graphene Oxide Facilitates Solvent-Free Synthesis of Well-Dispersed, Faceted Zeolite Crystals	ANGEWANDTE CHEMIE-INTERNATIONAL EDITION	56	45	14090	Li, Hui; Liu, Xing; Qi, Siqi
115	Ultra-Broadband THz Antireflective Coating with Polymer Composites	POLYMERS	9	11	574	Cai, Bin; Chen, Haitao; Xu, Gongjie
116	Ion sieving in graphene oxide membranes via cationic control of interlayer spacing	NATURE	550	7676		Chen, Liang; Shi, Guosheng; Shen, Jie
117	Preparation of graphene oxides with different sheet sizes by temperature control	CHINESE PHYSICS B	26	10	106101	Qian, Zhe; Chen, Liang; Li, De-Yuan
118	Dynamic Cooperation of Hydrogen Binding and pi Stacking in ssDNA Adsorption on Graphene Oxide	CHEMISTRY-A EUROPEAN JOURNAL	23	53	13100	Xu, Zhen; Lei, Xiaoling; Tu, Yusong
119	Inert Gas Deactivates Protein Activity by Aggregation	SCIENTIFIC REPORTS	7		10176	Zhang, Lijuan; Zhang, Yuebin; Cheng, Jie
120	Catalytic role of vacancy diffusion in ceria supported atomic gold catalyst	CHEMICAL COMMUNICATIONS	53	65	9125	Han, Zhong-Kang; Wang, Yang-Gang; Gao, Yi
121	Defect-Induced Wetting Behavior on Solid Polar Surfaces with Small Charge Dipole Length	JOURNAL OF PHYSICAL CHEMISTRY C	121	32	17365	Qiu, Yifei; Liu, Yang; Tu, Yusong
122	Ti12Xe: A twelve-coordinated Xe-containing molecule	PHYSICS LETTERS A	381	29	2363	Miao, Junjian; Xu, Wenwu; Zhu, Beien
123	Au-3(mu(3)-S)(0e) elementary block: new insights into ligated gold clusters with mu(3)-sulfido motifs	NANOSCALE	9	26	8990	Xu, Wen Wu; Zeng, Xiao Cheng; Gao, Yi

124	Terahertz Spectra of Ninhydrin and Indane-1,2,3-Trione	JOURNAL OF INFRARED MILLIMETER AND TERAHERTZ WAVES	38	7	896	Zou, Tao; Li, Shaoping; Pan, Tingting
125	Formation and Stability of Bulk Nanobubbles Generated by Ethanol-Water Exchange	CHEMPHYSCHEM	18	10	1345	Qiu, Jie; Zou, Zhenglei; Wang, Shuo
126	Terahertz spectra of L-phenylalanine and its monohydrate	SPECTROCHIMICA ACTA PART A-MOLECULAR AND BIOMOLECULAR SPECTROSCOPY	178		19	Pan, Tingting; Li, Shaoping; Zou, Tao
127	Au-13(8e): A secondary block for describing a special group of liganded gold clusters containing icosahedral Au-13 motifs	CHEMICAL PHYSICS LETTERS	675		35	Xu, Wen Wu; Zeng, Xiao Cheng; Gao, Yi
128	Mechanism of degradation of a nitrogenous heterocycle induced by a reductive radical: decomposition of a sym-triazine ring	PHYSICAL CHEMISTRY CHEMICAL PHYSICS	19	14	9354	Lyu, Gengxin; Shi, Guosheng; Tang, Liang
129	Accelerated evaporation of water on graphene oxide	PHYSICAL CHEMISTRY CHEMICAL PHYSICS	19	13	8843	Wan, Rongzheng; Shi, Guosheng;
130	DNA origami-based shape IDs for single-molecule nanomechanical genotyping	NATURE COMMUNICATIONS	8		14738	Zhang, Honglu; Chao, Jie; Pan, Dun
131	Supersonic thermal excitation-induced shock wave in black phosphorene	PHYSICAL REVIEW B	95	13	134301	Chen, Jige; Chen, Shunda; Gao, Yi
132	Asymmetric nanoparticle may go "active" at room temperature	SCIENCE CHINA-PHYSICS MECHANICS & ASTRONOMY	60	4	40511	Sheng, Nan; Tu, YuSong; Guo, Pan
133	Flow effect on I-135 and Xe-135 evolution behavior in a molten salt reactor	NUCLEAR ENGINEERING AND DESIGN	314		318	Wu, Jianhui; Guo, Chen; Cai, Xiangzhou
134	Equilibrium Shape of Metal Nanoparticles under Reactive Gas Conditions	JOURNAL OF PHYSICAL CHEMISTRY C	121	10	5629	Zhu, Beien; Meng, Jun; Gao, Yi
135	A nonmonotonic dependence of the contact angles on the surface polarity for a model solid surface	PHYSICAL CHEMISTRY CHEMICAL PHYSICS	19	9	6665	Qi, Chonghai; Zhou, Bo; Wang, Chunlei
136	Design of High-Performance Pd-Based Alloy Nanocatalysts for Direct Synthesis of H2O2	ACS CATALYSIS	7	3	2164	Xu, Haoxiang; Cheng, Daojian; Gao, Yi
137	Water flow in carbon-based nanoporous membranes impacted by interactions	NANOTECHNOLOGY	28	8	84004	Liu, Jian; Shi, Guosheng; Fang,

	between hydrated ions and aromatic rings					Haiping
138	Graphene Oxide Restricts Growth and Recrystallization of Ice Crystals	ANGEWANDTE CHEMIE-INTERNATIONAL EDITION	56	4	997	Geng, Hongya; Liu, Xing; Shi, Guosheng
139	The switch of the binding behaviours between Xe and pi system induced by the change of oxidation state of Cu	MOLECULAR SIMULATION	43	13-16	1256	Miao, Junjian; Gao, Yi;
140	Effect of water molecules on nanoscale wetting behaviour of molecular ethanol on hydroxylated SiO2 substrate	MOLECULAR SIMULATION	43	13-16	1377	Nie, Xuechuan; Chen, Jige; Sheng, Nan
141	Minor actinide incineration and Th-U breeding in a small FLiNaK Molten Salt Fast Reactor	ANNALS OF NUCLEAR ENERGY	99		335	Yu, Chenggang; Li, Xiaoxiao; Cai, Xiangzhou
142	FEA-based structural optimization design of a side cooling collimating mirror at SSRF	NUCLEAR SCIENCE AND TECHNIQUES	28	11	159	Jin, Li-Min; Wang, Na-Xiu; Zhu, Wan-Qian
143	Cleaning of carbon-contaminated optics using O-2/Ar plasma	NUCLEAR SCIENCE AND TECHNIQUES	28	9	127	Zhang, Yi-Fei; Luo, Hong-Xin; Guo, Zhi
144	Normal tracing deflectometry using a secondary light source	JOURNAL OF SYNCHROTRON RADIATION	24		765	Peng, Chuanqian; He, Yumei; Wang, Jie
145	Measurement of the spatial coherence of hard synchrotron radiation using a pencil beam	CHINESE OPTICS LETTERS	15	3	33401	Hua, Wenqiang; Zhou, Guangzhao; Wang, Yuzhu
146	Injection transient study using a two-frequency bunch length measurement system at the SSRF	NUCLEAR SCIENCE AND TECHNIQUES	28	7	93	Duan, Li-Wu; Leng, Yong-Bin; Yuan, Ren-Xian
147	Beam test results of high Q CBPM prototype for SXFEL	NUCLEAR SCIENCE AND TECHNIQUES	28	4	51	Chen, Jian; Leng, Yong-Bin; Yu, Lu-Yang
148	In vitro anticoagulant activity of polyanionic graft chains modified poly(vinyl alcohol) particles	RADIATION PHYSICS AND CHEMISTRY	134		27	Li, Rong; Wu, Guozhong; Cai, Ximing
149	Microstructure variations induced by excess PbX2 or AX within perovskite thin films	CHEMICAL COMMUNICATIONS	53	96	12966	Zheng, Guanhaojie; Zhu, Cheng; Chen, Yihua
150	The crystal structure of Pyrococcus furiosus RecJ implicates it as an ancestor of eukaryotic Cdc45	NUCLEIC ACIDS RESEARCH	45	21	12551	Li, Min-Jun; Yi, Gang-Shun; Yu, Feng
151	Detailed structure of a new bioactive glass	JOURNAL OF	475		10	Li, Ailing; Ren,

	composition for the design of bone repair materials	NON-CRYSTALLINE SOLIDS				Huihui; Cui, Yang
152	Facile Construction of Novel 3-Dimensional Graphene/Amorphous Porous Carbon Hybrids with Enhanced Lithium Storage Properties	ACS APPLIED MATERIALS & INTERFACES	9	40	35191	Zhu, Daming; Liu, Huaqiu; Tai, Lixuan
153	Discovery of a novel small inhibitor RJ19 targeting to human Hsp90	NUCLEAR SCIENCE AND TECHNIQUES	28	10	148	Cao, Hui-Ling; Lyu, Kai-Kai; Liu, Bin
154	In Situ Observation of Thermal Proton Transport through Graphene Layers	ACS NANO	11	9	8970	Zhu, Daming; Liu, Xing; Gao, Yi
155	Enhanced Crystalline Phase Purity of CH3NH3PbI3-XClX Film for High-Efficiency Hysteresis-Free Perovskite Solar Cells	ACS APPLIED MATERIALS & INTERFACES	9	27	23141	Yaug, Yingguo; Feng, Shanglei; Xu, Weidong
156	Mini-beam modes on standard MX beamline BL17U at SSRF	REVIEW OF SCIENTIFIC INSTRUMENTS	88	7	73301	Wang, Qisheng; Yu, Feng; Cui, Ying
157	Atomic pair distribution function method development at the Shanghai Synchrotron Radiation Facility	CHINESE PHYSICS B	26	7	76101	Zhou, Xiao-Juan; Tao, Ju-Zhou; Guo, Han
158	Novel phenomenon of magnetism and superconductivity in Fe-doped superconductor Bi4-xFexO4S3 (0 <= x <= 0.1)	APPLIED PHYSICS A-MATERIALS SCIENCE & PROCESSING	123	6	427	Li, Qing; Wang, Difei; Feng, Zhenjie
159	Annealing Induced Re-crystallization in CH3NH3PbI3-xClx for High Performance Perovskite Solar Cells	SCIENTIFIC REPORTS	7		46724	Yang, Yingguo; Feng, Shanglei; Li, Meng
160	Facile synthesis the nitrogen and sulfur co-doped carbon dots for selective fluorescence detection of heavy metal ions	MATERIALS LETTERS	193		236	Pang, Yuqian; Gao, Hui; Wu, Shaohui
161	Dehydration behaviour and structural evolution of graphene oxide membranes on silicon substrate	CARBON	114		23	Wang, Rui; Gao, Hui; Zhu, Daming
162	Microwave Hydrothermal Synthesis of Terbium Ions Complexed with Porous Graphene for Effective Absorbent for Organic Dye	NANOSCALE RESEARCH LETTERS	12		204	Chen, Keqin; Gao, Hui; Bai, Bowei
163	Origin of Magnetism in Hydrothermally Aged 2-Line Ferrihydrite Suspensions	ENVIRONMENTAL SCIENCE & TECHNOLOGY	51	5	2643	Cao, Liang; Jiang, Zhao-Xia; Du, Yong-Hua
164	Interfacial electronic structures revealed at the rubrene/CH3NH3PbI3 interface	PHYSICAL CHEMISTRY CHEMICAL PHYSICS	19	9	6546	Ji, Gengwu; Zheng,

						Guanhaojie; Zhao, Bin
165	Local structural characteristics of Sb2Te3 films studied by reverse Monte Carlo modeling	NUCLEAR SCIENCE AND TECHNIQUES	28	3	38	Zhang, Ling; Song, San-Nian; Lin, He
166	The structure of filled skutterudites and the local vibration behavior of the filling atom	PHYSICA B-CONDENSED MATTER	507		131	Zhou, Xiaojuan; Zong, Peng-an; Chen, Xihong
167	The Evidence of Giant Surface Flexoelectric Field in (111) Oriented BiFeO3 Thin Film	ACS APPLIED MATERIALS & INTERFACES	9	6	5600	Yang, Tieying; Zhang, Xingmin; Chen, Bin
168	The energy level alignment at the CH3NH3PbI3/pentacene interface	APPLIED SURFACE SCIENCE	393		417	Ji, Gengwu; Zhao, Bin; Song, Fei
169	Structural consistency analysis of recombinant and wild-type human serum albumin	JOURNAL OF MOLECULAR STRUCTURE	1127		1	Cao, Hui-Ling; Sun, Li-Hua; Liu, Li
170	Thermal Stable Perovskite Solar Cells Improved by ZnO/Graphene Oxide as Electron Transfer Layers	JOURNAL OF INORGANIC MATERIALS	32	1	96	Jiang Wen-Long; Zhou Wei; Ying Ji-Fei
171	STRESS ANALYSIS AND STRUCTURAL INTEGRITY EVALUATIONS OF PRESSURE VESSEL IN MOLTEN SALT REACTOR	PROCEEDINGS OF THE ASME PRESSURE VESSELS AND PIPING CONFERENCE, 2016, VOL 3			UNSP V003T03 A036	Wang, Xiaoyan; Zhu, Shifeng; Wang, Xiao
172	The critical role of Si doping in enhancing the stability of M6C carbides	JOURNAL OF ALLOYS AND COMPOUNDS	728		917	Jiang, Li; Ye, Xiang-Xi; Wang, Zhi-Qiang
173	Grain boundary engineering for control of tellurium diffusion in GH3535 alloy	JOURNAL OF NUCLEAR MATERIALS	497		76	Fu, Cai-Tao; Wang Yinling; Chu, Xiang-Wei
174	Effect of thermal exposure time on tellurium-induced embrittlement of Ni-16Mo-7Cr-4Fe alloy	NUCLEAR SCIENCE AND TECHNIQUES	28	12	178	Chu, Xiang-Wei; Cheng, Hong-Wei; Fu, Cai-Tao
175	Microstructure and Mechanical Properties of Fiber Laser Welded GH3535 Superalloy	JOURNAL OF MATERIALS SCIENCE & TECHNOLOGY	33	11	1289	Yu, Kun; Jiang, Zhenguo; Li, Chaowen
176	Control rod drop dynamic analysis in the TMSR-SF1 based on numerical simulation and experiment	NUCLEAR ENGINEERING AND DESIGN	322		131	Lin, Zuokang; Zhai, Lifang; Zhu, Lin
177	Characteristics of the laminar convective heat transfer of molten salt in concentric tube	APPLIED THERMAL ENGINEERING	125		995	Chen, Yu-Shuang; Tian, Jian; Sun, Shen-De

178	Preparation and Characterization of Vanadium Carbide Coating on 3Cr13 Steel by Thermal Diffusion Process with Fluoride Salt Bath	RARE METAL MATERIALS AND ENGINEERING	46	7	2028	Zhang Jie; Jiang Li; Xie Deming
179	DEM-CFD simulation of modular PB-FHR core with two-grid method	NUCLEAR SCIENCE AND TECHNIQUES	7		10.1007/s41365-017-0246-3	Liu, Feng-Rui; Chen, Xing-Wei; Li, Zhong
180	Microstructure and local strains in GH3535 alloy heat affected zone and their influence on the mechanical properties	MATERIALS SCIENCE AND ENGINEERING A-STRUCTURAL MATERIALS PROPERTIES MICROSTRUCTURE AND PROCESSING	699		48	Chen, Shuangjian; Tsang, D. K. L.; Jiang, Li
181	Convective heat transfer characteristics in the laminar and transition region of molten salt in concentric tube	APPLIED THERMAL ENGINEERING	117		682	Chen, Y. S.; Zhu, H. H.; Tian, J.
182	Microstructure and mechanical properties of UNS N10003 alloy welded joints	MATERIALS SCIENCE AND ENGINEERING A-STRUCTURAL MATERIALS PROPERTIES MICROSTRUCTURE AND PROCESSING	682		168	Chen, Shuangjian; Ye, Xiang-Xi; Yu, Kun
183	EVALUATION ON MICROSTRUCTURE AND MECHANICAL PROPERTIES OF WELDED JOINTS BY GMAW IN UNS N10003 ALLOY	PROCEEDINGS OF THE ASME PRESSURE VESSELS AND PIPING CONFERENCE, 2017, VOL 6B			UNSP V06BT06A019	Yu, Kun; Jiang, Zhenguo; Shi, Xianwu
184	An insight into the effects of B-site transition metals on the activity, activation effect and stability of perovskite oxygen electrodes for solid oxide electrolysis cells	JOURNAL OF POWER SOURCES	363		470	Bi, Jiaxin; Yang, Shengbing; Zhong, Shaohua
185	Thermodynamic modeling of the Ca(NO3)(2)-MNO3 (M: alkali metal) systems	CALPHAD-COMPUTER COUPLING OF PHASE DIAGRAMS AND THERMOCHEMISTRY	59		90	Li, Xiang; Wang, Kun; Shen, Miao
186	Probing the Influence of Acidity and Temperature to Th(IV) on Hydrolysis, Nucleation, and Structural Topology	INORGANIC CHEMISTRY	56	22	14198	Lin, Jian; Qie, Meiying; Zhang, Linjuan
187	A perspective on hydrogen production via high temperature steam electrolysis	SCIENCE CHINA-CHEMISTRY	60	11	1379	Chen, Xinbing; Guan, Chengzhi; Xiao, Guoping
188	Thermodynamic modeling of the GdF3-MF (M: Li, K, Rb, Cs) systems	FLUID PHASE EQUILIBRIA	449		18	Li, Xiang; Wang, Kun; Xie, Leidong

189	Thermodynamic Description of the MCl2-ThCl4 (M: Mg, Ca, Sr, Ba) Systems	CHEMICAL RESEARCH IN CHINESE UNIVERSITIES	33	5	794	Xie Mengya; Li Xiang; Ding Yaping
190	Investigation on molecular structure of molten Li2BeF4 (FLiBe) salt by infrared absorption spectra and density functional theory (DFT)	JOURNAL OF MOLECULAR LIQUIDS	242		1052	Liu, Shuting; Su, Tao; Cheng, Jinhui
191	Insight into the Role of Metal-Oxygen Bond and O 2p Hole in High-Voltage Cathode LiNixMn2-xO4	JOURNAL OF PHYSICAL CHEMISTRY C	121	30	16079	Liu, Hengjie; Zhou, Jing; Zhang, Linjuan
192	Identification of Superoxide O-2(-) during Thermal Decomposition of Molten KNO3-NaNO2-NaNO3 Salt by Electron Paramagnetic Resonance and UV-Vis Absorption Spectroscopy	CHINESE JOURNAL OF CHEMICAL PHYSICS	30	4	372	Liu, Shu-ting; Su, Tao; Zhang, Peng
193	Adsorption of uranium (VI) onto amidoxime-functionalized ultra-high molecular weight polyethylene fibers from aqueous solution	NUCLEAR SCIENCE AND TECHNIQUES	28	7	94	Xie, Chun-Yu; Jing, Shi-Pei; Wang, Yu
194	A Breakthrough Efficiency of 19.9% Obtained in Inverted Perovskite Solar Cells by Using an Efficient Trap State Passivator Cu(thiourea)I	JOURNAL OF THE AMERICAN CHEMICAL SOCIETY	139	22	7504	Ye, Senyun; Rao, Haixia; Zhao, Ziran
195	Investigating the influence of F- on U4+ in molten LiCl-KCl-UF4 system and electro-deposition of U	JOURNAL OF RADIOANALYTICAL AND NUCLEAR CHEMISTRY	3		48510.1007/s10967-017-5242-x	Zhu, Tiejian; Huang, Wei; Zheng, Haiyang
196	Thermodynamic Reevaluation and Experimental Validation of the CsNO3-KNO3-NaNO3 System and Its Subsystems	CHEMICAL RESEARCH IN CHINESE UNIVERSITIES	33	1	122	An Xuehui; Zhang Peng; Cheng Jinhui
197	Simulation study of slow extraction for the Shanghai Advanced Proton Therapy facility	NUCLEAR SCIENCE AND TECHNIQUES	28	9	120	Yang, Yu-Hui; Zhang, Man-Zhou; Li, De-Ming
198	Low emittance lattice design with Robinson wiggler in the arc section	NUCLEAR SCIENCE AND TECHNIQUES	28	1	9	Tian, Shun-Qiang; Zhang, Qing-Lei; Zhang, Man-Zhou
199	Investigation on demagnetization of Nd2Fe14B permanent magnets induced by irradiation	NUCLEAR INSTRUMENTS & METHODS IN PHYSICS RESEARCH SECTION B-BEAM INTERACTIONS	413		68	Li, Zhefu; Jia, Yanyan; Liu, Renduo

		WITH MATERIALS AND ATOMS				
200	Eddy current effects in a high field dipole	NUCLEAR SCIENCE AND TECHNIQUES	28	12	173	Zhang, Man-Zhou; Zhang, Miao; Xie, Xiu-Cui
201	Development of a Superconducting Undulator Prototype at the SSRF	IEEE TRANSACTIONS ON APPLIED SUPERCONDUCTIVITY	27	4	4100304	Xu, Jieping; Ding, Yi; Wang, Shuhua
202	Low energy analysis techniques for CUORE	EUROPEAN PHYSICAL JOURNAL C	77	12	857	Alduino, C.; Alfonso, K.; Artusa, D. R.
203	Coherent diffractive photoproduction of rho(0) mesons on gold nuclei at 200 GeV/nucleon-pair at the Relativistic Heavy Ion Collider	PHYSICAL REVIEW C	96	5	54904	Adamczyk, L.; Adkins, J. K.; Agakishiev, G.
204	Bulk properties of the medium produced in relativistic heavy-ion collisions from the beam energy scan program	PHYSICAL REVIEW C	96	4	44904	Adamczyk, L.; Adkins, J. K.; Agakishiev, G.
205	Scalar field quasinormal frequencies of Reissner-Nordstrom black hole surrounded by quintessence by using the continued fraction method	INTERNATIONAL JOURNAL OF MODERN PHYSICS D	26	10	1750111	Wu, Chen;;
206	The projected background for the CUORE experiment	EUROPEAN PHYSICAL JOURNAL C	77	8	543	Alduino, C.; Alfonso, K.; Artusa, D. R.
207	Measurements of jet quenching with semi-inclusive hadron plus jet distributions in Au plus Au collisions at root s(NN)=200 GeV	PHYSICAL REVIEW C	96	2	24905	Adamczyk, L.; Adkins, J. K.; Agakishiev, G.
208	Energy dependence of J/Psi production in Au plus Au collisions at root S-NN=39, 62.4 and 200 GeV	PHYSICS LETTERS B	771		13	Adamczyk, L.; Adkins, J. K.; Agakishiev, G.
209	Dijet imbalance measurements in Au plus Au and pp collisions at root s(NN)=200 GeV at STAR	PHYSICAL REVIEW LETTERS	119	6	62301	Adamczyk, L.; Adkins, J. K.; Agakishiev, G.
210	CUORE sensitivity to 0 nu beta beta decay	EUROPEAN PHYSICAL JOURNAL C	77	8	532	Alduino, C.; Alfonso, K.; Artusa, D. R.
211	Global Lambda hyperon polarization in nuclear collisions	NATURE	548	7665	62	Adamczyk, L.; Adkins, J. K.; Agakishiev, G.
212	Direct virtual photon production in Au plus Au collisions at root s(NN)=200 GeV	PHYSICS LETTERS B	770		451	Adamczyk, L.; Adkins, J. K.;

	STAR Collaboration					Agakishiev, G.
213	Measurement of D-0 Azimuthal Anisotropy at Midrapidity in Au plus Au Collisions at root S-NN=200 GeV	PHYSICAL REVIEW LETTERS	118	21	212301	Adamczyk, L.; Adkins, J. K.; Agakishiev, G.
214	The CUORE cryostat and its bolometric detector	JOURNAL OF INSTRUMENTATION	12		C02055	Santone, D.; Alduino, C.; Alfonso, K.
215	Measurement of the two-neutrino double-beta decay half-life of Te-130 with the CUORE-0 experiment	EUROPEAN PHYSICAL JOURNAL C	77	1	13	Alduino, C.; Alfonso, K.; Artusa, D. R.
216	Charge-Dependent Directed Flow in Cu plus Au Collisions at root S-NN=200 GeV	PHYSICAL REVIEW LETTERS	118	1	12301	Adamczyk, L.; Adkins, J. K.; Agakishiev, G.
217	Mean free path and shear viscosity in central Xe-129+Sn-119 collisions below 100 MeV/nucleon	PHYSICAL REVIEW C	96	6	64604	Liu, H. L.; Ma, Y. G.; Bonasera, A.
218	Revisiting directed flow in relativistic heavy-ion collisions from a multiphase transport model	EUROPEAN PHYSICAL JOURNAL A	53	12	1233	Guo, Chong-Qiang; Zhang, Chun-Jian; Xu, Jun
219	Electromagnetic field effects on nucleon transverse momentum for heavy ion collisions around 100 A MeV	NUCLEAR SCIENCE AND TECHNIQUES	28	12	182	Deng, Xian-Gai; Ma, Yu-Gang;
220	Measurements of the total cross section of Be-nat with thermal neutrons from a photo-neutron source	NUCLEAR INSTRUMENTS & METHODS IN PHYSICS RESEARCH SECTION B-BEAM INTERACTIONS WITH MATERIALS AND ATOMS	410		158	Liu, L. X.; Wang, H. W.; Ma, Y. G.
221	Dark Matter Results from 54-Ton-Day Exposure of PandaX-II Experiment	PHYSICAL REVIEW LETTERS	119	18	181302	Cui, Xiangyi; Abdukerim, Abdusalam; Chen, Wei
222	Simulating spin dynamics with spin-dependent cross sections in heavy-ion collisions	PHYSICAL REVIEW C	96	4	44618	Xia, Yin; Xu, Jun; Li, Bao-An
223	Effects of hadronic mean-field potentials on Hanbury-Brown-Twiss correlations in relativistic heavy-ion collisions	PHYSICAL REVIEW C	96	4	44907	Zhang, Chun-Jian; Xu, Jun;
224	Chemical freeze-out in relativistic heavy-ion collisions	PHYSICS LETTERS B	772		290	Xu, Jun; Ko, Che Ming;
225	Collective Flows of O-16+O-16 Collisions with alpha-Clustering Configurations	CHINESE PHYSICS LETTERS	34	9	92101	Guo, Chen-Chen; He, Wan-Bing;

226	Nuclear cluster structure effect on elliptic and triangular flows in heavy-ion collisions	PHYSICAL REVIEW C	95	6	64904	Ma, Yu-Gang Zhang, S.; Ma, Y. G.; Chen, J. H.
227	Alpha-clustering effects on O-16(gamma, np)N-14 in the quasi-deuteron region	EUROPEAN PHYSICAL JOURNAL A	53	6	119	Huang, Bo-Song; Ma, Yu-Gang; He, Wan-Bing
228	A Photonuclear Reaction Model Based on IQMD in Intermediate-Energy Region	CHINESE PHYSICS LETTERS	34	7	72401	Huang, Bo-Song; Ma, Yu-Gang;
229	Isovector dipole resonance and shear viscosity in low energy heavy-ion collisions	PHYSICAL REVIEW C	95	5	54622	Guo, C. Q.; Ma, Y. G.; He, W. B.
230	Investigation of giant dipole resonances in heavy deformed nuclei with an extended quantum molecular dynamics model	PHYSICAL REVIEW C	95	5	54615	Wang, S. S.; Ma, Y. G.; Cao, X. G.
231	Production of light nuclei and hypernuclei at High Intensity Accelerator Facility energy region	NUCLEAR SCIENCE AND TECHNIQUES	28	4	55	Liu, Peng; Chen, Jin-Hui; Ma, Yu-Gang
232	Constraining simultaneously nuclear symmetry energy and neutron-proton effective mass splitting with nucleus giant resonances using a dynamical approach	PHYSICAL REVIEW C	95	3	34324	Kong, Hai-Yun; Xu, Jun; Chen, Lie-Wen
233	Photonuclear reaction as a probe for a-clustering nuclei in the quasi-deuteron region	PHYSICAL REVIEW C	95	3	34606	Huang, B. S.; Ma, Y. G.; He, W. B.
234	Medium effect on the nuclear modification factor of protons and pions in intermediate-energy heavy ion collisions	PHYSICAL REVIEW C	95	2	24614	Lv, M.; Ma, Y. G.; Chen, J. H.
235	Alignment calibration and performance study of the STAR PXL detector	NUCLEAR SCIENCE AND TECHNIQUES	28	2	25	Ma, Long; Dong, Xin; Qiu, Hao
236	Giant dipole resonance in proton capture reactions using an extended quantum molecular dynamics model	PHYSICAL REVIEW C	95	1	14608	Wang, K.; Ma, Y. G.; Zhang, G. Q.
237	beta-decay study of the T-z =-2 proton-rich nucleus Mg-20	PHYSICAL REVIEW C	95	1	14314	Sun, L. J.; Xu, X. X.; Fang, D. Q.
238	Reconstructed jets in a multi-phase transport model	NUCLEAR AND PARTICLE PHYSICS PROCEEDINGS	289		363	Ma, Guo-Liang;;
239	Measurement of D*-meson triggered correlations in p plus p collisions at RHIC	NUCLEAR AND PARTICLE PHYSICS PROCEEDINGS	289		329	Ma, Long;;
240	Measurement of bottom contribution to the non-photonic electron production in p plus p collisions at STAR	16TH INTERNATIONAL CONFERENCE ON STRANGENESS IN QUARK MATTER (SQM2016)	779		UNSP 012053	Li, Wei;;
241	Omega and phi in Au plus Au collisions at	CHINESE PHYSICS C	41	8	84101	Ye, Y. J.; Chen,

	root S-NN=200 and 11.5 GeV from a multiphase transport model					J. H.; Ma, Y. G.
242	Measurement of the cross section and longitudinal double-spin asymmetry for dijet production in polarized pp collisions at root s=200 GeV	PHYSICAL REVIEW D	95	7	71103	Adamczyk, L.; Adkins, J. K.; Agakishiev, G.
243	Cyclic thermal characterization of a molten-salt packed-bed thermal energy storage for concentrating solar power	APPLIED ENERGY	195		761	Zhao, Bing-chen; Cheng, Mao-song; Liu, Chang
244	A Wind Power Plant with Thermal Energy Storage for Improving the Utilization of Wind Energy	ENERGIES	10	12	2126	Liu, Chang; Cheng, Mao-Song; Zhao, Bing-Chen
245	Treatment of radioactive spent extraction solvent by supercritical water oxidation	JOURNAL OF RADIOANALYTICAL AND NUCLEAR CHEMISTRY	314	2	1169	Qin, Qiang; Wang, Shuai; Wang, Hongyu
246	Design of PC-based quantitative split charging device for hydrogen isotope elemental gases	INTERNATIONAL JOURNAL OF HYDROGEN ENERGY	42	29	18484	Cheng, Honghui; Xi, Chenyu; Liu, Jingjing
247	Source apportionment of carbonaceous particulate matter during haze days in Shanghai based on the radiocarbon	JOURNAL OF RADIOANALYTICAL AND NUCLEAR CHEMISTRY	313	1	145	Wei, Nannan; Wang, Guanghua; Zhouga, Deqing
248	Effects of alloying substitutions on the anti-disproportionation behavior of ZrCo alloy	INTERNATIONAL JOURNAL OF HYDROGEN ENERGY	42	24	15782	Yang, Guo; Liu, Wenguan; Han, Xingbo
249	Theoretical study of the interaction between hydrogen and 4d alloying atom in nickel	NUCLEAR SCIENCE AND TECHNIQUES	6		10.1007/s 41365-01 7-0235-6	Liu, Wen-Guan; Qian, Yuan; Zhang, Dong-Xun
250	Extraction of lanthanide ions with N,N,N',N'-tetrabutyl-3-oxa-diglycolamide from nitric acid media	NUCLEAR SCIENCE AND TECHNIQUES	28	6	87	Peng, Xiu-Jing; Cui, Yu; Ma, Ji-Fei
251	A theoretical study of the effects of sp-elements on hydrogen in nickel-based alloys	COMPUTATIONAL MATERIALS SCIENCE	128		37	Liu, Wenguan; Qian, Yuan; Zhang, Dongxun
252	Analysis of atmospheric pollutant metals by laser ablation inductively coupled plasma mass spectrometry with a radial line-scan dried-droplet approach	SPECTROCHIMICA ACTA PART B-ATOMIC SPECTROSCOPY	138		18	Tang, Xiaoxing; Qian, Yuan; Guo, Yanchuan
253	Synchrotron radiation X-ray powder diffraction techniques applied in hydrogen storage materials - A review	PROGRESS IN NATURAL SCIENCE-MATERIALS INTERNATIONAL	27	1	72	Cheng, Honghui; Lu, Chen; Liu, Jingjing

254	Radiolysis products and degradation mechanism studies on di-1-methyl heptyl methyl phosphonate	JOURNAL OF RADIOANALYTICAL AND NUCLEAR CHEMISTRY	314	3	1715	Li, Ruifen; Cao, Xiaojun; Zhao, Haogui
255	High-performance functionalized polyethylene fiber for the capture of trace uranium in water	JOURNAL OF RADIOANALYTICAL AND NUCLEAR CHEMISTRY	314	3	2393	Pang, Li-juan; Zhang, Lin-juan; Hu, Jiang-tao
256	Reprocessing Th-based spent fuels with di-1-methyl heptyl methyl phosphonate using centrifugal extractors	HYDROMETALLURGY	174		84	Li, Ruifen; Zhao, Haogui; Liu, Chunxia
257	Supercritical CO2 foaming of radiation crosslinked polypropylene/high-density polyethylene blend: Cell structure and tensile property	RADIATION PHYSICS AND CHEMISTRY	141		276	Yang, Chenguang; Xing, Zhe; Zhang, Mingxing
258	The recovery of uranium from irradiated thorium by extraction with di-1-methyl heptyl methylphosphonate (DMHMP)/n-dodecane	SEPARATION AND PURIFICATION TECHNOLOGY	188		219	Li, Ruifen; Zhao, Haogui; Liu, Chunxia
259	Potential application of graphene oxide membranes for removal of Cs(I) and Sr(II) from high level-liquid waste	SEPARATION AND PURIFICATION TECHNOLOGY	188		523	Ma, Fuyin; Li, Zheng; Zhao, Haogui
260	Matrix Infrared Spectra of Manganese and Iron Isocyanide Complexes	JOURNAL OF PHYSICAL CHEMISTRY A	121	46	8835	Chen, Xiuting; Li, Qingnuan; Andrews, Lester
261	Preparation of antimicrobial MnO4--doped nylon-66 fibers with excellent laundering durability	APPLIED SURFACE SCIENCE	422		1067	Zhang, Mingxing; Gao, Qianhong; Yang, Chenguang
262	Determination of Trace Fission Products Associated with Thorium and HCl Matrix by Inductively Coupled Plasma Mass Spectrometry after Anion Exchange Separation	ANALYTICAL SCIENCES	33	11	1265	He, Shuhua; Chen, Mumei; Li, Zheng
263	Infrared Spectroscopic and Theoretical Studies on the OMF2 and OMF (M = Cr, Mo, W) Molecules in Solid Argon	JOURNAL OF PHYSICAL CHEMISTRY A	121	40	7603	Wei, Rui; Li, Qingnuan; Gong, Yu
264	Coordination Structure and Fragmentation Chemistry of the Tripositive Lanthanide-Thio-Diglycolamide Complexes	JOURNAL OF PHYSICAL CHEMISTRY A	121	49	9429	Chen, Xiuting; Li, Qingnuan; Gong, Yu
265	Formation and Fragmentation Chemistry of Tripositive Ln(TMGA)(3)(3+) Complexes in the Gas Phase	JOURNAL OF THE AMERICAN SOCIETY FOR MASS SPECTROMETRY	28	8	1696	Chen, Xiuting; Li, Qingnuan; Gong, Yu
266	Preparation of Cu2+-Chitosan Quaternary Ammonium Salt-g-Poly(acrylicacid) with	CHEMICAL JOURNAL OF CHINESE	38	5	902	Li Hui; Xing Zhe; Li Rong

	Efficient Antibacterial Activity	UNIVERSITIES-CHINESE				
267	Formation and Characterization of Homoleptic Thorium Isocyanide Complexes	INORGANIC CHEMISTRY	56	9	5060	Chen, Xiuting; Li, Qingnuan; Gong, Yu
268	The extraction of uranium using graphene aerogel loading organic solution	TALANTA	166		284	Chen, Mumei; Li, Zheng; Li, Jihao
269	More wear-resistant and ductile UHMWPE composite prepared by the addition of radiation crosslinked UHMWPE powder	JOURNAL OF APPLIED POLYMER SCIENCE	134	13	44643	Wang, Honglong; Xu, Lu; Zhang, Mingxing
270	Optimization of molar content of amidoxime and acrylic acid in UHMWPE fibers for improvement of seawater uranium adsorption capacity	JOURNAL OF RADIOANALYTICAL AND NUCLEAR CHEMISTRY	311	3	1771	Li, Rong; Pang, Lijuan; Ma, Hongjuan
271	Electrochemical behavior and electrowinning of uranium(IV) from FLiNaK molten salt	JOURNAL OF RADIOANALYTICAL AND NUCLEAR CHEMISTRY	3		189710.1007/s10967-016-5160-3	Jiang, Feng; Huang, Wei; Zheng, Haiyang
272	Application of polyantimonic acid-polyacrylonitrile for removal of strontium(II) from simulated high-level liquid waste	JOURNAL OF RADIOANALYTICAL AND NUCLEAR CHEMISTRY	311	3	2007	Ma, Fuyin; Li, Zheng; Zhou, Wei
273	Radiation effects on the foaming of atactic polypropylene with supercritical carbon dioxide	RADIATION PHYSICS AND CHEMISTRY	131		35	Yang, Chenguang; Zhe, Xing; Zhang, Mingxing
274	Di-1-methyl heptyl methylphosphonate (DMHMP): A promising extractant in Th-based fuel reprocessing	SEPARATION AND PURIFICATION TECHNOLOGY	173		105	Li, Ruifen; Liu, Chunxia; Zhao, Haogui
275	Electrochemical Behavior of Graphite Anode in LiF-NaF-KF Eutectic with YF3	ELECTROCHIMICA ACTA	225		392	Tian, Lifang; Huang, Wei; Jiang, Feng
276	Pyrohydrolysis of SmF3 in moist air	JOURNAL OF FLUORINE CHEMISTRY	193		106	Peng, Jia; Zheng, Xiaobei; Qiu, Tingting
277	The evaporation behaviors of rare-earth-doped FLiNaK melts during low-pressure distillation	JOURNAL OF RADIOANALYTICAL AND NUCLEAR CHEMISTRY	311	1	637	Wang, Zihao; Fu, Haiying; Yang, Yang
278	Radiation-induced graft polymerization for the preparation of a highly efficient UHMWPE fibrous adsorbent for Cr(VI) removal	RADIATION PHYSICS AND CHEMISTRY	130		92	Gao, Qianhong; Hua, Jiangtao; Li, Rong
279	An efficient tank size estimation strategy	SOLAR ENERGY	153		104	Zhao, Bingchen;

	for packed-bed thermocline thermal energy storage systems for concentrated solar power					Cheng, Maosong; Liu, Chang
280	Growth and Scintillation Properties of GdI3:Ce Crystal	JOURNAL OF INORGANIC MATERIALS	32	4	346	Ye Le; Shi Jiang; Li Huan-Ying
281	Radionuclides in primary coolant of a fluoride salt-cooled high-temperature reactor during normal operation	NUCLEAR SCIENCE AND TECHNIQUES	28	3	41	Zhang, Guo-Qing; Wang, Shuai; Zhang, Hai-Qing
282	Thermal performance analysis of a thermocline thermal energy storage system with FLiNaK molten salt	INTERNATIONAL CONFERENCE ON ENERGY ENGINEERING AND ENVIRONMENTAL PROTECTION (EEEP2016)	52		UNSP 012039	Liu, C.; Cheng, M. S.; Zhao, B. C.
283	Neutronics physics analysis of a large fluoride-salt-cooled solid-fuel fast reactor with Th-based fuel	NUCLEAR SCIENCE AND TECHNIQUES	28	11	158	Peng, Yu; Zhu, Gui-Feng; Zou, Yang
284	The feasibility research of thorium breeding using fast reactor coolant fluoride salt as a	PROGRESS IN NUCLEAR ENERGY	101		199	Peng, Yu; Zhu, Guifeng; Zou, Yang
285	Transition toward thorium fuel cycle in a molten salt reactor by using plutonium	NUCLEAR SCIENCE AND TECHNIQUES	28	10	152	Cui, De-Yang; Xia, Shao-Peng; Li, Xiao-Xiao
286	Evaluation of the fraction of delayed photoneutrons for TMSR-SF1	NUCLEAR SCIENCE AND TECHNIQUES	28	9	135	Ji, Rui-Min; Dai, Ye; Zhu, Gui-Feng
287	Development of a GPU-accelerated 3D neutron dynamics code for PB-FHR	NUCLEAR ENGINEERING AND DESIGN	320		88	E, Yanzhi; Zou, Yang; Guo, Wei
288	A specialized code for operation transient analysis and its application in fluoride salt-cooled high-temperature reactors	NUCLEAR SCIENCE AND TECHNIQUES	28	8	119	Ruan, Jian; Xu, Bo; Li, Ming-Hai
289	Influences of Li-7 enrichment on Th-U fuel breeding for an Improved Molten Salt Fast Reactor (IMSFR)	NUCLEAR SCIENCE AND TECHNIQUES	28	7	97	Li, Guang-Chao; Zou, Yang; Yu, Cheng-Gang
290	Impact of photoneutrons on reactivity measurements for TMSR-SF1	NUCLEAR SCIENCE AND TECHNIQUES	6		10.1007/s41365-017-0234-7	Ji, Rui-Min; Li, Ming-Hai; Zou, Yang
291	Projector Augmented Wave Method Incorporated into Gauss-Type Atomic Orbital Based Density Functional Theory	JOURNAL OF CHEMICAL THEORY AND COMPUTATION	13	7	3236	Xiong, Xiao-Gen; Yanai, Takeshi;
292	Effect of Cr contents on the diffusion behavior of Te in Ni-based alloy	JOURNAL OF NUCLEAR MATERIALS	497		101	Jia, Yanyan; Li, Zhefu; Ye, Xiangxi
293	Behaviors of fine (IG-110) and ultra-fine	NUCLEAR SCIENCE AND	28	10	144	Qi, Wei; He,

	(HPG-510) grain graphite irradiated by 7 MeV Xe26+ ions	TECHNIQUES				Zhou-Tong; Zhang, Bao-Liang
294	Infiltration of graphite by molten 2LiF-BeF2 salt	JOURNAL OF MATERIALS SCIENCE	52	19	11346	Tang, Hui; Qi, Wei; He, Zhoutong
295	Novel 3D metallic boron nitride containing only sp(2) bonds	JOURNAL OF PHYSICS D-APPLIED PHYSICS	50	38	385302	Wang, Hao; Zhang, Wei; Huai, Ping
296	High temperature in-situ synchrotron-based XRD study on the crystal structure evolution of C/C composite impregnated by FLiNaK molten salt	SCIENTIFIC REPORTS	7		10673	Feng, Shanglei; Yang, Yingguo; Li, Li
297	First-principles study of helium clustering at initial stage in ThO2	CHINESE PHYSICS B	26	9	97101	Shao, Kuan; Han, Han; Zhang, Wei
298	First-principles study of fission product stability and clustering in ThO2	COMPUTATIONAL MATERIALS SCIENCE	137		186	Shao, Kuan; Han, Han; Zhang, Wei
299	Evaluating Young's modulus of porous nuclear graphite by a novel multi-scale method	JOURNAL OF MATERIALS SCIENCE	18		1097110.1007/s10853-017-1259-3	Yang, Xiong; Tsang, D. K. L.;
300	First-principles prediction of interstitial carbon, nitrogen, and oxygen effects on the helium behavior in nickel	JOURNAL OF APPLIED PHYSICS	122	6	65901	Zhang, Xun; Ren, Cui-Lan; Han, Han
301	Effect of Mg on the Microstructure and Corrosion Resistance of the Continuously Hot-Dip Galvanizing Zn-Mg Coating	MATERIALS	10	8	980	Dong, Anping; Li, Baoping; Lu, Yanling
302	Effects of SO42- ions on the corrosion of GH3535 weld joint in FLiNaK molten salt	JOURNAL OF NUCLEAR MATERIALS	492		122	Zhu, Yasheng; Qiu, Jie; Hou, Juan
303	First-principles study of noble gas stability in ThO2	JOURNAL OF NUCLEAR MATERIALS	490		181	Shao, Kuan; Han, Han; Zhang, Wei
304	First-principles investigation on the geometries, stabilities and defective properties of fluoride surfaces	COMPUTATIONAL MATERIALS SCIENCE	133		159	Han, Han; Yin, Gen; Wang, Hui
305	Pressure-induced structural transformations and polymerization in ThC2	SCIENTIFIC REPORTS	7		45872	Guo, Yongliang; Yu, Cun; Lin, Jun
306	The Effect of Milling Time on the Microstructural Characteristics and	MATERIALS	10	4	389	Yang, Chao; Muransky,

	Strengthening Mechanisms of NiMo-SiC Alloys Prepared via Powder Metallurgy					Ondrej; Zhu, Hanliang
307	Probing Chemical Bonding and Electronic Structures in ThO- by Anion Photoelectron Imaging and Theoretical Calculations	JOURNAL OF PHYSICAL CHEMISTRY A	121	10	2108	Li, Yanli; Zou, Jinghan; Xiong, Xiao-Gen
308	The influence of FLiNaK salt impregnation on the mechanical properties of a 2D woven C/C composite	JOURNAL OF NUCLEAR MATERIALS	485		74	Zhang, Dongsheng; Xia, Huihao; Yang, Xinmei
309	First-Principles Study of Vacancies in Ti3SiC2 and Ti3AlC2	MATERIALS	10	2	UNSP 103	Wang, Hui; Han, Han; Yin, Gen
310	On the origin of strengthening mechanisms in Ni-Mo alloys prepared via powder metallurgy	MATERIALS & DESIGN	113		223	Yang, Chao; Muransky, Ondrej; Zhu, Hanliang
311	Theoretical study of the substitutional solute effect on the interstitial carbon in nickel-based alloy	RSC ADVANCES	7	33	20567	Zhang, Xun; Ren, Cui-Lan; Han, Han
312	Diffusion of tellurium at nickel grain boundaries: a first-principles study	RSC ADVANCES	7	14	8421	Wang, C. Y.; Han, H.; Wickramaratne, D.
313	Effects of Cr3+ on the corrosion of SiC in LiF-NaF-KF molten salt	CORROSION SCIENCE	114		96	Xue, Wandong; Yang, Xinmei; Qiu, Jie
314	The Fabrication of Multifunctional SLIPS Films by Electrospinning	CHEMNANOMAT	3	12	869	Wu, Jingxia; Zhang, Bowu; Wang, Bingjie
315	Stretchable Ionic-Liquid-Based Gel Polymer Electrolytes for Lithium Ion Batteries	INDUSTRIAL & ENGINEERING CHEMISTRY RESEARCH	56	44	12456	Guan, Jipeng; Li, Yongjin; Li, Jingye
316	Green and efficient synthesis of an adsorbent fiber by preirradiation-induced grafting of PDMAEMA and its Au(III) adsorption and reduction performance	JOURNAL OF APPLIED POLYMER SCIENCE	134	25	44955	Liu, Xiyan; Ao, Junxuan; Yang, Xiaojuan
317	Radiation graft of acrylamide onto polyethylene separators for lithium-ion batteries	NUCLEAR SCIENCE AND TECHNIQUES	28	6	77	Miao, Xiao-Li; Li, Ji-Hao; Xiang, Qun
318	Amidoxime-based adsorbents prepared by cografting acrylic acid with acrylonitrile onto HDPE fiber for the recovery of uranium from seawater	NUCLEAR SCIENCE AND TECHNIQUES	28	4	45	Xu, Lu; Hu, Jiang-Tao; Ma, Hong-Juan
319	Preparation of Dynamic Superhydrophobic	ACTA POLYMERICA		2	315	Li, Jing-ye;

	Cotton Fabric via Radiation-induced Graft Polymerization	SINICA				Wang, Zi-qiang; Yu, Ming
320	Uranium Adsorption Tests of Amidoxime-Based Ultrahigh Molecular Weight Polyethylene Fibers in Simulated Seawater and Natural Coastal Marine Seawater from Different Locations	INDUSTRIAL & ENGINEERING CHEMISTRY RESEARCH	56	4	1103	Ling, Changjian; Liu, Xiyan; Yang, Xiaojuan
321	Poly (vinylidene fluoride) dielectric composites with both ionic nanoclusters and well dispersed graphene oxide	COMPOSITES SCIENCE AND TECHNOLOGY	138		98	Guan, Jipeng; Xing, Chenyang; Wang, Yanyuan
322	Preparation of freestanding graphene-based laminar membrane for clean-water intake via forward osmosis process	RSC ADVANCES	7	3	1326	Yan, Feng; Yu, Chuhong; Zhang, Bowu
323	Temperature dependence of nickel ion irradiation damage in GH3535 alloy weld metal	JOURNAL OF NUCLEAR MATERIALS	497		108	Huang, Hefei; Zhou, Xiaoling; Li, Chaowen
324	Raman spectra and modulus measurement on the cross section of proton-irradiated graphite	NUCLEAR INSTRUMENTS & METHODS IN PHYSICS RESEARCH SECTION B-BEAM INTERACTIONS WITH MATERIALS AND ATOMS	412		221	Huang, Qing; Lei, Qiantao; Deng, Qi
325	Encapsulation of metal-based phase change materials using ceramic shells prepared by spouted bed CVD method	SOLAR ENERGY MATERIALS AND SOLAR CELLS	170		137	Zhang, Feng; Zhong, Yajuan; Yang, Xu
326	In-core fuel management strategy for the basket-fuel-assembly molten salt reactor	NUCLEAR SCIENCE AND TECHNIQUES	28	9	130	Xue, Chun; Zhu, Zhi-Yong; Zhang, Hai-Qing
327	Characterization the microstructure and defects of matrix graphite irradiated with Xe ions	NUCLEAR INSTRUMENTS & METHODS IN PHYSICS RESEARCH SECTION B-BEAM INTERACTIONS WITH MATERIALS AND ATOMS	406		638	Xu, H. X.; Lin, J.; Li, J. J.
328	Effect of irradiation damage on corrosion of 4H-SiC in FLiNaK molten salt	CORROSION SCIENCE	125		194	Li, Jianjian; Huang, Hefei; Huang, Qing
329	PL and ESR study for defect centers in 4H-SiC induced by oxygen ion implantation	NUCLEAR SCIENCE AND TECHNIQUES	28	8	105	Cheng, Guo-Dong; Chen, Ye; Yan, Long
330	The elemental move characteristic of nickel-based alloy in molten salt corrosion	NUCLEAR INSTRUMENTS & METHODS IN PHYSICS	404		185	Lei, Qiantao; Liu, Ke; Gao, Jie

	by using nuclear microprobe	RESEARCH SECTION B-BEAM INTERACTIONS WITH MATERIALS AND ATOMS				
331	Surface morphology and microstructure evolution of IG-110 graphite after xenon ion irradiation and subsequent annealing	JOURNAL OF NUCLEAR MATERIALS	491		213	Huang, Qing; Li, Jianjian; Liu, Renduo
332	Mesocarbon microbead based graphite for spherical fuel element to inhibit the infiltration of liquid fluoride salt in molten salt reactor	JOURNAL OF NUCLEAR MATERIALS	490		34	Zhong, Yajuan; Zhang, Junpeng; Lin, Jun
333	Synthesis of thorium sol for fabricating fuel kernels	NUCLEAR SCIENCE AND TECHNIQUES	28	7	96	Wang, Feng-Xia; Yan, Chao; Cao, Chang-Qing
334	Ion irradiation-induced swelling and hardening effect of Hastelloy N alloy	JOURNAL OF NUCLEAR MATERIALS	489		180	Zhang, S. J.; Li, D. H.; Chen, H. C.
335	Reactions of Triplet-State Difloxacin with Amino Acids and dGMP: A Laser Flash Photolysis Study	ACTA PHYSICO-CHIMICA SINICA	33	5	1051	Li Hai-Xia; Liu Yan-Cheng; Tang Rui-Zhi
336	ERDA, RBS, TEM and SEM characterization of microstructural evolution in helium-implanted Hastelloy N alloy	NUCLEAR INSTRUMENTS & METHODS IN PHYSICS RESEARCH SECTION B-BEAM INTERACTIONS WITH MATERIALS AND ATOMS	399		62	Gao, Jie; Bao, Liangman; Huang, Hefei
337	Investigation of the damage behavior in CVD SiC irradiated with 70 keV He ions by NEXAFS, Raman and TEM	JOURNAL OF THE EUROPEAN CERAMIC SOCIETY	37	4	1253	Liu, Min; Yang, Xinmei; Gao, Yantao
338	Radical-Induced Degradation of Fluoxetine in Aqueous Solution by Pulse and Steady-State Radiolysis Studies	ACTA PHYSICO-CHIMICA SINICA	33	4	823	Ji Tian-Yi; Liu Yan-Cheng; Zhao Jian-Feng
339	Structural Phase Transition of ThC Under High Pressure	SCIENTIFIC REPORTS	7		96	Yu, Cun; Lin, Jun; Huai, Ping
340	A paramagnetic neutral CBVN center in hexagonal boron nitride monolayer for spin qubit application	COMPUTATIONAL MATERIALS SCIENCE	129		247	Cheng, G. D.; Zhang, Y. G.; Yan, L.
341	Theory of sulfur-vacancy defect in diamond: a comparable NV-1 isoelectronic center	OPTIK	136		151	Cheng, G. D.; Huang, Q.; Shen, Y. H.
342	Synthesis of a ceria-supported iron-ruthenium oxide catalyst and its structural transformation from subnanometer clusters to single atoms	INORGANIC CHEMISTRY FRONTIERS	4	12	2059	Wang, Xu; Fu, Xin-Pu; Yu, Wen-Zhu

	during the Fischer-Tropsch synthesis reaction					
343	Effects of Multiple Platinum Species on Catalytic Reactivity Distinguished by Electron Microscopy and X-ray Absorption Spectroscopy Techniques	JOURNAL OF PHYSICAL CHEMISTRY C	121	46	25805	Nan, Bing; Hu, Xiu-Cui; Wang, Xu
344	Ternary organic solar cells: compatibility controls for morphology evolution of active layers	JOURNAL OF MATERIALS CHEMISTRY C	5	41	10801	Ai, Qingyun; Zhou, Weihua; Zhang, Lin
345	Investigating microstructure of Longmaxi shale in Shizhu area, Sichuan Basin, by optical microscopy, scanning electron microscopy and micro-computed tomography	NUCLEAR SCIENCE AND TECHNIQUES	28	11	163	Wang, Yu; Wang, Li-Hua; Wang, Jian-Qiang
346	Improving the efficiency of small-angle x-ray scattering computed tomography using the OSEM algorithm	APPLIED OPTICS	56	30	8326	Hu, Tao; Wang, Yudan; Du, Guohao
347	Investigation of atom distribution in Mg-9wt.%Al melt using small-angle X-ray scattering and molecular dynamics simulation	JOURNAL OF NON-CRYSTALLINE SOLIDS	473		47	Huang, Xiusong; Dong, Xixi; Yang, Chunming
348	Improved Glass Transition Temperature towards Thermal Stability via Thiols Solvent Additive versus DIO in Polymer Solar Cells	MACROMOLECULAR RAPID COMMUNICATIONS	38	20	1700428	Yin, Jingping; Zhou, Weihua; Zhang, Lin
349	Morphology and structure improvement of the hybrid CH3NH3PbI3 perovskite film via external doping	THIN SOLID FILMS	636		296	Shen, Kongchao; Hu, Jinbang; Sun, Haoliang
350	High Extinction Coefficient Thieno[3,4-b]thiophene-Based Copolymer for Efficient Fullerene-Free Solar Cells with Large Current Density	CHEMISTRY OF MATERIALS	29	16	6766	Bao, Xichang; Zhang, Yongchao; Wang, Junyi
351	Co3O4-Al2O3 mesoporous hollow spheres as efficient catalyst for Fischer-Tropsch synthesis	APPLIED CATALYSIS B-ENVIRONMENTAL	211		176	Fu, Xin-Pu; Shen, Qi-Kai; Shi, Dong
352	Manifestation of the structural stability of Mg-doped Zn4Sb3 via atomic fine structure investigation	SOLID STATE COMMUNICATIONS	261		26	Wang, Y.; Feng, S. L.; Shen, K. C.
353	Investigation of the fine structure around the copper site in copper/zinc superoxide dismutase by XANES combined with ab initio calculations	RADIATION PHYSICS AND CHEMISTRY	137		88	Wang, Yu; Jin, Sheng; Li, Jiong
354	Disorder effects on EXAFS modeling for catalysts working at elevated temperatures	RADIATION PHYSICS AND CHEMISTRY	137		93	Sun, Xueping; Sun, Fanfei; Sun,

						Zhihu
355	Zn Single Atom Catalyst for Highly Efficient Oxygen Reduction Reaction	ADVANCED FUNCTIONAL MATERIALS	27	28	1700802	Song, Ping; Luo, Mi; Liu, Xiaozhi
356	High performance platinum single atom electrocatalyst for oxygen reduction reaction	NATURE COMMUNICATIONS	8		15938	Liu, Jing; Jiao, Menggai; Lu, Lanlu
357	Photoelectron spectroscopy study of the electronic structures at CoPc/Bi(111) interface	SURFACE SCIENCE	661		34	Sun, Haoliang; Liang, Zhaofeng; Shen, Kongchao
358	Achieving Remarkable Activity and Durability toward Oxygen Reduction Reaction Based on Ultrathin Rh-Doped Pt Nanowires	JOURNAL OF THE AMERICAN CHEMICAL SOCIETY	139	24	8152	Huang, Hongwen; Li, Kan; Chen, Zhao
359	Catalytically active ceria-supported cobalt-manganese oxide nanocatalysts for oxidation of carbon monoxide	PHYSICAL CHEMISTRY CHEMICAL PHYSICS	19	22	14533	Wang, Xu; Du, Lin-Ying; Du, Meng
360	Probing intermediates of the induction period prior to nucleation and growth of semiconductor quantum dots	NATURE COMMUNICATIONS	8		15467	Liu, Mingyang; Wang, Kun; Wang, Linxi
361	Enhanced electrochemical sensing arsenic(III) with excellent anti-interference using amino-functionalized graphene oxide decorated gold microelectrode: XPS and XANES evidence	SENSORS AND ACTUATORS B-CHEMICAL	245		230	Yang, Meng; Jiang, Tian-Jia; Wang, Yu
362	Poly(3-hexylthiophene) coated graphene oxide for improved performance of bulk heterojunction polymer solar cells	ORGANIC ELECTRONICS	44		149	Zheng, Fei; Yang, Xiao-Yu; Bi, Peng-Qing
363	Supported Rhodium Catalysts for Ammonia-Borane Hydrolysis: Dependence of the Catalytic Activity on the Highest Occupied State of the Single Rhodium Atoms	ANGEWANDTE CHEMIE-INTERNATIONAL EDITION	56	17	4712	Wang, Liangbing; Li, Hongliang; Zhang, Wenbo
364	Synthesis and Self-Assembly of Shape Amphiphiles Based on POSS-Dendron Conjugates	MOLECULES	22	4	622	Shao, Yu; Ding, Minyuan; Xu, Yujie
365	WAXD/SAXS study and 2D fitting (SAXS) of the microstructural evolution of PAN-based carbon fibers during the pre-oxidation and carbonization process	NEW CARBON MATERIALS	32	2	130	Li Xiao-yun; Tian Feng; Gao Xue-ping
366	The Influence of Epitaxial Crystallization on the Mechanical Properties of Polyamide 66/Reduced Graphene Oxide Nanocomposite Injection Bar	CRYSTALS	7	12	384	Chi, Enyi; An, Minfang; Yao, Guibin
367	Microfocus small-angle X-ray scattering at	CHINESE PHYSICS C	41	4	48001	Hua,

	SSRF BL16B1					Wen-Qiang; Wang, Yu-Zhu; Zhou, Ping
368	Synthesis and metal-support interaction of subnanometer copper-palladium bimetallic oxide clusters for catalytic oxidation of carbon monoxide	INORGANIC CHEMISTRY FRONTIERS	4	4	668	Du, Pei-Pei; Hu, Xiu-Cui; Wang, Xu
369	Facile synthesis and hierarchical assembly of polystyrene-block- poly (perfluorooctylethyl acrylates)	POLYMER	113		46	Dai, Hui; Yin, Guang-Zhong; Zhao, Fang-Jia
370	Performance on absolute scattering intensity calibration and protein molecular weight determination at BL16B1, a dedicated SAXS beamline at SSRF	JOURNAL OF SYNCHROTRON RADIATION	24		509	Zeng, Jianrong; Bian, Fenggang; Wang, Jie
371	Local structural evolutions of CuO/ZnO/Al2O3 catalyst for methanol synthesis under operando conditions studied by in situ quick X-ray absorption spectroscopy	NUCLEAR SCIENCE AND TECHNIQUES	28	2	21	Sun, Xue-Ping; Sun, Fan-Fei; Gu, Song-Qi
372	Crystal Plane Effect of Ceria on Supported Copper Oxide Cluster Catalyst for CO Oxidation: Importance of Metal-Support Interaction	ACS CATALYSIS	7	2	1313	Wang, Wei-Wei; Yu, Wen-Zhu; Du, Pei-Pei
373	Unveiling orbital coupling at the CoPc/Bi(111) surface by ab initio calculations and photoemission spectroscopy	RSC ADVANCES	7	82	52143	Liang, Zhaofeng; Sun, Haoliang; Shen, Kongchao
374	Recent Progress in the Fabrication of Low Dimensional Nanostructures via Surface-Assisted Transforming and Coupling	JOURNAL OF NANOMATERIALS			4796538	Hu, Jinbang; Liang, Zhaofeng; Shen, Kongchao
375	On-surface manipulation of atom substitution between cobalt phthalocyanine and the Cu(111) substrate	RSC ADVANCES	7	23	13827	Shen, Kongchao; Narsu, Bai; Ji, Gengwu
376	In-situ high-energy-resolution X-ray absorption spectroscopy for UO2 oxidation at SSRF	NUCLEAR SCIENCE AND TECHNIQUES	28	1	2	Duan, Pei-Quan; Bao, Hong-Liang; Li, Jiong
377	A three-crystal spectrometer for high-energy resolution fluorescence-detected X-ray absorption spectroscopy and X-ray emission spectroscopy at SSRF	X-RAY SPECTROMETRY	46	1	12	Duan, Peiquan; Gu, Songqi; Cao, Hanjie
378	Au6S2 monolayer sheets: metallic and	MATERIALS HORIZONS	4	6	1085	Wu, Qisheng;

	semiconducting polymorphs					Xu, Wen Wu; Qu, Bingyan
379	J/ ψ azimuthal anisotropy in Au+Au collisions at √ sNN = 200 GeV	Journal of Physics: Conference Series	832	1		Zhou, Chensheng;;
380	Analysis on partial coherence propagation using the four-dimensional coherence function	Proceedings of SPIE - The International Society for Optical Engineering	10388			Meng, Xiangyu; Xue, Chaofan; Yu, Huaina
381	Evaluation on microstructure and mechanical properties of welded joints by GMAW in UNS N10003 alloy	American Society of Mechanical Engineers, Pressure Vessels and Piping Division (Publication) PVP	6B-2017			Yu, Kun; Jiang, Zhenguo; Shi, Xianwu
382	Research of the rod drop time based on the control rod system of TMSR - SF1	International Conference on Nuclear Engineering, Proceedings, ICONE	2			Lin, Zuokang; Zhu, Lin; Zhao, Chunfeng
383	The feasibility research of thorium breeding using fluoride salt as a fast reactor coolant	Progress in Nuclear Energy	101		199	Peng, Yu; Zhu, Guifeng; Zou, Yang
384	RESEARCH OF THE ROD DROP TIME BASED ON THE CONTROL ROD SYSTEM OF TMSR-SF1	PROCEEDINGS OF THE 25TH INTERNATIONAL CONFERENCE ON NUCLEAR ENGINEERING, 2017, VOL 2			V002T03A073-1	Lin, Zuokang; Zhu, Lin; Zhao, Chunfeng
385	TMSR FUEL CYCLE EVALUATION UNDER A SCREENING AND DECISION-MAKING FRAMEWORK	PROCEEDINGS OF THE 25TH INTERNATIONAL CONFERENCE ON NUCLEAR ENGINEERING, 2017, VOL 7			V007T10A024	Wu Jian-hui; Chen Jin-gen; Cai Xiang-zhou
386	ANALYSIS OF SUSTAINABLE THORIUM FUEL UTILIZATION IN MOLTEN SALT REACTORS STARTING FROM ENRICHED URANIUM	PROCEEDINGS OF THE 25TH INTERNATIONAL CONFERENCE ON NUCLEAR ENGINEERING, 2017, VOL 5			V005T05A033-1	Cui, Deyang; Cai, Xiangzhou; Chen, Jingen
387	AN INNOVATIVE SPHERICAL FUEL ELEMENT TO INHIBIT THE INFILTRATION OF LIQUID FLUORIDE SALT IN MOLTEN SALT REACTOR	PROCEEDINGS OF THE 25TH INTERNATIONAL CONFERENCE ON NUCLEAR ENGINEERING, 2017, VOL 3			UNSP V003T02A0023-1	Zhong, Yajuan; Lin, Jun; Xu, Liujun
388	THERMAL HYDRAULICS ANALYSIS OF THE FLUORIDE-SALT-COOLED, HIGH TEMPERATURE REACTOR	PROCEEDINGS OF THE 25TH INTERNATIONAL CONFERENCE ON NUCLEAR ENGINEERING, 2017, VOL 5			V005T05A020	Fu, Yao; Sun, Qiang; Zhou, Chong
389	BREEDING PROPERTIES STUDY ON HIGH POWER THORIUM MOLTEN	PROCEEDINGS OF THE 25TH INTERNATIONAL			V005T05A026	Liu, Yafen; Guo, Rui; Cai,

	SALT REACTOR	CONFERENCE ON NUCLEAR ENGINEERING, 2017, VOL 5				Xiangzhou
390	CONTROL SCHEME RESEARCH OF 10MW FLUORIDE SALT COOLED HIGH TEMPERATURE EXPERIMENT REACTOR	PROCEEDINGS OF THE 25TH INTERNATIONAL CONFERENCE ON NUCLEAR ENGINEERING, 2017, VOL 5			V005T05 A009	Ruan, Jian; Zou, Yang; Li, Minghai
391	Application of the Probability-Based Safety Analysis for the Reliability Evaluation of a Special Fuel Salt Release System Design in the Molten Salt Reactor	PROCEEDINGS OF THE 25TH INTERNATIONAL CONFERENCE ON NUCLEAR ENGINEERING, 2017, VOL 5			V005T05 A027	Yang Qun; Li Minghai; Hou Jie
392	In situ investigations of structures evolution of Mg doped Zn4Sb3	Key Engineering Materials	727		178	Wang, Yu; Li, Hong; Yang, Ying-Guo
393	Thorium molten salt reactor nuclear energy system (TMSR)	MOLTEN SALT REACTORS AND THORIUM ENERGY			531	Dai, Zhimin;;
394	高温剪断式触发吸收球非能动停堆装置可行性分析	核技术	40	7	70605	乔延凯;曹云; 程懋松
395	高温原位氟化熔盐红外吸收光谱装置研制	核技术	40	7	70604	刘舒婷;苏涛; 张鹏
396	g 射线辐照对超高分子量聚乙烯/改性纳米伊蒙土复合材料的拉伸性能及热稳定性的影响	辐射研究与辐射工艺学报	35	4	40303	董鹏刚;陈有双; 唐忠锋
397	聚焦太阳能热发电用熔盐腐蚀研究现状与展望	腐蚀科学与防护技术	29	3	282	孙华;苏兴治; 张鹏
398	辐射接枝法制备动态超疏水棉织物及其性能研究	高分子学报		2	315	李景烨;王自强; 虞鸣
399	基于氢同位素研究商用钯银合金膜的渗氚性能	原子能科学技术	51	8	1494	黄豫;韩兴博; 姚剑
400	低放废水沉淀/蒸发/离子交换处理系统的调试	中国给水排水	33	6	135	秦强;王帅; 马洪军
401	质谱在锕系配位化学研究中的应用	核化学与放射化学	39	1	1	陈秀婷;李晴暖; 龚昱
402	钍基熔盐堆核能系统中熔盐的蒸馏纯化与分离	核化学与放射化学	39	1	36	耿俊霞;窦强; 王子豪
403	NaF 吸附剂上 MoF_6 的脱附	核化学与放射化学	39	1	43	李杨娟;程治强; 窦强
404	固态燃料熔盐堆自适应功率控制器设计及分析	核技术	40	9	90602	王京华;程懋松; 戴志敏
405	FHR 在全厂断电事故下对 RVACS 散热能力的要求	核技术	40	9	90603	赵晶;王凯; 焦小伟

406	翅片管熔盐对流传热特性研究	核技术	40	7	70602	樊奇伟;朱海华; 陈玉爽
407	一体化小型氟盐冷却高温堆瞬态特性分析	核技术	40	6	60603	谢雪松;程懋松; 何兆忠
408	熔盐球床堆堆芯入口热工水力特性数值分析	核技术	40	9	90601	冯权胜;徐博; 潘登
409	超级均匀化方法用于球床氟盐冷却高温堆扩散计算	核技术	40	9	90604	戴明;朱贵凤; 戴叶
410	基于 SCALE/TRITON 的单流双区熔盐堆燃耗计算方法	核技术	40	8	80602	崔德阳;夏少鹏; 余呈刚
411	GPU 加速的球床式氟盐冷却高温堆堆芯热工水力程序研发	核技术	40	7	70603	鄂彦志;邹杨; 郭威
412	固态燃料熔盐堆稳态核热耦合程序开发	核动力工程	38	2	1	彭玉;邹杨; 戴叶
413	钍基液态燃料熔盐实验堆氙毒分析	核技术	40	4	40602	郭晨;冀锐敏; 陈金根
414	基于球床密实实验装置的熔盐堆分流板设计	核技术	40	4	40605	梅牡丹;林大富; 陈兴伟
415	氟盐冷却高温堆主冷却剂放射性源项研究	原子能科学技术	51	3	462	周波;严睿; 邹杨
416	圆柱容器内生成单粒径颗粒堆积的两阶段重力落球算法	核技术	40	2	20601	刘峰瑞;黄建平; 黎忠
417	基于熔盐快堆的模型优化与 Th-U 增殖性能研究	核技术	40	2	20603	李光超;邹杨; 余呈刚
418	基于 CITATION-ORIGEN2 球床堆平衡态计算程序的实现	原子能科学技术	51	1	113	戴明;朱贵凤; 戴叶
419	纳米压痕技术表征 T800 碳纤维的弹性模量和硬度	宇航材料工艺	47	4	79	张东生;李新涛; 夏汇浩
420	上海软 X 射线装置中纯永磁移相器的积分场垫补	核技术	40	7	70102	王建军;张伟; 周巧根
421	V 型凹口对液态熔盐堆用核石墨构件应力分析的影响	核技术	40	7	70601	杨雄;曾广礼; 顾晨光
422	三种不同碳纤维的纳米压痕行为	复合材料学报	34	6	1340	张东生;李新涛; 夏汇浩
423	微束分析仪器在金属材料研究中的应用	电子显微学报	36	3	293	贾彦彦;赵同新; 李哲夫
424	犬骨型核石墨四点弯曲实验与模拟	核技术	40	5	50601	顾晨光;曾广礼; 杨雄
425	10 MW 固态燃料钍基熔盐堆稳态物理-热工耦合	核技术	40	8	80603	陈家豪;张海青; 朱智勇
426	胺肟基尼龙66纤维的制备及其对模拟核工业废水中铀的选择性吸附	辐射研究与辐射工艺学报	35	4	40304	张明星;李荣; 邢哲
427	聚丙烯腈纳米纤维的辐射氧化及热性能变化	高分子材料科学与工程	33	6	60	徐翔宇;刘伟华; 王谋华
428	辐射接枝制备聚丙烯纤维基海水提铀吸	核技术	40	5	50301	李荣;庞利娟; 张

	附剂					明星
429	伽马射线辐照技术制备石墨烯基功能材料的研究进展	辐射研究与辐射工艺学报	35	2	20101	张伯武;俞初红;沈蓉芳
430	外泌体定量检测的研究进展及其在疾病诊疗中的应用	辐射研究与辐射工艺学报	35	3	30101	苏静;宋世平;

2018

No.	论文名称	期刊名称	期	卷	页	作者
1	Ultrabroad and Angle Tunable THz Filter Based on Multiplexed Metallic Bar Resonators	IEEE PHOTONICS TECHNOLOGY LETTERS	30	24	2103	Liu, Weiwei; Dai, Zijie; Yang, Jing
2	A novel input power control strategy for high-power dynamic dipole power supply for proton therapy	NUCLEAR INSTRUMENTS & METHODS IN PHYSICS RESEARCH SECTION A-ACCELERATORS SPECTROMETERS DETECTORS AND ASSOCIATED EQUIPMENT	911		25	Tan, Songqing; Li, Rui; Guo, Chunlong
3	First-principle atomistic thermodynamic study on the early-stage corrosion of NiCr alloy under fluoride salt environment	PHYSICAL CHEMISTRY CHEMICAL PHYSICS	20	45	28832	Yin, Ya-Ru; Ren, Cui-Lan; Han, Han
4	Influence of alpha-clustering nuclear structure on the rotating collision system	NUCLEAR SCIENCE AND TECHNIQUES	29	12	186	Xu, Zhi-Wan; Zhang, Song; Ma, Yu-Gang
5	Formation and Characterization of Zr4+ Stabilized by Neutral Tridentate Ligands in the Gas Phase	JOURNAL OF THE AMERICAN SOCIETY FOR MASS SPECTROMETRY	29	12	2327	Chen, Xiuting; Li, Qingnuan; Gong, Yu
6	Nonlinear energy chirp compensation with corrugated structures	NUCLEAR SCIENCE AND TECHNIQUES	29	12	175	Wang, Zhen; Feng, Chao; Huang, Da-Zhang
7	Stress analysis of the TMSR graphite component under irradiation conditions	NUCLEAR SCIENCE AND TECHNIQUES	29	12	173	Yang, Xiong; Gao, Yan-Tao; Zhong, Yang
8	Crystal structure of the periplasmic domain of TssL, a key membrane component of Type VI secretion system	INTERNATIONAL JOURNAL OF BIOLOGICAL MACROMOLECULES	120		1474	Wang, Xiangbei; Sun, Bo; Xu, Mengxue
9	Molecular dynamics investigation on the local structures and transport properties of uranium ion in LiCl-KCl molten salt	JOURNAL OF NUCLEAR MATERIALS	511		75	Dai, Jian-Xing; Zhang, Wei; Ren, Cui-Lan
10	Th-U breeding performance in a Channel-type molten salt Fast reactor with different starting fuels	ANNALS OF NUCLEAR ENERGY	122		91	Yu, Chenggang; He, Long; Zou, Chunyan
11	The packing factor of the pebble bed in molten salt reactor	ANNALS OF NUCLEAR ENERGY	122		118	Chen, Xingwei; Zou, Yang; Yan, Rui

12	Preliminary study on TRUs utilization in a small modular Th-based molten salt reactor (smTMSR)	NUCLEAR ENGINEERING AND DESIGN	339		75	Zou, Chunyan; Zhu, Guifeng; Yu, Chenggang
13	Studies of particle size distribution of Non-Exchangeable Organically Bound Tritium activities in the soil around Qinshan Nuclear Power Plant	JOURNAL OF ENVIRONMENTAL RADIOACTIVITY	192		362	Zhang, Qin; Du, Lin; Dai, Zhong-qin
14	Uniform Pt quantum dots-decorated porous g-C3N4 nanosheets for efficient separation of electron-hole and enhanced solar-driven photocatalytic performance	JOURNAL OF COLLOID AND INTERFACE SCIENCE	531		119	Sun, Fanfei; Tan, Siyu; Zhang, Hao
15	Unexpectedly High Salt Accumulation inside Carbon Nanotubes Soaked in Dilute Salt Solutions	PHYSICAL REVIEW LETTERS	121	22	226102	Wang, Xueliang; Shi, Guosheng; Liang, Shanshan
16	Controlling crystal polymorphism of isotactic poly(1-butene) by incorporating long chain branches	SOFT MATTER	14	44	8872	Maimaitiming, Aizezi; Zhang, Maojiang; Hu, Jiangtao
17	Better scCO(2) Foaming of Polypropylene via Earlier Crystallization with the Addition of Composite Nucleating Agent	INDUSTRIAL & ENGINEERING CHEMISTRY RESEARCH	57	46	15916	Yang, Chenguang; Xing, Zhe; Wang, Mouhua
18	Reexamining the isospin-relaxation time in intermediate-energy heavy-ion collisions	PHYSICAL REVIEW C	98	5	54608	Wang, Han-Sheng; Xu, Jun; Li, Bao-An
19	Synchrotron Big Data Science	SMALL	14	46	1802291	Wang, Chunpeng; Steiner, Ullrich; Sepe, Alessandro
20	Effects of nanobubbles on peptide self-assembly	NANOSCALE	10	42	20007	Wang, Yujiao; Shen, Zhiwei; Guo, Zhen
21	Anionic uranyl oxyfluorides as a bifunctional platform for highly selective ion-exchange and photocatalytic degradation of organic dyes	DALTON TRANSACTIONS	47	42		Yue, Zenghui; Lin, Jian; Silver, Mark A.
22	Electrochemical and Spectroscopic Study of Homo- and Hetero-Dimetallic Phthalocyanines as Catalysts for the Oxygen Reduction Reaction in Acidic Media	CHEMELECTROCHEM	5	22	3478	Wang, Xiaojiang; Liu, Yang; Wang, Ying
23	Design of a 7-MeV APF DTL with robust considerations	NUCLEAR INSTRUMENTS & METHODS IN PHYSICS RESEARCH SECTION A-ACCELERATORS SPECTROMETERS DETECTORS AND	908		49	Xie, Xiucui; Pu, Yuehu; Yang, Fan

24	The high level application architecture of the control system for SHINE	ASSOCIATED EQUIPMENT NUCLEAR INSTRUMENTS & METHODS IN PHYSICS RESEARCH SECTION A-ACCELERATORS SPECTROMETERS DETECTORS AND ASSOCIATED EQUIPMENT	908		167	Lv, Huihui; Leng, Yongbin; Yan, Yingbing
25	Investigating different Lambda and (Lambda)over-bar polarizations in relativistic heavy-ion collisions	PHYSICS LETTERS B	786		255	Han, Zhang-Zhu; Xu, Jun;
26	Nanoplatelet modulation in 2D/3D perovskite targeting efficient light-emitting diodes	NANOSCALE	10	41	19322	Wu, Tian; Yang, Yingguo; Zou, Yatao
27	Graphene oxide-silver nanocomposites modulate biofilm formation and extracellular polymeric substance (EPS) production	NANOSCALE	10	41	19603	Liu, Shima; Cao, Shuting; Guo, Jingyang
28	The effects of aerogen-bonding on the geometries and spectral properties of several small molecular clusters containing XeO3	JOURNAL OF PHYSICS-CONDENSED MATTER	30	44	444001	Miao, Junjian; Xiong, Zhenhai; Gao, Yi
29	Application of Electronic Counting Rules for Ligand-Protected Gold Nanoclusters	ACCOUNTS OF CHEMICAL RESEARCH	51	11	2739	Xu, Wen Wu; Zeng, Xiao Cheng; Gao, Yi
30	Formation and stability of ultrasonic generated bulk nanobubbles	CHINESE PHYSICS B	27	11	118104	Mo, Chen-Ran; Wang, Jing; Fang, Zhou
31	Neutronics modeling and analysis of the TMSR-SF1 fuel lattice and full core with explicit fuel particle distribution and random pebble loadings	PROGRESS IN NUCLEAR ENERGY	109		171	Sun, Kaichao; Wilson, Jarod; Hauptman, Sara
32	The wave optical whole process design of the soft X-ray interference lithography beamline at SSRF	JOURNAL OF SYNCHROTRON RADIATION	25		1869	Xue, Chaofan; Meng, Xiangyu; Wu, Yanqing
33	Effect of SO42- on the corrosion of 316L stainless steel in molten FLiNaK salt	CORROSION SCIENCE	144		224	Qiu, Jie; Leng, Bin; Liu, Huajian
34	The effect of moisture on the desorption behavior of UF6 from NaF adsorbent	JOURNAL OF RADIOANALYTICAL AND NUCLEAR CHEMISTRY	318	2	1325	Cheng, Zhiqiang; Hu, Congwei; Cui, Rongrong
35	Chemical and electrochemical studies on the solubility of UO2 in molten FLINAK with ZrF4 additive	JOURNAL OF NUCLEAR MATERIALS	510		256	Peng, Hao; Shen, Miao; Zuo, Yong
36	Improving the ceramic yield of polycarbosilane by radiation cross-linking	INTERNATIONAL JOURNAL OF APPLIED	15	6	1510	Zhou, Lulu; Cheng, Yong; Zhang, Wenfa

	in the presence of multifunctional monomers	CERAMIC TECHNOLOGY				
37	Review of fully coherent free-electron lasers	NUCLEAR SCIENCE AND TECHNIQUES	29	11	160	Feng, Chao; Deng, Hai-Xiao;
38	The morphology and structure of crystals in Qing Dynasty purple-gold glaze excavated from the Forbidden City	JOURNAL OF THE AMERICAN CERAMIC SOCIETY	101	11	5229	Liu, Zhen; Jia, Cui; Li, Li
39	DNA Nanostructure-Based Systems for Intelligent Delivery of Therapeutic Oligonucleotides	ADVANCED HEALTHCARE MATERIALS	7	20	1701153	Hu, Qinqin; Wang, Sheng; Wang, Lihua
40	Combustion Fabrication of Nanoporous Graphene for Ionic Separation Membranes	ADVANCED FUNCTIONAL MATERIALS	28	43	1805026	Li, Zhan; Zhang, Xin; Tan, Hongxin
41	DNA Nanostructure-Programmed Like-Charge Attraction at the Cell-Membrane Interface	ACS CENTRAL SCIENCE	4	10	1344	Ding, Hongming; Li, Jiang; Chen, Nan
42	Effect of confinement on water rotation via quantum tunnelling	NANOSCALE	10	39	18622	Zhang, Depeng; Zhang, Zhiyuan; Jiang, Wanrun
43	Antinuclei in heavy-ion collisions	PHYSICS REPORTS-REVIEW SECTION OF PHYSICS LETTERS	760		1	Chen, Jinhui; Keane, Declan; Ma, Yu-Gang
44	Nanodiamond autophagy inhibitor allosterically improves the arsenical-based therapy of solid tumors	NATURE COMMUNICATIONS	9		4347	Cui, Zhifen; Zhang, Yu; Xia, Kai
45	Simulating the chiral magnetic wave in a box system	PHYSICAL REVIEW C	98	4	44904	Zhou, Wen-Hao; Xu, Jun;
46	The beam-based alignment for soft X-ray free-electron lasers via genetic algorithm	NUCLEAR INSTRUMENTS & METHODS IN PHYSICS RESEARCH SECTION A-ACCELERATORS SPECTROMETERS DETECTORS AND ASSOCIATED EQUIPMENT	905		104	Zeng, Li; Feng, Chao; Gu, Duan
47	Serum protein corona-responsive autophagy tuning in cells	NANOSCALE	10	37	18055	Kong, Huating; Xia, Kai; Ren, Ning
48	Theoretical study of fluorine-induced surface segregation of Cr in non-passivated Ni-based alloys	JOURNAL OF APPLIED PHYSICS	124	13	135302	Yin, Ya-Ru; Ren, Cui-Lan; Han, Han
49	Formation and Stability of Surface/Bulk Nanobubbles Produced by Decompression at Lower Gas Concentration	JOURNAL OF PHYSICAL CHEMISTRY C	122	39	22418	Fang, Zhou; Wang, Lei; Wang, Xingya
50	Achieving a Record-High Yield Rate of 120.9 mu g(NH3) mg(cat)(-1). h(-1) for	ADVANCED MATERIALS	30	40	1803498	Geng, Zhigang; Liu, Yan; Kong,

	N-2 Electrochemical Reduction over Ru Single-Atom Catalysts					Xiangdong
51	Operando X-ray spectroscopic tracking of self-reconstruction for anchored nanoparticles as high-performance electrocatalysts towards oxygen evolution	ENERGY & ENVIRONMENTAL SCIENCE	11	10	2945	Song, Sanzhao; Zhou, Jing; Su, Xiaozhi
52	Assessment of Catalytic Activities of Gold Nanoclusters with Simple Structure Descriptors	ACS CATALYSIS	8	10	9702	Xu, Haoxiang; Cheng, Daojian; Gao, Yi
53	Effects of silicon carbide on the corrosion of metallic materials in molten LiF-NaF-KF salt	CORROSION SCIENCE	143		157	Xue, Wandong; Yang, Xinmei; Ye, Xiang-Xi
54	Effects of alloying elements on the corrosion behavior of Ni-based alloys in molten NaCl-KCl-MgCl(2)salt at different temperatures	CORROSION SCIENCE	143		187	Sun, Hua; Zhang, Peng; Wang, Jianqiang
55	Corrosion performance of Ni-16%wt.Mo-X%wt.SiC alloys in FLiNaK molten salt	CORROSION SCIENCE	143		240	Yang, Chao; Muransky, Ondrej; Zhu, Hanliang
56	Oscillator Strengths and Integral Cross Sections of the Valence-shell Excitations of the Oxygen Molecule Studied by Fast Electron and Inelastic X-Ray Scattering	ASTROPHYSICAL JOURNAL SUPPLEMENT SERIES	238	2	26	Liu, Ya-Wei; Xu, Long-Quan; Xiong, Tao
57	Contact angle measurement in lattice Boltzmann method	COMPUTERS & MATHEMATICS WITH APPLICATIONS	76	7	1686	Wen, Binghai; Huang, Bingfang; Qin, Zhangrong
58	Preparation and investigation of multicomponent alkali nitrate/nitrite salts for low temperature thermal energy storage	ENERGY	160		1021	Li, Xiang; Wang, Yang; Wu, Shuang
59	Real-time label-free analysis of the thermostability of DNA structures using GelRed	NUCLEAR SCIENCE AND TECHNIQUES	29	10	138	Hao, Ya-Ya; Liu, Lei; Zhang, Lu-Hao
60	Numerical study of the dynamic characteristics of a single-layer graphite core in a thorium molten salt reactor	NUCLEAR SCIENCE AND TECHNIQUES	29	10	141	Zhong, Yang; Yang, Xiong; Ding, Dong
61	ESR study of free radicals in polysilazane irradiated by gamma rays	RADIATION PHYSICS AND CHEMISTRY	151		108	Zhou, Lulu; Zhao, Chenxuan; Liu, Weihua
62	Theoretical investigation of Ti and Ni co-doping on the anti-disproportionation ability of ZrCo alloy	MATERIALS RESEARCH EXPRESS	5	10	105501	Yang, Guo; Liu, Wenguan; Wu, Shengwei
63	Effect of concentration of Cr3+ in LiF-NaF-KF salt on the corrosion of SiC	JOURNAL OF NUCLEAR MATERIALS	509		527	Xue, Wandong; Yang, Xinmei; Zhou,

						Xingtai
64	Sm-149 evolution behavior in a small modular molten salt reactor	ANNALS OF NUCLEAR ENERGY	120		100	Wu, Jianhui; Chen, Jingen; Yu, Chenggang
65	Infrared Spectra of the SO2F2- Anion in Solid Argon and Neon	JOURNAL OF PHYSICAL CHEMISTRY A	122	38	7723	Wei, Rui; Chen, Xiuting; Gong, Yu
66	Fabricating Quasi-Free-Standing Graphene on a SiC(0001) Surface by Steerable Intercalation of Iron	JOURNAL OF PHYSICAL CHEMISTRY C	122	37	21484	Shen, Kongchao; Sun, Haoliang; Hu, Jinping
67	Anomalous behavior of membrane fluidity caused by copper-copper bond coupled phospholipids	SCIENTIFIC REPORTS	8		14093	Jiang, Xiankai; Zhang, Jinjin; Zhou, Bo
68	Uranium-Induced Changes in Crystal-Field and Covalency Effects of Th4+ in Th1-xUxO2 Mixed Oxides Probed by High-Resolution X-ray Absorption Spectroscopy	INORGANIC CHEMISTRY	57	18	11404	Bao, Hongliang; Duan, Peiquan; Zhou, Jing
69	Highly Efficient CO2 Electroreduction on ZnN4-based Single-Atom Catalyst	ANGEWANDTE CHEMIE-INTERNATIONAL EDITION	57	38	12303	Yang, Fa; Song, Ping; Liu, Xiaozhi
70	System-level performance optimization of molten-salt packed-bed thermal energy storage for concentrating solar power	APPLIED ENERGY	226		225	Zhao, Bing-chen; Cheng, Mao-song; Liu, Chang
71	Hindered Gas Transport through an Aqueous Salt Solution Interface	JOURNAL OF PHYSICAL CHEMISTRY C	122	36	20774	Fang, Gang; Chen, Jige;
72	Operando Spectroscopic Identification of Active Sites in NiFe Prussian Blue Analogues as Electrocatalysts: Activation of Oxygen Atoms for Oxygen Evolution Reaction	JOURNAL OF THE AMERICAN CHEMICAL SOCIETY	140	36	11286	Su, Xiaozhi; Wang, Yu; Zhou, Jing
73	A numerical comparison between internal cooling and side cooling of the reflection mirror for Spatial and Spin (S-2) beam-line at SSRF	NUCLEAR INSTRUMENTS & METHODS IN PHYSICS RESEARCH SECTION A-ACCELERATORS SPECTROMETERS DETECTORS AND ASSOCIATED EQUIPMENT	902		190	Jin, Li-Min; Zhu, Wan-Qian; Wang, Yong
74	Observation of beta-delayed He-2 emission from the proton-rich nucleus Al-22	PHYSICS LETTERS B	784		12	Wang, Y. T.; Fang, D. Q.; Wang, K.
75	Chemical interaction dictated energy level alignment at the N,N '-dipentyl-3,4,9,10-perylenedicarboximide/ CH3NH3PbI3 interface	APPLIED PHYSICS LETTERS	113	11	113901	Zhang, Xiaonan; Su, Zhenhuang; Zhao, Bin

76	Accelerated active phase transformation of NiO powered by Pt single atoms for enhanced oxygen evolution reaction	CHEMICAL SCIENCE	9	33	6803	Lin, Chao; Zhao, Yonghui; Zhang, Haojie
77	Infrared Spectroscopic and Theoretical Studies of Group 3 Metal Isocyanide Molecules	JOURNAL OF PHYSICAL CHEMISTRY A	122	35	7099	Chen, Xiuting; Li, Qingnuan; Andrews, Lester
78	Multiparticle azimuthal cumulants in p plus Pb collisions from a multiphase transport model	PHYSICAL REVIEW C	98	3	34903	Nie, Mao-Wu; Huo, Peng; Jia, Jiangyong
79	Synchrotron Radiation Based Study of the Catalytic Mechanism of Ag+ to Chalcopyrite Bioleaching by Mesophilic and Thermophilic Cultures	MINERALS	8	9	382	Nie, Zhenyuan; Zhang, Weiwei; Liu, Hongchang
80	Improvement of Corrosion Resistance of Hastelloy-N Alloy in LiF-NaF-KF Molten Salt by Laser Cladding Pure Metallic Coatings	COATINGS	8	9	322	Zhu, Hongmei; Li, Baichun; Chen, Minghui
81	Formation of chromium carbide coatings on HT250 steel by thermal diffusion processes in fluoride molten salt bath	VACUUM	155		219	Su, Xingzhi; Zhao, Sufang; Hou, Juan
82	Optimization of Th-U fuel breeding based on a single-fluid double-zone thorium molten salt reactor	PROGRESS IN NUCLEAR ENERGY	108		144	Li, G. C.; Cong, P.; Yu, C. G.
83	Fuel pebble optimization for the thorium-fueled Pebble Bed Fluoride salt-cooled high-temperature reactor (PB-TFHR)	PROGRESS IN NUCLEAR ENERGY	108		179	Fang, Y. H.; Li, X. X.; Yu, C. G.
84	AlN coatings on Hastelloy-N alloy offering superior corrosion resistance in LiF-KF-NaF molten salt	JOURNAL OF FLUORINE CHEMISTRY	213		80	Zhu, Hongmei; Li, Baichun; Chen, Minghui
85	Influence of alpha-Al2O3 and AlF(3)on pyrohydrolysis of Li3AlF6	NUCLEAR SCIENCE AND TECHNIQUES	9		10.1007/s41365-018-0465-2	Peng, Jia; Zheng, Xiao-Bei; Liu, Yu-Xia
86	Mechanical-force-promoted peptide assembly: a general method	NUCLEAR SCIENCE AND TECHNIQUES	29	9	131	Yuan, Yue; Du, Qi-Qi-Ge; Wang, Yu-Jiao
87	Electronic structure tuning during facile construction of two-phase tungsten based electrocatalyst for hydrogen evolution reaction	ELECTROCHIMICA ACTA	283		834	Shi, Meiqin; Li, Wang; Fang, Jun
88	Molten-salt synthesis of porous La0.6Sr0.4CO0.2Fe0.8O2.9 perovskite as	NANO RESEARCH	11	9	4796	Song, Sanzhao; Zhou, Jing; Zhang,

	an efficient electrocataiyst for oxygen evolution					Shuo
89	Preliminary in situ teeth study of the narrow-ridged finless porpoises remains using microsynchrotron radiation X-ray fluorescence and laser ablation inductively coupled plasma mass spectrometry	X-RAY SPECTROMETRY	47	5	388	Zheng, Yi; Zhang, Ya; Tang, Wenqiao
90	First-principles study on structural, mechanical and electronic properties of thorium dichalcogenides under high pressure	JOURNAL OF NUCLEAR MATERIALS	508		147	Guo, Yongliang; Chen, Juncai; Wang, Changying
91	Research on chemical durability of iron phosphate glass wasteforms vitrifying SrF2 and CeF3	JOURNAL OF NUCLEAR MATERIALS	508		286	Liu, Xueyang; Qiao, Yanbo; Qian, Zhenghua
92	Microstructural evolution of amorphous Si2BC3N nanopowders upon heating at high temperatures: High pressures reverse the nucleation order of SiC and BN(C)	JOURNAL OF THE AMERICAN CERAMIC SOCIETY	101	9	4321	Liang, Bin; Jia, Dechang; Liao, Xingqi
93	A Green and lower-temperature synthesis of two-color fluorescent nitrogen dopedgraphene quantum dots	DYES AND PIGMENTS	156		379	Xue, Zhipeng; Gao, Hui; Li, Xiaolong
94	Directed flow in an extended multiphase transport model	PHYSICAL REVIEW C	98	2	24914	Guo, Chong-Qiang; Liu, He; Xu, Jun
95	Hydrogen embrittlement susceptibility of a Ni-16Mo-7Cr base superalloy	MATERIALS SCIENCE AND ENGINEERING A-STRUCTURAL MATERIALS PROPERTIES MICROSTRUCTURE AND PROCESSING	733		291	Han, Fenfen; He, Suixia; Liu, Min
96	Understanding and prediction of the structures of ligand-protected gold nanoclusters using electron counting rule	ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY	256			Gao, Yi; Xu, Wenwu; Zeng, Xiao
97	Structural evolution of metal nanoparticles in operando conditions	ABSTRACTS OF PAPERS OF THE AMERICAN CHEMICAL SOCIETY	256			Gao, Yi; Zhu, Beien;
98	Irradiation resistance study of binderless nanopore-isotropic graphite for use in molten salt nuclear reactors	NUCLEAR ENGINEERING AND DESIGN	335		231	Liu, Min; Zhang, Wenting; Song, Jinliang
99	Dynamic characteristics identification of two graphite bricks in molten salt reactor considering fluid-structure interaction	NUCLEAR ENGINEERING AND DESIGN	335		409	Zhong, Yang; Yang, Xiong; Ding, Dong
100	Unexpected refacetting of palladium nanoparticles under atmospheric N-2 conditions	CHEMICAL COMMUNICATIONS	54	62	8587	Zhang, Xun; Meng, Jun; Zhu, Beien

101	Sol-Gel Technology Plus Radiation Curing: A Novel and Facile Technique for Preparing Thick, Large-Area Hyperbranched Polysiloxane Hybrids	INDUSTRIAL & ENGINEERING CHEMISTRY RESEARCH	57	31	10372	Chen, Shaoyun; Zhuo, Dongxian; Hu, Jiangtao
102	Gain-guided X-ray free-electron laser oscillator	APPLIED PHYSICS LETTERS	113	6	61106	Li, Kai; Deng, Haixiao;
103	pH-sensitive microfiltration membrane prepared from polyethersulfone grafted with poly(itaconic acid) synthesized by simultaneous irradiation in homogeneous phase	WATER SCIENCE AND TECHNOLOGY	78	3	602	Fan, Kai; Zhou, Guoqing; Zhang, Jinjin
104	A 1-m non-resonant inelastic x-ray scattering spectrometer at BL15U, Shanghai Synchrotron Radiation Facility	REVIEW OF SCIENTIFIC INSTRUMENTS	89	8	85108	Ni, Dong-Dong; Kang, Xu; Yan, Shuai
105	The properties of surface nanobubbles formed on different substrates	CHINESE PHYSICS B	27	8	86803	Zou, Zheng-Lei; Quan, Nan-Nan; Wang, Xing-Ya
106	A modular process for the treatment of high level liquid waste (HLLW) using solvent-impregnated graphene aerogel	HYDROMETALLURGY	179		167	Chen, Mumei; Li, Zheng; Geng, Yiyun
107	Stress and thickness calculation of a bolted flat cover with double metal sealing rings	NUCLEAR SCIENCE AND TECHNIQUES	8		10.1007/s41365-018-0457-2	Wang, Xiao-Yan; Zhu, Shi-Feng; Wang, Xiao
108	Analysis of Th-U breeding capability for an accelerator-driven subcritical molten salt reactor	NUCLEAR SCIENCE AND TECHNIQUES	29	8	121	Zhao, Xue-Chao; Cui, De-Yang; Cai, Xiang-Zhou
109	Helium ion irradiation-induced microstructure evolution on the surfaces of thin nickel foils	NUCLEAR INSTRUMENTS & METHODS IN PHYSICS RESEARCH SECTION B-BEAM INTERACTIONS WITH MATERIALS AND ATOMS	428		24	Gao, Jie; Huang, Hefei; Liu, Xiang
110	Spatially correlated coherent diffractive imaging method	APPLIED OPTICS	57	22	6527	Tao, Xulei; Xu, Zijian; Liu, Haigang
111	Solubility of radioactive inorganic salt in supercritical water	JOURNAL OF RADIOANALYTICAL AND NUCLEAR CHEMISTRY	317	2	947	Qin, Qiang; Wang, Shuai; Peng, Honghua
112	Poly-adenine-mediated fluorescent spherical nucleic acid probes for live-cell imaging of endogenous tumor-related mRNA	NANOMEDICINE-NANOTECHNOLOGY BIOLOGY AND MEDICINE	14	6	1797	Zhu, Dan; Zhao, Dongxia; Huang, Jiaxuan
113	Upgrade of the X-ray pinhole camera	NUCLEAR SCIENCE AND	29	8	115	Gao, Bo; Leng,

	system at SSRF	TECHNIQUES				Yong-Bin; Chen, Han-Jiao
114	Effects of fuel salt composition on fuel salt temperature coefficient (FSTC) for an under-moderated molten salt reactor (MSR)	NUCLEAR SCIENCE AND TECHNIQUES	29	8	110	Li, Xiao-Xiao; Ma, Yu-Wen; Yu, Cheng-Gang
115	Bunch-by-bunch longitudinal phase monitor at SSRF	NUCLEAR SCIENCE AND TECHNIQUES	29	8	113	Zhou, Yi-Mei; Chen, Han-Jiao; Cao, Shan-Shan
116	Visualizing glioma margins by real-time tracking of gamma-glutamyltranspeptidase activity	BIOMATERIALS	173		1	Liu, Yingchao; Tan, Jie; Zhang, Yi
117	Wavelet analysis of extended X-ray absorption fine structure data: Theory, application	PHYSICA B-CONDENSED MATTER	542		12	Xia, Zhaoming; Zhang, Hao; Shen, Kongchao
118	Commentary and introduction to the virtual special issue on nanocarbons for electrochemistry	CARBON	134		539	Yang, Nianjun; Swain, Greg M.; Einaga, Yasuaki
119	Facile synthesis of the nitrogen-doped graphene quantum dots at low temperature for cellular labeling	MATERIALS RESEARCH BULLETIN	104		83	Pang, Yuqian; Gao, Hui; Lai, Luhao
120	Complex silica composite nanomaterials templated with DNA origami	NATURE	559	7715	593	Liu, Xiaoguo; Zhang, Fei; Jing, Xinxin
121	Effect of plasmonic near field on the emittance of plasmon-enhanced photocathode	NUCLEAR INSTRUMENTS & METHODS IN PHYSICS RESEARCH SECTION A-ACCELERATORS SPECTROMETERS DETECTORS AND ASSOCIATED EQUIPMENT	897		14	Jiang, Zenggong; Li, Xudong; Huang, Dazhang
122	Engineering the Coordination Environment of Single-Atom Platinum Anchored on Graphdiyne for Optimizing Electrocatalytic Hydrogen Evolution	ANGEWANDTE CHEMIE-INTERNATIONAL EDITION	57	30	9382	Yin, Xue-Peng; Wang, Hong-Juan; Tang, Shang-Feng
123	Manipulation of facet orientation in hybrid perovskite polycrystalline films by cation cascade	NATURE COMMUNICATIONS	9		2793	Zheng, Guanhaojie; Zhu, Cheng; Ma, Jingyuan
124	Doping Ti to achieve microstructural refinement and strength enhancement in a high volume fraction Y2O3 dispersion strengthened Cu	JOURNAL OF ALLOYS AND COMPOUNDS	753		18	Zhou, Dengshan; Wang, Xinkai; Zeng, Wei
125	Structural and thermodynamic stability of uranyl-deferiprone complexes and the	DALTON TRANSACTIONS	47	26	8764	Wang, Xiaomei; Ji, Guoxun; Shi, Cen

	removal efficacy of U(vi) at the cellular level					
126	Equally sloped tomography based X-ray full-field nano-CT at Shanghai Synchrotron Radiation Facility	NUCLEAR INSTRUMENTS & METHODS IN PHYSICS RESEARCH SECTION A-ACCELERATORS SPECTROMETERS DETECTORS AND ASSOCIATED EQUIPMENT	896		108	Wang, Yudan; Ren, Yuqi; Zhou, Guangzhao
127	Highly Active Surface Structure in Nanosized Spinel Cobalt-Based Oxides for Electrocatalytic Water Splitting	JOURNAL OF PHYSICAL CHEMISTRY C	122	26	14447	Zhou, Jing; Li, Jiong; Zhang, Linjuan
128	Atomic inner-shell radiation seeded free-electron lasers	PHYSICAL REVIEW ACCELERATORS AND BEAMS	21	7	70701	Zhang, Han; Li, Kai; Yan, Jiawei
129	Highly Durable and Robust Superhydrophobic/Superoleophilic Cotton Fabric with Well-designed Roughness for Oil/Water Separation	FIBERS AND POLYMERS	19	7	1522	Hu, Jiangtao; Gao, Qianhong; Xu, Lu
130	Bifunctional Nitrogen and Cobalt Codoped Hollow Carbon for Electrochemical Syngas Production	ADVANCED SCIENCE	5	7	1800177	Song, Xiaokai; Zhang, Hao; Yang, Yuqi
131	Kinoform and saw-tooth X-ray refractive lenses development at SSRF	JOURNAL OF INSTRUMENTATION	13		C07005	Xu, J.; Liu, G.; Huang, Q.
132	Multiple Amplified Electrochemical Detection of MicroRNA-21 Using Hierarchical Flower-like Gold Nanostructures Combined with Gold-enriched Hybridization Chain Reaction	ELECTROANALYSIS	30	7	1349	Zhu, Dan; Liu, Wei; Cao, Wenfang
133	Elastic squared form factor and binding effect of carbon dioxide studied by the high resolution X-ray scattering	JOURNAL OF ELECTRON SPECTROSCOPY AND RELATED PHENOMENA	226		41	Huang, Xin-Chao; Xu, Long-Quan; Ni, Dong-Bong
134	Extraction and structural investigation of jute cellulose nanofibers	NUCLEAR SCIENCE AND TECHNIQUES	29	7	106	Bian, Zhong-Xuan; Miao, Xia-Ran; Lin, Jin-You
135	Immobilization of radioactive fluoride waste in aluminophosphate glass: a molecular dynamics simulation	NUCLEAR SCIENCE AND TECHNIQUES	29	7	92	Gao, Ling-Wei; Xia, Xiao-Bin; Xu, Xiu-Qing
136	Implantation-decay method to study the beta-delayed charged particle decay	NUCLEAR SCIENCE AND TECHNIQUES	29	7	98	Wang, Yu-Ting; Fang, De-Qing; Xu, Xin-Xing
137	Two-dimensional Na-Cl crystals of unconventional stoichiometries on	NATURE CHEMISTRY	10	7	776	Shi, Guosheng; Chen, Liang; Yang,

	graphene surface from dilute solution at ambient conditions					Yizhou
138	Preparation and adsorption performance of a NiO/MgF2 composite adsorbent	JOURNAL OF RADIOANALYTICAL AND NUCLEAR CHEMISTRY	317	1	287	Li, Sasa; Cheng, ZhiQiang; Zhang, Linjuan
139	Systematic design and three-dimensional simulation of X-ray FEL oscillator for Shanghai Coherent Light Facility	NUCLEAR INSTRUMENTS & METHODS IN PHYSICS RESEARCH SECTION A-ACCELERATORS SPECTROMETERS DETECTORS AND ASSOCIATED EQUIPMENT	895		40	Li, Kai; Deng, Haixiao;
140	Development and application of optimal burnup estimation methodology for pebble bed reactor	ANNALS OF NUCLEAR ENERGY	117		343	Tang, Haibo; Han, Jianlong; Li, XiaoXiao
141	Anion photoelectron spectroscopy and chemical bonding of ThO2- and ThO3-	JOURNAL OF CHEMICAL PHYSICS	148	24	244304	Li, Yanli; Zou, Jinghan; Xiong, Xiao-Gen
142	Thermally-induced reversible structural isomerization in colloidal semiconductor CdS magic-size clusters	NATURE COMMUNICATIONS	9		2499	Zhang, Baowei; Zhu, Tingting; Ou, Mingyang
143	beta-delayed particle emission from Mg-21	EUROPEAN PHYSICAL JOURNAL A	54	6	107	Wang, Yu-Ting; Fang, De-Qing; Wang, Kang
144	A general synthetic approach for hexagonal phase tungsten nitride composites and their application in the hydrogen evolution reaction	JOURNAL OF MATERIALS CHEMISTRY A	6	23	10967	Jin, Haiyan; Zhang, Hao; Chen, Jiayi
145	Immobilization of Alkali Metal Fluorides via Recrystallization in a Cationic Lamellar Material, [Th(MoO4)(H2O)(4)Cl]Cl center dot H2O	INORGANIC CHEMISTRY	57	12	6778	Lin, Jian; Bao, Hongliang; Qie, Meiying
146	Conceptual design and preliminary performance analysis of a hybrid nuclear-solar power system with molten-salt packed-bed thermal energy storage for on-demand power supply	ENERGY CONVERSION AND MANAGEMENT	166		174	Zhao, Bing-chen; Cheng, Mao-song; Liu, Chang
147	A Rechargeable High-Temperature Molten Salt Iron-Oxygen Battery	CHEMSUSCHEM	11		1886102/cssc.201800237	Peng, Cheng; Guan, Chengzhi; Lin, Jun
148	A remark on the sign change of the four-particle azimuthal cumulant in small	PHYSICS LETTERS B	781		117	Bzdak, Adam; Ma, Guo-Liang;

	systems					
149	In Situ Reduction from Uranyl Ion into a Tetravalent Uranium Trimer and Hexamer Featuring Ion-Exchange Properties and the Alexandrite Effect	INORGANIC CHEMISTRY	57	11	6753	Lin, Jian; Yue, Zenghui; Silver, Mark A.
150	The effect of Ar ion beam irradiation on mesocarbon microbead-densified graphite as the matrix of fuel elements in molten-salt nuclear reactors	NEW CARBON MATERIALS	33	3	268	Xu Liu-jun; Wang Hao-ran; Lin Jun
151	Thermodynamic Evaluation of NaF-MFn(M=Be, U, Th) Systems for Molten Salt Reactor	CHEMICAL RESEARCH IN CHINESE UNIVERSITIES	34	3	457	Wu Shuang; Li Xiang; Zhang Peng
152	Experimental Investigation and Thermodynamic Modeling of the NaCl-NaNO3-Na2SO4 Ternary System	CHEMICAL RESEARCH IN CHINESE UNIVERSITIES	34	3	475	Li Xiang; Fei Zejie; Wang Yang
153	Phosphate-Based Ultrahigh Molecular Weight Polyethylene Fibers for Efficient Removal of Uranium from Carbonate Solution Containing Fluoride Ions	MOLECULES	23	6	1245	Li, Rong; Li, Yuna; Zhang, Maojiang
154	Emerging Characterizing Techniques in the Fine Structure Observation of Metal Halide Perovskite Crystal	CRYSTALS	8	6	232	Shen, Kongchao; Hu, Jinping; Liang, Zhaofeng
155	Enhancement of water self-diffusion at super-hydrophilic surface with ordered water	CHINESE PHYSICS B	27	6	60101	Yu, Xiao-Meng; Qi, Chong-Hai; Wang, Chun-Lei
156	Pt Single Atoms Embedded in the Surface of Ni Nanocrystals as Highly Active Catalysts for Selective Hydrogenation of Nitro Compounds	NANO LETTERS	18	6	3785	Peng, Yuhan; Geng, Zhigang; Zhao, Songtao
157	Bunch-by-bunch beam size measurement during injection at Shanghai Synchrotron Radiation Facility	NUCLEAR SCIENCE AND TECHNIQUES	29	6	79	Chen, Han-Jiao; Chen, Jie; Gao, Bo
158	Study of the crosstalk evaluation for cavity BPM	NUCLEAR SCIENCE AND TECHNIQUES	29	6	83	Chen, Jian; Leng, Yong-Bin; Yu, Lu-Yang
159	X-ray fluorescence microtomography based on polycapillary-focused X-rays from laboratory source	NUCLEAR SCIENCE AND TECHNIQUES	29	6	85	Feng, Bing-Gang; Tao, Fen; Yang, Yi-Ming
160	A density functional theory study on the interaction between UO22+ and the carbamoylphosphoramidic acid ligand for uranium extraction from seawater	NUCLEAR SCIENCE AND TECHNIQUES	29	6	90	Guo, Xiao-Jing; Li, Cheng; Hu, Jiang-Tao
161	Electron-beam radiation effects on the structure and properties of polypropylene	NUCLEAR SCIENCE AND TECHNIQUES	29	6	87	Wang, Heng-Ti; Jiang, Hai-Qing;

	at low dose rates					Shen, Rong-Fang
162	Study on neutronics design of ordered-pebble-bed fluoride-salt-cooled high-temperature experimental reactor	NUCLEAR SCIENCE AND TECHNIQUES	29	6	81	Yan, Rui; Yu, Shi-He; Zou, Yang
163	2.856 GHz microwave signal extraction from mode-locked Er-fiber lasers with sub-100 femtosecond timing jitter	NUCLEAR SCIENCE AND TECHNIQUES	29	6	91	Zhang, Wen-Yan; Liu, Xiao-Qing; Feng, Lie
164	Decay modes of highly excited nuclei	NUCLEAR SCIENCE AND TECHNIQUES	29	6	78	Zhang, Zhen-Fang; Fang, De-Qing; Ma, Yu-Gang
165	Enormously improved CH3NH3PbI3 film surface for environmentally stable planar perovskite solar cells with PCE exceeding 19.9%	NANO ENERGY	48		10	Yang, Yingguo; Feng, Shanglei; Li, Meng
166	Functional reliability analysis of a molten salt natural circulation system	NUCLEAR ENGINEERING AND DESIGN	332		127	Jiao, X.; Shao, S.; Wang, K.
167	A novel atmospheric tritium sampling system	NUCLEAR INSTRUMENTS & METHODS IN PHYSICS RESEARCH SECTION A-ACCELERATORS SPECTROMETERS DETECTORS AND ASSOCIATED EQUIPMENT	892		127	Qin, Lailai; Xia, Zhenghai; Gu, Shaozhong
168	Theoretical study of ZrCoH3 and the anti-disproportionation ability of alloying elements	INTERNATIONAL JOURNAL OF HYDROGEN ENERGY	43	22	10410	Yang, Guo; Liu, Wenguan; Tan, Jie
169	Chemically activating MoS2 via spontaneous atomic palladium interfacial doping towards efficient hydrogen evolution	NATURE COMMUNICATIONS	9		2120	Luo, Zhaoyan; Ouyang, Yixin; Zhang, Hao
170	Reconstruction of Supported Metal Nanoparticles in Reaction Conditions	ANGEWANDTE CHEMIE-INTERNATIONAL EDITION	57	22	6464	Duan, Manyi; Yu, Jian; Meng, Jun
171	Synergistic effects on microstructural evolution and hardening of the Hastelloy N alloy under subsequent He and Xe ion irradiation	JOURNAL OF APPLIED PHYSICS	123	20	205901	Gao, Jie; Huang, Hefei; Liu, Jizhao
172	The structural isomerism in gold nanoclusters	NANOSCALE	10	20	9476	Xu, Wen Wu; Zeng, Xiao Cheng; Gao, Yi
173	Formation of nano-sized M2C carbides in Si-free GH3535 alloy	SCIENTIFIC REPORTS	8		8158	Jiang, Li; Wang Yinling; Hu, Rui
174	The effect of He bubbles on the swelling and hardening of UNS N10003 alloy	JOURNAL OF ALLOYS AND COMPOUNDS	746		153	Lei, Guanhong; Xie, Ruobing; Huang, Hefei

175	Angiopep-2-conjugated Ag2S Quantum Dot for NIR-II Imaging of Brain Tumors	ACTA CHIMICA SINICA	76	5	393	Xu Yi; Zhao Yan; Zhang Yejun
176	Systematic Study in Mammalian Cells Showing No Adverse Response to Tetrahedral DNA Nanostructure	ACS APPLIED MATERIALS & INTERFACES	10	18	15442	Xia, Kai; Kong, Huating; Cui, Yunzhi
177	Evaporation of nanoscale water on a uniformly complete wetting surface at different temperatures	PHYSICAL CHEMISTRY CHEMICAL PHYSICS	20	17	12272	Guo, Yuwei; Wan, Rongzheng;
178	Charge Neutralization Drives the Shape Reconfiguration of DNA Nanotubes	ANGEWANDTE CHEMIE-INTERNATIONAL EDITION	57	19	5418	Liu, Pi; Zhao, Yan; Liu, Xiaoguo
179	An ATP-Responsive Linear DNA Hydrogel	ACTA POLYMERICA SINICA		5	553	Wang, Fei; Zhong, Rui-bo; Tang, Qian
180	One-Dimensional Zinc Oxide Nanomaterials for Application in High-Performance Advanced Optoelectronic Devices	CRYSTALS	8	5	223	Ding, Meng; Guo, Zhen; Zhou, Lianqun
181	Ionic Liquids Incorporating Polyamide 6: Miscibility and Physical Properties	POLYMERS	10	5	562	Zheng, Xin; Lin, Qingqing; Jiang, Pan
182	Framework-Nucleic-Acid-Enabled Biosensor Development	ACS SENSORS	3	5	903	Yang, Fan; Li, Qian; Wang, Lihua
183	Intergranular stress study of TC11 titanium alloy after laser shock peening by synchrotron-based high-energy X-ray diffraction	AIP ADVANCES	8	5	55126	Su, R.; Li, L.; Wang, Y. D.
184	Sub-picosecond electron bunch length measurement using coherent transition radiation at SXFEL	NUCLEAR SCIENCE AND TECHNIQUES	29	5	74	Bian, Yu; Zhang, Wen-Yan; Liu, Bo
185	Tritium concentrations in precipitation in Shanghai	NUCLEAR SCIENCE AND TECHNIQUES	29	5	63	Deng, Ke; Wang, Ling; Xia, Zheng-Hai
186	Upgrade of macromolecular crystallography beamline BL17U1 at SSRF	NUCLEAR SCIENCE AND TECHNIQUES	29	5	68	Wang, Qi-Sheng; Zhang, Kun-Hao; Cui, Yin
187	Coexistence of Polaronic States and Superconductivity in Iron-Pnictide Compound Ba2Ti2Fe2As4O	CHINESE PHYSICS LETTERS	35	5	57401	Rong, Li-Yuan; Shi, Xun; Richard, Pierre
188	Deciphering active biocompatibility of iron oxide nanoparticles from their intrinsic antagonism	NANO RESEARCH	11	5	2746	Wang, Lu; Wang, Zejun; Li, Xiaoming
189	The dynamic micro computed tomography at SSRF	JOURNAL OF INSTRUMENTATION	13		C05006	Chen, R.; Xu, L.; Du, G.
190	Nanoscale delivery systems for cancer immunotherapy	MATERIALS HORIZONS	5	3	344	Wang, Zejun; Liu, Wenhan; Shi, Jiye

191	A sagittally confined high-resolution spectrometer in the 'water window'	JOURNAL OF SYNCHROTRON RADIATION	25		738	Li, Zhuo; Li, Bin;
192	Thickness-dependent structural characteristics for a sputtering-deposited chromium monolayer and Cr/C and Cr/Sc multilayers	JOURNAL OF SYNCHROTRON RADIATION	25		785	Jiang, Hui; Wang, Hua; Zhu, Jingtao
193	Thermodynamic modeling of LiF-NaF-KF-CrF3 system	JOURNAL OF FLUORINE CHEMISTRY	209		6	Yin, Huiqin; Zhang, Peng; An, Xuehui
194	Microstructure, hardness and modulus of carbon-ion-irradiated new SiC fiber (601-4)	JOURNAL OF NUCLEAR MATERIALS	503		91	Huang, Qing; Lei, Guanhong; Liu, Renduo
195	Influence of graphite-alloy interactions on corrosion of Ni-Mo-Cr alloy in molten fluorides	JOURNAL OF NUCLEAR MATERIALS	503		116	Ai, Hua; Hou, Juan; Ye, Xiang-Xi
196	Phase-retrieval-based synchrotron X-ray micro-tomography for 3D structural characterization and quantitative analysis of agalloch eaglewood	WOOD SCIENCE AND TECHNOLOGY	52	3	839	Liu, Huiqiang; Lin, Fanghua; Lin, Jianhuan
197	Experimental investigation of the bed structure in liquid salt cooled pebble bed reactor	NUCLEAR ENGINEERING AND DESIGN	331		24	Chen, Xingwei; Zhang, Jie; Dai, Ye
198	X-ray absorption spectroscopy study of synthetic cobalt blue pigments similar to Kangxi blue and white porcelain	JOURNAL OF THE AMERICAN CERAMIC SOCIETY	101	5	2130	Luo, Mi; Zhang, Maolin; Yan, Wensheng
199	Adsorption behavior of thorium on N,N,N',N '-tetraoctyldiglycolamide (TODGA) impregnated graphene aerogel	TALANTA	181		311	Chen, Mumei; Li, Zheng; Geng, Yiyun
200	Preparation of highly fluorescent sulfur doped graphene quantum dots for live cell imaging	JOURNAL OF LUMINESCENCE	197		147	Jin, Kaixiang; Gao, Hui; Lai, Luhao
201	Sharing of Na+ by Three -COO- Groups at Deprotonated Carboxyl-Terminated Self-Assembled Monolayer-Charged Aqueous Interface	JOURNAL OF PHYSICAL CHEMISTRY C	122	16	9111	Liu, Xing; Huang, Gang; Hu, Kuan-Kan
202	Facet-specific interaction between methanol and TiO2 probed by sum-frequency vibrational spectroscopy	PROCEEDINGS OF THE NATIONAL ACADEMY OF SCIENCES OF THE UNITED STATES OF AMERICA	115	17	E3888	Yang, Deheng; Li, Yadong; Liu, Xinyi
203	High brightness fully coherent x-ray amplifier seeded by a free-electron laser oscillator	PHYSICAL REVIEW ACCELERATORS AND BEAMS	21	4	40702	Li, Kai; Yan, Jiawei; Feng, Chao
204	The irradiation hardening of Ni-Mo-Cr and Ni-W-Cr alloy under Xe26+ ion	NUCLEAR INSTRUMENTS & METHODS IN PHYSICS	421		50	Chen, Huaican; Hai, Yang; Liu, Renduo

	irradiation	RESEARCH SECTION B-BEAM INTERACTIONS WITH MATERIALS AND ATOMS				
205	Transition to thorium fuel cycle for TMSR	NUCLEAR ENGINEERING AND DESIGN	330		420	Zou, C. Y.; Cai, C. Z.; Yu, C. G.
206	Nucleic acid-based electrochemical nanobiosensors	BIOSENSORS & BIOELECTRONICS	102		479	Abi, Alireza; Mohammadpour, Zahra; Zuo, Xiaolei
207	Functionalization of cotton fabrics with highly durable polysiloxane-TiO2 hybrid layers: potential applications for photo-induced water-oil separation, UV shielding, and self-cleaning	JOURNAL OF MATERIALS CHEMISTRY A	6	14	6085	Hu, Jiangtao; Gao, Qianhong; Xu, Lu
208	Electrostatic force spectroscopy revealing the degree of reduction of individual graphene oxide sheets	BEILSTEIN JOURNAL OF NANOTECHNOLOGY	9		1146	Shen, Yue; Wang, Ying; Zhou, Yuan
209	Terahertz time-domain spectroscopy of L-histidine hydrochloride monohydrate	JOURNAL OF MOLECULAR STRUCTURE	1157		486	Zong, Siqi; Ren, GuanHua; Li, Shaoping
210	Elimination technology of noise introduced by top-up injection in synchrotron radiation infrared beamline	JOURNAL OF INFRARED AND MILLIMETER WAVES	37	2	251	Zhu Hua-Chun; Tong Ya-Jun; Ji Te
211	An efficient and reusable quaternary ammonium fabric adsorbent prepared by radiation grafting for removal of Cr(VI) from wastewater	ENVIRONMENTAL SCIENCE AND POLLUTION RESEARCH	25	11	11045	Pang, Li-juan; Hu, Jiang-tao; Zhang, Mao-jiang
212	Corrosion of Incoloy 800H alloys with nickel cladding in FLiNaK salts at 850 degrees C	CORROSION SCIENCE	133		349	Dai, Qilong; Ye, Xiang-Xi; Ai, Hua
213	Magnetic field stability of PrFeB magnets developed by GBD for cryogenic permanent magnet undulators	JOURNAL OF RARE EARTHS	36	4	385	He, Yongzhou; Bao, Xiaoqing; Zhou, Qiaogen
214	Study on inherent neutron sources in MSR	NUCLEAR SCIENCE AND TECHNIQUES	29	4	47	Ji, Rui-Min; Yu, Cheng-Gang; Li, Ming-Hai
215	Omega and phi production in Au plus Au collisions at root s(NN),=11.5 and 7.7 GeV in a dynamical quark coalescence model	NUCLEAR SCIENCE AND TECHNIQUES	29	4	54	Jin, Xiao-Hai; Chen, Jin-Hui; Ma, Yu-Gang
216	The effect of ball-milling time and annealing temperature on fracture toughness of Ni-3 wt.% SiC using small punch testing	MATERIALS CHARACTERIZATION	138		289	Yang, Chao; Wei, Tao; Muransky, Ondrej

217	The control of magnetic vortex state in rectangular nanomagnet	JOURNAL OF MAGNETISM AND MAGNETIC MATERIALS	451		379	Li, Junqin; Wang, Yong; Cao, Jiefeng
218	Electron-beam-induced post-grafting polymerization of acrylic acid onto the surface of Kevlar fibers	RADIATION PHYSICS AND CHEMISTRY	145		74	Xu, Lu; Hu, Jiangtao; Ma, Hongjuan
219	Identification of binuclear Co2N5 active sites for oxygen reduction reaction with more than one magnitude higher activity than single atom CoN4 site	NANO ENERGY	46		396	Xiao, Meiling; Zhang, Hao; Chen, Yongting
220	A special coarsening mechanism for intergranular helium bubbles upon heating: A combined experimental and numerical study	SCRIPTA MATERIALIA	147		93	Gao, Jie; Huang, Hefei; Liu, Xiang
221	Direct Growth of Graphene on Silicon by Metal-Free Chemical Vapor Deposition	NANO-MICRO LETTERS	10	2	20	Tai, Lixuan; Zhu, Daming; Liu, Xing
222	pH and thermal-dependent ultrafiltration membranes prepared from poly (methacrylic acid) grafted onto polyethersulfone synthesized by simultaneous irradiation in homogenous phase (vol 543, pg 335, 2017)	JOURNAL OF MEMBRANE SCIENCE	551		222	Fan, Kai;;
223	Possible scenarios for the transition to thorium fuel cycle in molten salt reactor by using enriched uranium	PROGRESS IN NUCLEAR ENERGY	104		75	Cui, D. Y.; Li, X. X.; Xia, S. P.
224	The Scanning Magnets for Proton Therapy Designed by SINAP	IEEE TRANSACTIONS ON APPLIED SUPERCONDUCTIVITY	28	3	4400904	Jia, Bolei; Zhao, Zhentang; Ouyang, Lianhua
225	The Design and Magnetic Measurement of a SuperBend Dipole Magnet at SSRF	IEEE TRANSACTIONS ON APPLIED SUPERCONDUCTIVITY	28	3	4002403	Qian, Maofei; Zhou, Qiaogen; Wang, Hongfei
226	Comparison of heavy-ion transport simulations: Collision integral in a box	PHYSICAL REVIEW C	97	3	34625	Zhang, Ying-Xun; Wang, Yong-Jia; Colonna, Maria
227	Investigation on Molecular Structures of Electron-Beam-Irradiated Low-Density Polyethylene by Rheology Measurements	INDUSTRIAL & ENGINEERING CHEMISTRY RESEARCH	57	12	4298	Wang, Hengti; Li, Linfan; Guan, Jipeng
228	Imaging of Colorectal Cancers Using Activatable Nanoprobes with Second Near-Infrared Window Emission	ANGEWANDTE CHEMIE-INTERNATIONAL EDITION	57	14	3626	Xu, Ge; Yan, Qinglong; Lv, Xiaoguang
229	Effect of in-medium nucleon-nucleon cross section on proton-proton momentum correlation in intermediate-energy heavy-ion collisions	PHYSICAL REVIEW C	97	3	34617	Wang, Ting-Ting; Ma, Yu-Gang; Zhang, Chun-Jian

230	Shape Evolution of Metal Nanoparticles in Binary Gas Environment	JOURNAL OF PHYSICAL CHEMISTRY C	122	11	6144	Meng, Jun; Zhu, Beien; Gao, Yi
231	Reactivating Catalytic Surface: Insights into the Role of Hot Holes in Plasmonic Catalysis	SMALL	14	12	1703510	Peng, Tianhuan; Miao, Junjian; Gao, Zhaoshuai
232	An overview on the research of Sr2IrO4-based system probed by X-ray absorption spectroscopy	MODERN PHYSICS LETTERS B	32	8	1850094	Cheng, Jie; Zhu, Chaomin; Ma, Jingyuan
233	Nanoscale mapping of dielectric properties based on surface adhesion force measurements	BEILSTEIN JOURNAL OF NANOTECHNOLOGY	9		900	Wang, Ying; Shen, Yue; Wang, Xingya
234	Unraveling the oxygen vacancy structures at the reduced CeO2(111) surface	PHYSICAL REVIEW MATERIALS	2	3	35802	Han, Zhong-Kang; Yang, Yi-Zhou; Zhu, Beien
235	Comprehensive Understanding of the Spatial Configurations of CeO2 in NiO for the Electrocatalytic Oxygen Evolution Reaction: Embedded or Surface-Loaded	ADVANCED FUNCTIONAL MATERIALS	28	11	1706056	Gao, Wei; Xia, Zhaoming; Cao, Fangxian
236	Investigating the quark flavor dependence of the chiral magnetic effect with a multiphase transport model	PHYSICAL REVIEW C	97	3	34909	Huang, Ling; Ma, Chun-Wang; Ma, Guo-Liang
237	Bandwidth broadening of X-ray free electron laser pulses with the natural gradient of planar undulator	NUCLEAR INSTRUMENTS & METHODS IN PHYSICS RESEARCH SECTION A-ACCELERATORS SPECTROMETERS DETECTORS AND ASSOCIATED EQUIPMENT	884		11	Song, Minghao; Yan, Jiawei; Li, Kai
238	MoS2 Nanoprobe for MicroRNA Quantification Based on Duplex-Specific Nuclease Signal Amplification	ACS APPLIED MATERIALS & INTERFACES	10	9	7852	Xiao, Mingshu; Man, Tiantian; Zhu, Changfeng
239	Efficient selection methods for black phosphorene nanoribbons	NANOSCALE	10	9	4385	Wei, Ning; Chen, Yang; Zhang, Yingyan
240	Experimental study of heat transfer enhancement for molten salt with transversely grooved tube heat exchanger in laminar-transition-turbulent regimes	APPLIED THERMAL ENGINEERING	132		95	Chen, Y. S.; Tian, J.; Fu, Y.
241	Experimental investigation and thermodynamic modeling of the LiNO3-RbNO3-AgNO3 system and its subsystems	JOURNAL OF ALLOYS AND COMPOUNDS	736		124	Li, Xiang; Xie, Leidong;
242	Laser test of the prototype of CEE time projection chamber	NUCLEAR SCIENCE AND TECHNIQUES	29	3	41	Huang, Wen; Lu, Fei; Li, He

243	Preliminary design of a femtosecond timing system for large accelerator facilities	NUCLEAR SCIENCE AND TECHNIQUES	29	3	32	Liu, Ming; Dai, Xiao-Lei; Yin, Chong-Xian
244	Determination of boron concentration in uranium fuel samples by ICP-OES following a separation step by cation exchange resin	NUCLEAR SCIENCE AND TECHNIQUES	29	3	44	Luo, Yan; Cong, Hai-Xia; Cui, Rong-Rong
245	Study on Nondestructive Testing for CuAz Preservative-Treated Bamboo with Synchrotron Radiation X-Ray	SPECTROSCOPY AND SPECTRAL ANALYSIS	38	3	901	Peng Guan-yun; Liu Xing-e; Yang Shu-min
246	Hydrophobic nanochannel self-assembled by amphipathic Janus particles confined in aqueous nano-space	CHINESE PHYSICS B	27	3	30505	Fang, Gang; Sheng, Nan; Jin, Tan
247	Nucleon effective masses in neutron-rich matter	PROGRESS IN PARTICLE AND NUCLEAR PHYSICS	99		29	Li, Bao-An; Cai, Bao-Jun; Chen, Lie-Wen
248	Shannon information entropy in heavy-ion collisions	PROGRESS IN PARTICLE AND NUCLEAR PHYSICS	99		120	Ma, Chun-Wang; Ma, Yu-Gang;
249	Functionalized polyethylene fibers for the selective capture of palladium ions from aqueous solution	APPLIED SURFACE SCIENCE	433		116	Pang, Li-juan; Li, Rong; Hu, Jiang-tao
250	A First-Principles Study on the Vibrational and Electronic Properties of Zr-C MXenes	COMMUNICATIONS IN THEORETICAL PHYSICS	69	3	336	Wang, Chang-Ying; Guo, Yong-Liang; Zhao, Yuan-Yuan
251	Tris-amidoximate uranyl complexes via eta(2) binding mode coordinated in aqueous solution shown by X-ray absorption spectroscopy and density functional theory methods	JOURNAL OF SYNCHROTRON RADIATION	25		514	Zhang, Linjuan; Qie, Meiying; Su, Jing
252	Radiolysis products and degradation mechanism studies on tri-isoamyl phosphate (TiAP)	RADIOCHIMICA ACTA	106	3	239	Li, Ruifen; Cao, Xiaojun; Zhao, Haogui
253	Effect of Ti additions on structure and phase stability of Sb2Te3 thin films by experimental and theoretical methods	JOURNAL OF MATERIALS SCIENCE-MATERIALS IN ELECTRONICS	29	6	4704	Zhang, Ling; Song, Sannian; Xi, Wei
254	Synergistic effects between hydroxyl radicals and hydrated electrons on strengthening decomposition of an s-triazine compound: A combined experimental and theoretical study	CHEMOSPHERE	195		365	Tang, Liang; Lyu, Geng-xin; Mao, Wen
255	Evaluation of thermal physical properties of molten nitrate salts with low melting temperature	SOLAR ENERGY MATERIALS AND SOLAR CELLS	176		36	Zhang, Peng; Cheng, Jinhui; Jin, Yuan
256	Bacterial Analysis Using an	ACS APPLIED MATERIALS	10	8	6895	Li, Lanying; Wang,

	Electrochemical DNA Biosensor with Poly-Adenine-Mediated DNA Self-Assembly	& INTERFACES				Lele; Xu, Qin
257	Eliminating the microbunching-instability-induced sideband in a soft x-ray self-seeding free-electron laser	NUCLEAR INSTRUMENTS & METHODS IN PHYSICS RESEARCH SECTION A-ACCELERATORS SPECTROMETERS DETECTORS AND ASSOCIATED EQUIPMENT	882		22	Zhang, Kaiqing; Zeng, Li; Qi, Zheng
258	Temperature dependence of spherical micelles of PS3000-b-PAA(5000) studied by in-situ small angle X-ray scattering	ACTA PHYSICA SINICA	67	4	48301	Jin Xin; Yang Chun-Ming; Hua Wen-Qiang
259	Electromagnetic fields in small systems from a multiphase transport model	PHYSICAL REVIEW C	97	2	24910	Zhao, Xin-Li; Ma, Yu-Gang; Ma, Guo-Liang
260	Experimental investigation and thermodynamic modeling of an innovative molten salt for thermal energy storage (TES)	APPLIED ENERGY	212		516	Li, Xiang; Wu, Shuang; Wang, Yang
261	Optimizing the Crystallinity and Phase Separation of PTB7:PC71BM Films by Modified Graphene Oxide	JOURNAL OF PHYSICAL CHEMISTRY C	122	5	2572	Lv, Cheng-Kun; Zheng, Fei; Yang, Xiao-Yu
262	Identifying the Genotypes of Hepatitis B Virus (HBV) with DNA Origami Label	SMALL	14	6	UNSP 1701718	Liu, Ke; Pan, Dun; Wen, Yanqin
263	Merits of the Addition of PTFE Micropowder in Supercritical Carbon Dioxide Foaming of Polypropylene: Ultrahigh Cell Density, High Tensile Strength, and Good Sound Insulation	INDUSTRIAL & ENGINEERING CHEMISTRY RESEARCH	57	5	1498	Yang, Chenguang; Xing, Zhe; Wang, Mouhua
264	A Large Family of Centrosymmetric and Chiral f-Element-Bearing Iodate Selenates Exhibiting Coordination Number and Dimensional Reductions	INORGANIC CHEMISTRY	57	3	1676	Qie, Meiying; Lin, Jian; Kong, Fang
265	Design of wide-range energy material beamline at the Shanghai Synchrotron Radiation Facility	NUCLEAR SCIENCE AND TECHNIQUES	29	2	26	Chen, Zhen-Hua; Sun, Fan-Fei; Zou, Ying
266	New design for multi-crystal data collection at SSRF	NUCLEAR SCIENCE AND TECHNIQUES	29	2	21	Li, Bing; Huang, Sheng; Pan, Qiang-Yan
267	Wetting behaviors of methanol, ethanol, and propanol on hydroxylated SiO2 substrate	NUCLEAR SCIENCE AND TECHNIQUES	29	2	18	Nie, Xue-Chuan; Zhou, Bo; Wang, Chun-Lei

268	Spectroscopic study of beta-delayed particle emission from proton-rich nucleus Si-23	INTERNATIONAL JOURNAL OF MODERN PHYSICS E-NUCLEAR PHYSICS	27	2	1850014	Wang, K.; Fang, D. Q.; Wang, Y. T.
269	Anomalous compression behaviour in Nd2O3 studied by x-ray diffraction and Raman spectroscopy	AIP ADVANCES	8	2	25019	Jiang, Sheng; Liu, Jing; Bai, Ligang
270	Protection-against-water-attack determined difference between strengths of backbone hydrogen bonds in kinesin's neck zipper region	CHINESE PHYSICS B	27	2	28704	Qin, Jing-Yu; Geng, Yi-Zhao; Lu, Gang
271	Microstructural evolution and hardening of GH3535 alloy under energetic Xe ion irradiation at room temperature and 650 degrees C	JOURNAL OF NUCLEAR MATERIALS	499		431	Huang, Hefei; Gao, Jie; Radiguet, Bertrand
272	Scalar field coupling to Einstein tensor in regular black hole spacetime	GENERAL RELATIVITY AND GRAVITATION	50	2	18	Zhang, Chi; Wu, Chen;
273	Study on the microstructure evolution of TiO2-reinforced HDPE nanocomposites by synchrotron small angle X-ray scattering	POLYMER COMPOSITES	39	2	580	Li, Xiaoyun; Liu, Guoming; Tang, Zhongfeng
274	Effect of CrF3 on the corrosion behaviour of Hastelloy-N and 316L stainless steel alloys in FLiNaK molten salt	CORROSION SCIENCE	131		355	Yin, Huiqin; Qiu, Jie; Liu, Huajian
275	A study on K*(892)(0) and phi(1020) production in p-Pb and Pb-Pb collisions at the LHC from a multiphase transport model	JOURNAL OF PHYSICS G-NUCLEAR AND PARTICLE PHYSICS	45	2	25102	Liu, X. Y.; Chen, J. H.; Ma, C. W.
276	Targeted Imaging of Brain Tumors with a Framework Nucleic Acid Probe	ACS APPLIED MATERIALS & INTERFACES	10	4	3414	Tian, Tian; Li, Jiang; Xie, Cao
277	Microstructural characterization of Ni-201 weld cladding onto 304 stainless steel	SURFACE & COATINGS TECHNOLOGY	334		19	Shi, Xianwu; Yu, Kun; Jiang, Li
278	In Situ Probing of the Particle-Mediated Mechanism of WO3-Networked Structures Grown inside Confined Mesoporous Channels	SMALL	14	4	UNSP 1702565	Zhang, Lingling; Li, Jiang; You, Hongjun
279	In Situ Spatial Complementation of Aptamer-Mediated Recognition Enables Live-Cell Imaging of Native RNA Transcripts in Real Time	ANGEWANDTE CHEMIE-INTERNATIONAL EDITION	57	4	972	Wang, Zejun; Luo, Yao; Xie, Xiaodong
280	Electrochemical deposition of neodymium in LiF-CaF2 from Nd2O3 assisted by AlF3	ELECTROCHIMICA ACTA	261		289	Chen, Zi; She, Changfeng; Zheng, Haiyang
281	Nanomanipulation of Individual DNA	JOURNAL OF PHYSICAL	122	2	612	Wang, Ying; Shen,

	Molecules Covered by Single-Layered Reduced Graphene Oxide Sheets on a Solid Substrate	CHEMISTRY B				Yue; Li, Bin
282	Elliptic flow coefficients from transverse momentum conservation	PHYSICAL REVIEW C	97	1	14903	Bzdak, Adam; Ma, Guo-Liang;
283	Epitope Binning Assay Using an Electron Transfer-Modulated Aptamer Sensor	ACS APPLIED MATERIALS & INTERFACES	10	1	341	Li, Min; Guo, Xudong; Li, Hui
284	Carboxylic Acid Group-Induced Oxygen Vacancy Migration on an Anatase (101) Surface	LANGMUIR	34	1	546	Li, Yadong; Gao, Yi;
285	Unveiling the Atomic Structures of the Minority Surfaces of TiO2 Nanocrystals	CHEMISTRY OF MATERIALS	30	1	288	Yuan, Wentao; Meng, Jun; Zhu, Beien
286	Effect of proton irradiation on microstructure evolution of permanent magnet	ACTA PHYSICA SINICA	67	1	16104	Li Zhe-Fu; Jia Yan-Yan; Liu Ren-Duo
287	Criticality Properties and Control Rod Worth of the Critical Experiment Device for MSR Research	NUCLEAR TECHNOLOGY	204	2	203	Liu, Yafen; Yan, Rui; Zou, Yang
288	Uranium thermochemical cycle: hydrogen production demonstration	ENERGY SOURCES PART A-RECOVERY UTILIZATION AND ENVIRONMENTAL EFFECTS	40	21	2542	Chen, Aimei; Zheng, Xiaobei; Liu, Chunxia
289	Enhanced removal of heavy metals by zerovalent iron in designed magnetic reactors	ENVIRONMENTAL TECHNOLOGY	39	19	2542	Fan, Peng; Jiang, Xiao; Qiao, Junlian
290	Coherent nanoscale cobalt/cobalt oxide heterostructures embedded in porous carbon for the oxygen reduction reaction	RSC ADVANCES	8	50	28625	Li, Xue-Cheng; She, Fa-Shuang; Shen, Dong
291	Study on the Electrochemical Co-Reduction of Gd(III) and Al(III) in LiF-CaF2 Melt	JOURNAL OF THE ELECTROCHEMICAL SOCIETY	165	9	D411	Chen, Zi; She, Changfeng; Zheng, Haiyang
292	Electrochemical Behavior of UO2F2 and Its Electrodeposition from UO2F2-FLiNaK Melt	JOURNAL OF THE ELECTROCHEMICAL SOCIETY	165	7	D301	Han, Dong; She, ChangFeng; Peng, Jia
293	Development of a Coupled Code for Steady-State Analysis of the Graphite-Moderated Channel Type Molten Salt Reactor	SCIENCE AND TECHNOLOGY OF NUCLEAR INSTALLATIONS			405325 4	He, Long; Yu, Cheng-Gang; Guo, Wei
294	Development of the Tritium Transport Analysis Code for the Thorium-Based Molten Salt Reactor	NUCLEAR TECHNOLOGY	203	1	48	Zeng, Youshi; Wu, Shengwei; Liu, Wei
295	A new promising nucleating agent for	RSC ADVANCES	8	36	20061	Yang, Chenguang;

	polymer foaming: effects of hollow molecular-sieve particles on polypropylene supercritical CO2 microcellular foaming					Wang, Mouhua; Xing, Zhe
296	The preparation of a three dimensional terbium doped reduced graphene oxide aerogel with photoluminescence and paramagnetic properties	RSC ADVANCES	8	17	9287	Chen, Keqin; Gao, Hui; Wang, Dongdong
297	Determination of the Mercury Isotopic Ratio by Cold Vapor Generation Sector Field-Inductively Coupled Plasma-Mass Spectrometry Using Lead as the Internal Standard	ANALYTICAL LETTERS	51	12	1944	Tang, Xiaoxing; Qian, Yuan; Li, Yulan
298	Surrogate Fluid Experimental Study and CFD Simulation on the Hydraulic Characteristics of Vortex Diode	NUCLEAR SCIENCE AND ENGINEERING	189	3	282	Qu, Shi-Xiang; Wu, Yan-Hua; He, Zhao-Zhong
299	Thiolate-Protected Hollow Gold Nanospheres	ACTA PHYSICO-CHIMICA SINICA	34	7	770	Xu Wenwu; Gao Yi;
300	Study on the performance of a large-size CsI detector for high energy gamma-rays	NUCLEAR SCIENCE AND TECHNIQUES	29	1	7	Dong, He; Fang, De-Qing; Li, Chen
301	Transverse phase space reconstruction study in Shanghai soft X-ray FEL facility	NUCLEAR SCIENCE AND TECHNIQUES	29	1	9	Yu, Qing-Lin; Gu, Duan; Zhang, Meng
302	Protein-mimicking nanoparticle (Protmin)-based nanosensor for intracellular analysis of metal ions	NUCLEAR SCIENCE AND TECHNIQUES	29	1	5	Zhu, Dan; Zhao, Dong-Xia; Huang, Jia-Xuan
303	Fabrication of polyacrylamide-carbon nanotubes by One-Step Radiation-Induced Graft Polymerization	FULLERENES NANOTUBES AND CARBON NANOSTRUCTURES	26	1	12	Fan, Kai; Li, Jihao; Li, Linfan
304	A facile approach to fabricate few-layer chemically modified and reduced graphene oxide sheets: Combination of stitching, reduction and functionaliztion	FULLERENES NANOTUBES AND CARBON NANOSTRUCTURES	26	1	30	Fan, Kai; Li, Jihao; Li, Linfan
305	Electric field distribution and initial jet motion induced by spinneret configuration for molecular orientation in electrospun fibers	EUROPEAN POLYMER JOURNAL	98		330	Li, Xiang; Lin, Jinyou; Zeng, Yongchun
306	Structure and performances changes during tensile of aromatic copolysulfonamide fibers under different thermal temperatures via in-situ synchrotron SAXS/WAXS	EUROPEAN POLYMER JOURNAL	98		354	Li, Xiaoyun; Yu, Jinchao; Wang, Jianning
307	Optimization of pencil beam f-theta lens for high-accuracy metrology	OPTICAL ENGINEERING	57	1	15101	Peng, Chuanqian; He, Yumei; Wang,

						Jie
308	The role of EDTA on rutile flotation using Al3+ ions as an activator	RSC ADVANCES	8	9	4872	Xiao, Wei; Fang, Chaojun; Wang, Jun
309	Evolution of carbide precipitates in Hastelloy N joints during welding and post weld heat treatment	MATERIALS CHARACTERIZATION	135		311	Wang, Wanxia; Li, Chaowen; Jiang, Li
310	Insight into the Formation of Co@Co2C Catalysts for Direct Synthesis of Higher Alcohols and Olefins from Syngas	ACS CATALYSIS	8	1	228	Zhao, Ziang; Lu, Wei; Yang, Ruoou
311	Graphene oxide as an additive to improve perovskite film crystallization and morphology for high-efficiency solar cells	RSC ADVANCES	8	2	987	Zhang, Xiaonan; Ji, Gengwu; Xiong, Dongbin
312	Synergistic effects of different co-monomers on the uranium adsorption performance of amidoximated polyethylene nonwoven fabric in natural seawater	JOURNAL OF RADIOANALYTICAL AND NUCLEAR CHEMISTRY	315	1	111	Li, Rong; Ma, Hongjuan; Xing, Zhe
313	Characterization of organic matter pores in typical marine and terrestrial shales, China	JOURNAL OF NATURAL GAS SCIENCE AND ENGINEERING	49		56	Wang, Yu; Wang, Lihua; Wang, Jianqiang
314	Transverse momentum spectra and nuclear modification factors of charged particles in pp, p-Pb and Pb-Pb collisions at the LHC	JOURNAL OF HIGH ENERGY PHYSICS		11	13	STAR 合作组;;
315	Measurement of D-0, D+, D*+ and D-s(+) production in Pb-Pb collisions at root s(NN)=5:02 TeV	JOURNAL OF HIGH ENERGY PHYSICS		10		STAR 合作组;;
316	Medium modification of the shape of small-radius jets in central Pb-Pb collisions at root s(NN)=2:76 TeV	JOURNAL OF HIGH ENERGY PHYSICS		10	139	STAR 合作组;;
317	Azimuthally-differential pion femtoscopy relative to the third harmonic event plane in Pb-Pbcollisions at root(NN)-N-S=2.76TeV	PHYSICS LETTERS B	785		320	STAR 合作组;;
318	Inclusive J/psi production in Xe-Xe collisions at root s(NN)=5.44 TeV	PHYSICS LETTERS B	785		419	STAR 合作组;;
319	Measurements of low-p(T) electrons from semileptonic heavy-flavour hadron decays at mid-rapidity in pp and Pb-Pb collisions at root s(NN)=2.A76 TeV	JOURNAL OF HIGH ENERGY PHYSICS		10	61	STAR 合作组;;
320	Searching for states analogous to the C-12 Hoyle state in heavier nuclei using the thick target inverse kinematics technique	PHYSICAL REVIEW C	98	4	44601	STAR 合作组;;
321	Harmonic decomposition of three-particle azimuthal correlations at energies	PHYSICAL REVIEW C	98	3	34918	STAR 合作组;;

	available at the BNL Relativistic Heavy Ion Collider					
322	Low-p(T) e(+)e(-) Pair Production in Au plus Au Collisions at root s(NN)=200 GeV and U plus U Collisions at root s(NN)=193 GeV at STAR	PHYSICAL REVIEW LETTERS	121	13	132301	STAR 合作组;;
323	Two-particle angular correlations in pp and p-Pb collisions at energies available at the CERN Large Hadron Collider from a multiphase transport model	PHYSICAL REVIEW C	98	3	34912	STAR 合作组;;
324	Anisotropic flow in Xe-Xe collisions at root s(NN)=5.44 TeV	PHYSICS LETTERS B	784		82	STAR 合作组;;
325	Anisotropic flow of identified particles in Pb-Pb collisions at root s(NN)=5.02 TeV	JOURNAL OF HIGH ENERGY PHYSICS		9	6	STAR 合作组;;
326	Longitudinal double-spin asymmetries for pi(0)s in the forward direction for 510 GeV polarized pp collisions	PHYSICAL REVIEW D	98	3	32013	STAR 合作组;;
327	Longitudinal double-spin asymmetries for dijet production at intermediate pseudorapidity in polarized pp collisions at root s=200 GeV	PHYSICAL REVIEW D	98	3	32011	STAR 合作组;;
328	Azimuthal anisotropy in Cu plus Au collisions at root s(NN)=200 GeV	PHYSICAL REVIEW C	98	1	14915	STAR 合作组;;
329	Inclusive J/psi production at forward and backward rapidity in p-Pb collisions at root s(NN)=8.16 TeV	JOURNAL OF HIGH ENERGY PHYSICS		7	160	STAR 合作组;;
330	Global polarization of Lambda hyperons in Au plus Au collisions at root s(NN)=200 GeV	PHYSICAL REVIEW C	98	1	14910	STAR 合作组;;
331	Beam Energy Dependence of Jet-Quenching Effects in Au plus Au Collisions at root s(NN)=7.7, 11.5, 14.5, 19.6, 27, 39, and 62.4 GeV	PHYSICAL REVIEW LETTERS	121	3	32301	STAR 合作组;;
332	Energy dependence and fluctuations of anisotropic fow in Pb-Pb collisions at root s(NN)=5:02 and 2:76 TeV	JOURNAL OF HIGH ENERGY PHYSICS		7	103	STAR 合作组;;
333	Measurement of the inclusive J/psi polarization at forward rapidity in pp collisions at root s=8 TeV	EUROPEAN PHYSICAL JOURNAL C	78	7	562	STAR 合作组;;
334	Prompt and non-prompt J/psi production and nuclear modification at mid-rapidity in p-Pb collisions at root s(NN)=5.02 TeV	EUROPEAN PHYSICAL JOURNAL C	78	6	466	STAR 合作组;;
335	Measurement of the H-3(Lambda) lifetime in Au plus Au collisions at the BNL	PHYSICAL REVIEW C	97	5	54909	STAR 合作组;;

336	Relativistic Heavy Ion Collider Search for neutrinoless beta(+) EC decay of Te-120 with CUORE-0	PHYSICAL REVIEW C	97	5	55502	STAR 合作组;;
337	First Results from CUORE: A Search for Lepton Number Violation via 0 nu ss ss Decay of Te-130	PHYSICAL REVIEW LETTERS	120	13	132501	STAR 合作组;;
338	Beam-Energy Dependence of Directed Flow of Lambda, (Lambda)over-bar, K-+/-, K-s(0), and phi in Au plus Au Collisions	PHYSICAL REVIEW LETTERS	120	6	62301	STAR 合作组;;
339	Azimuthal transverse single-spin asymmetries of inclusive jets and charged pions within jets from polarized-proton collisions at root s=500 GeV	PHYSICAL REVIEW D	97	3	32004	STAR 合作组;;
340	Thermal performance analysis of molten-salt heat storage system in mixed packed-bed	Taiyangneng Xuebao/Acta Energiae Solaris Sinica	39	2	475	Zhao, Bingchen; Cheng, Maosong; Liu, Chang
341	Foaming of Irradiation Cross-Linked Polypropylene Using Supercritical Carbon Dioxide	Gaofenzi Cailiao Kexue Yu Gongcheng/Polymeric Materials Science and Engineering	34	3	127	Li, Xiaohu; Cheng, Yong; Zhou, Lulu
342	Analysis of 16N Source Term in Primary Coolant System of FHR	Yuanzineng Kexue Jishu/Atomic Energy Science and Technology	52	4	652	Zhou, Bo; Yan, Rui; Zou, Yang
343	The Magnetic Field Measurement Systems for a Cryogenic Undulator and a Superconducting Undulator at SSRF	Journal of Physics: Conference Series	1067	8		Wang, H.F.; Zhang, J.M.; Qian, M.F.
344	Elastic, mechanical, electronic, and defective properties of Zr − Al − C nanolaminates from first principles	Journal of the American Ceramic Society	101	2	756	Wang, Changying; Han, Han; Zhao, Yuanyuan
345	Small-Angle X-Ray Scattering Tomography Based on Micro-Focusing Kirkpatrick-Baez Mirrors	Guangxue Xuebao/Acta Optica Sinica	38	1		Hu, Tao; Hua, Wenqiang; Wang, Yudan
346	Application of Fuzzy Control Method for Temperature Control of Molten Salt System	Hedongli Gongcheng/Nuclear Power Engineering	39	1	106	Ruan, Jian; Zou, Yang; Zhu, Haihua
347	A strategy for the preparation of closed-cell and crosslinked polypropylene foam by supercritical CO2foaming	Journal of Applied Polymer Science	135	6		Yang, Chenguang; Xing, Zhe; Zhao, Quan
348	An Efficient Family of Misfit-Layered Calcium Cobalt Oxide Catalyst for Oxygen Evolution Reaction	Advanced Materials Interfaces	5	23		Lin, Xiao; Bao, Hongliang; Zheng, Dehua
349	Interlock System for Soft X-ray Free-electron Laser in Shanghai	Yuanzineng Kexue Jishu/Atomic Energy Science	52	4	756	Yu, Chunlei; Zhao, Huan; Ding, Jianguo

		and Technology				
350	Fluoride-salt-cooled High-temperature Reactor Hardware-in-the-loop Simulation and Preliminary Test	Yuanzineng Kexue Jishu/Atomic Energy Science and Technology	52	4	659	Ruan, Jian; Zou, Yang; Kendrick, J.
351	Application of surface plasmon polaritons on charged particle beam diagnostics	Journal of Physics: Conference Series	1067	7		Jiang, Zenggong; Gu, Duan; Zhao, Minghua
352	Reconstruction Method of Attosecond Pulses Based on Ultrafast Dynamic Model	Guangxue Xuebao/Acta Optica Sinica	38	9		Shao, Renzhi; Li, Bin;
353	Influence of carboxyl and amide groups on in vitro hemocompatibility of sulfonated polypropylene non-woven fabric	Journal of Applied Polymer Science	135	9		Li, Rong; Cai, Xi-Ming; Ye, Yin
354	Corrosion behavior of 316SS and Ni-based alloys in a ternary NaCl-KCl-MgCl2molten salt	Solar Energy	171		320	Sun, Hua; Wang, Jianqiang; Li, Zhijun
355	Thermodynamic assessment of the SrBr2-MBr (M: alkali metal) binary systems	Calphad: Computer Coupling of Phase Diagrams and Thermochemistry	63		116	Li, Xiang; Xie, Leidong;
356	Uncertainty Analysis of Nuclear Data for Th-U and U-Pu Fuel Cycles in Molten Salt Reactor	Yuanzineng Kexue Jishu/Atomic Energy Science and Technology	52	7	1206	Hu, Jifeng; Wang, Xiaohe; Wu, Jianhui
357	Testing and Improvement Study on Neutron Detection Performance of GdI3:Ce Scintillator	Yuanzineng Kexue Jishu/Atomic Energy Science and Technology	52	2	365	Wang, Zhongqing; Huang, Yuefeng; Li, Yongping
358	Enhancing decontamination of zirconium and ruthenium in the Thorex process using acetohydroxamic acid	Hydrometallurgy	182		1	Li, Zheng; Zhao, Haogui; Chen, Mumei
359	Significantly reduced pre-oxidation period of PAN fibers by continuous electron beam irradiation: Optimization by monitoring radical variation	Polymer Degradation and Stability	158		72	Zhang, Wenli; Wang, Mouhua; Zhang, Wenfa
360	Design a high power pulse transformer for c-band klystron modulator	Journal of Physics: Conference Series	1067	8		Liu, Y.; Gu, M.; Yuan, Q.
361	基于超快动力学模型的阿秒脉冲复原方法	光学学报	38	9	932001	邵任之; 李宾;
362	梦之线光栅单色器温度起伏对能量漂移的影响	光学精密工程	26	9	2312	陈家华; 邹鹰; 卢启鹏
363	棒状氢化锆慢化钍基熔盐堆中子学性能优化	原子能科学技术	52	9	1656	朱帆; 伍建辉; 陈金根
364	快速原子力显微镜技术在细胞生物学中的应用新进展	南方医科大学学报	38	8	931	刘林; 魏余辉; 刘文静
365	同步光空间干涉仪缝距快速扫描系统	核技术	41	8	80101	高波; 冷用斌; 陈汉骄
366	嵌段共聚物 PS-b-PAA 自组装过程的原	核技术	41	8	80102	金鑫; 王建军; 李怡

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367	电转条件对Cas9核糖核蛋白基因编辑效率的影响	核技术	41	8	80502	夏凯; 韩玲; 孔华庭
368	熔盐燃料对加速器驱动的次临界堆中子学性能的影响	核技术	41	8	80601	赵学超; 蔡翔舟; 陈金根
369	熔盐添加剂对熔盐高温热稳定性的改性研究	核技术	41	8	80602	完志康; 安学会; 张鹏
370	正壬醇与苯乙烯膦酸在金红石表面的协同吸附作用研究	核技术	41	9	90501	王兴亚; 肖巍; 张立娟
371	巯基保护的中空金纳米球	物理化学学报	34	7	770	Xu Wenwu; Gao Yi;
372	非蒸散型吸气剂的研究进展	真空科学与技术学报	38	8	650	颜攀; 韩兴博; 冷海燕
373	基于 CR-39 固体探测器的粒子识别	辐射研究与辐射工艺学报	36	4	40401	徐秀清; 夏晓彬; 李洋
374	基于转化率法研究冰粉生成乙烯水合物的动力学及 THF 非常规抑制作用	高等学校化学学报	39	9	1968	施伟光; 卿红霞; 张尚尚
375	基于 Modelica 语言的塔式太阳能光热电站的熔盐回路建模与仿真	储能科学与技术	7	4	674	王楚航; 徐博; 周翀
376	熔盐堆钍铀、铀钚燃料循环核数据不确定度分析	原子能科学技术	52	7	1206	胡继峰; 王小鹤; 伍建辉
377	基于聚焦离子束-扫描电镜方法研究页岩有机孔三维结构	岩矿测试	37	3	235	王羽; 汪丽华; 王建强
378	一种用于波荡器磁中心高精度标定的磁靶标	强激光与粒子束	30	8	85104	俞成; 蒋志强; 周巧根
379	一种偕胺肟基纤维材料对模拟盐湖水中铀的吸附研究	中国科学. 化学	48	5	518	刘西艳; 许璐; 张晓敏
380	固相增密燃料元件基体石墨的氩离子辐照性能研究	新型炭材料	33	3	268	许六军; 王浩然; 林俊
381	基于干涉法的晶体表面微损伤的定位与表征	核技术	41	7	70101	金利民; 宋丽; 祝万钱
382	同步辐射 XAFS 技术研究 Th_(1-x)U_xO_(2+y)的微观结构	核技术	41	7	70102	解春雨; 曹罕杰; 岳增慧
383	自由电子激光装置数字化束流位置信号处理器研制及应用	核技术	41	7	70402	赖龙伟; 冷用斌; 阎映炳
384	钍基氯盐快堆燃耗性能分析	核技术	41	7	70602	彭一鹏; 余呈刚; 崔德阳
385	TMSR 云仿真平台初步设计与实现	核技术	41	7	70603	何越; 程懋松; 戴志敏
386	核石墨与熔盐相容性测试装置设计与实验	核技术	41	7	70605	唐辉; 贺周同; 张灿
387	一种评价三维控制网精度的方法	测绘通报		6	126	张翼飞; 金利民; 樊奕辰
388	伽马射线辐照制备还原氧化石墨烯	辐射研究与辐射工艺学报	36	1	10302	李吉豪; 黄泽茹; 黄卫兵

389	基于开环增益的 DCCT 线性误差测量方法	西北大学学报. 自然科学版	48	3	343	王东兴; 朱燕燕; 李瑞
390	磁调制零磁通电流传感器状态监测方法	西安电子科技大学学报	45	3	169	王东兴; 朱燕燕; 李瑞
391	ThF_4 -LiCl-KCl 熔盐体系中 F~-浓度对 Th(IV)电解提取的影响	辐射研究与辐射工艺学报	36	3	30301	徐千惠; 朱铁建; 郑海洋
392	单分子荧光共振能量转移用于生物大分子构象动态变化过程研究进展	分析化学	46	6	803	孙乐乐; 苏莹莹; 高延静
393	RFQ 低电平控制系统频率跟踪与幅相反馈的设计与实现	核技术	41	6	60202	李明达; 赵玉彬; 郑湘
394	Ln~(3+)在 LnF_3-LiCl-KCl 熔盐体系中的电化学行为	核技术	41	6	60301	王先彬; 龙德武; 朱铁建
395	熔盐冷冻壁传热平衡数值模拟及实验研究	核技术	41	6	60601	孙波; 周金豪; 窦强
396	熔盐堆中石墨吸附氚的理论研究	核技术	41	6	60602	吴喜军; 钱楠; 王广华
397	纳米 TiO_2 增强 NaNO_3-KNO_3-NaNO_2 熔盐的中温储热特性	核技术	41	6	60603	王义豪; 许茜; 唐忠锋
398	基于指数变换的三维六角形节块法动力学程序开发及验证	核技术	41	6	60604	程懋松; 林铭; 左献迪
399	ATP 触发快速响应的线性 DNA 凝胶	高分子学报		5	553	王飞; 钟睿博; 唐倩
400	BL17U 短波长 X 射线聚焦方案优化	核技术	41	5	50102	钟长游; 汪启胜; 刘科
401	大气环境中溶剂添加剂对制备钙钛矿薄膜的影响	核技术	41	5	50103	张晓楠; 郑官豪杰; 苏圳煌
402	Lynx-2D 在质子点扫描系统中的运用	核技术	41	5	50201	陈涛; 李秀芳; 虢梦雅
403	基于氢研究核石墨中氚的去除	核技术	41	5	50502	邓珂; 马玉华; 秦来来
404	外围熔盐层堵塞状态下熔盐堆内部温度分布分析	核技术	41	5	50601	何龙; 余呈刚; 郭威
405	基于双向流固耦合的换热管流致振动分析	核技术	41	5	50602	缪洪康; 陈玉爽; 吕刘帅
406	动态参数直接统计方法在 TMSR-SF1 中的应用	核技术	41	5	50603	朱贵凤; 严睿; 于世和
407	2 MW 钍基熔盐堆覆盖气净化系统失效事件下的辐射剂量分析	核技术	41	5	50604	陈畅其; 夏晓彬; 蔡军
408	Angiopep-2 修饰的 Ag_2S 量子点用于近红外二区脑胶质瘤成像	化学学报	76	5	393	徐毅; 赵彦; 张叶俊
409	Te 诱导纯 Ni 脆化的时效研究	功能材料	49	4	4077	贾彦彦; 李哲夫; 邱杰
410	熔盐堆中结构材料的腐蚀研究	核科学与工程	38	2	171	侯娟; 俞国军; 孙华
411	使用区域中值滤波算法降低同步辐射红	红外与毫米波学报	37	2	251	朱化春; 佟亚军; 吉

	外线站由 Top-Up 模式引入的噪声					特
412	退役核石墨中氚的去污	辐射研究与辐射工艺学报	36	2	20101	邓珂; 马玉华; 秦来来
413	聚醚砜接枝聚乙烯基吡咯烷酮超滤膜的制备及其抗污染性能	辐射研究与辐射工艺学报	36	2	20301	樊凯; 周国清; 杨海军
414	低能电子束辐射交联改性 PP/LLDPE 五层共挤 POF 热收缩膜的性能	高分子材料科学与工程	34	4	37	张茂江; 胡江涛; 王明磊
415	氟盐冷却高温堆主冷却剂系统~(16)N 源项分析	原子能科学技术	52	4	652	周波; 严睿; 邹杨
416	氟盐冷却高温堆半实物仿真及初步测试	原子能科学技术	52	4	659	阮见; 邹杨; Kendrick J
417	上海软 X 射线自由电子激光装置联锁保护系统	原子能科学技术	52	4	756	于春蕾; 赵欢; 丁建国
418	辐射交联聚丙烯的超临界二氧化碳发泡	高分子材料科学与工程	34	3	127	李小虎; 程勇; 周路路
419	乏燃料干法后处理中的熔盐减压蒸馏技术	核技术	41	4	40001	付海英; 耿俊霞; 杨洋
420	质子点扫描照射位置控制系统设计	核技术	41	4	40201	苗春晖; 刘鸣; 舒航
421	固体聚合物氚电解浓缩系统的性能研究	核技术	41	4	40502	刘佳煜; 李华; 秦来来
422	正常运行工况熔盐堆主回路衰变热特性研究	核技术	41	4	40602	周波; 严睿; 邹杨
423	高温光纤在熔盐中的腐蚀实验研究	核技术	41	4	40605	赵翠兰; 杨群; 周雪梅
424	基于石墨烯及纳米复合材料的抗菌性研究进展	生物学杂志	35	2	67	朱中杰; 黄青;
425	激光复合焊接7020铝合金的疲劳性能及损伤行为	中国激光	45	3	302003	胡雅楠; 吴圣川; 宋哲
426	上海软 X 射线自由电子激光装置束流分配系统设计	强激光与粒子束	30	4	45101	Gu Duan; Wang Zhen; Huang Dazhang
427	光栅单色器系统超环面镜转动机构优化设计	核技术	41	3	30101	陈家华; 徐中民; 甄香君
428	基于 Archiver Appliance 的束线数据管理系统	核技术	41	3	30102	赵子龙; 徐慧超; 龚培荣
429	高亮度电子束相空间重建技术的实验研究	核技术	41	3	30103	于清林; 张猛; 谷端
430	加速器电源电流突变补偿技术的研究	核技术	41	3	30104	黄山; 谭松清; 李瑞
431	移动式放射性气体监测仪能量响应的优化设计	核技术	41	3	30401	周雪梅; 刘桂民; 陈永忠
432	基于 EPICS 的质子注入器远程控制及监测系统的构建	核技术	41	3	30402	张根灿; 蒋舸扬; 李德明
433	模糊控制在熔盐系统温度控制中的应用	核动力工程	39	1	106	阮见; 邹杨; 朱海华
434	铜唑防腐剂处理竹材的同步辐射无损检	光谱学与光谱分析	38	3	901	彭冠云; 刘杏娥; 杨

	测研究					淑敏
435	质子辐照对永磁合金微观结构演化的研究	物理学报	67	1	16104	李哲夫; 贾彦彦; 刘仁多
436	PS_(3000)-b-PAA_(5000)球形胶束温度效应的原位小角 X 射线散射技术研究	物理学报	67	4	48301	金鑫; 杨春明; 滑文强
437	GdI_3:Ce 闪烁体中子探测性能测试与改进研究	原子能科学技术	52	2	365	王中庆; 黄跃峰; 李勇平
438	混合式填充床熔盐蓄热系统热性能分析	太阳能学报	39	2	475	赵炳晨; 程懋松; 刘畅
439	上海质子治疗装置动态电源控制系统	核技术	41	2	20404	蒋舸扬; 谭松清; 赵欢
440	基于 PostgreSQL 的 CRDM 数据存档系统	核技术	41	2	20602	郭冰; 魏永波;
441	ThorCon 堆氚产额分析研究	核技术	41	2	20606	钱楠; 王广华; 黄豫
442	伽马射线辐照对聚丙烯超临界二氧化碳发泡的影响	辐射研究与辐射工艺学报	36	1	10301	杨晨光; 赵全; 王谋华
443	预辐射引发气相接枝法制备 PE-g-PAN 材料	辐射研究与辐射工艺学报	36	1	10303	刘汉洲; 李林繁; 蒋海青
444	基于Kirkpatrick-Baez镜聚焦的X射线小角散射显微层析成像	光学学报	38	1	134001	胡涛; 滑文强; 王玉丹
445	Thorex 流程离心萃取器验证台架实验	核化学与放射化学	40	1	23	赵皓贵; 李峥; 于婷
446	MCNP5 在固态燃料熔盐堆功率分布计算的应用	强激光与粒子束	30	1	16003	彭红花; 严睿; 朱贵凤
447	压弯椭圆柱面镜的有限元分析	核技术	41	1	10101	秦超; 薛松; 王楠
448	氢和氘在 FLiNaK 熔盐中的渗透扩散行为	核技术	41	1	10604	曾友石; 吴胜伟; 钱渊
449	PB-FHR 的控制棒布局设计及物理效应	核技术	41	1	10605	于世和; 严睿; 冀锐敏
450	氟化物熔盐冷冻壁形成工艺研究	现代化工	38	1	149	周金豪; 孙波; 窦强
1	Ultrabroad and Angle Tunable THz Filter Based on Multiplexed Metallic Bar Resonators	IEEE PHOTONICS TECHNOLOGY LETTERS	30	24	2103	Liu, Weiwei; Dai, Zijie; Yang, Jing

附录 3

2017-2018 年专利授权一览表

Patents in 2017-2018

2017

No.	专利名称	申请号	申请日	授权日	类型	发明人
1	一种低剂量 CT 图像重建方法	201310608752.1	2013/11/25	2017/1/11	发明	周光照 杜国浩 佟亚军 陈荣昌 任玉琦 王玉丹 谢红兰 邓彪 肖体乔
2	一种氟盐中氧含量的测试方法	201410184920.3	2014/5/4	2017/1/11	发明	赵素芳 李明广 谢雷东 汪洋 苏兴治
3	一种交直流电流传感器	201410355923.9	2014/7/24	2017/1/18	发明	王东兴 卢宋林 李瑞 朱燕燕 胡志敏 黄毛毛 刘洪 武万锋 谭松清 郭春龙 许瑞年
4	一种测量放射性气体产生的β射线的探测系统及方法	201410455841.1	2014/9/9	2017/3/1	发明	陈明明 蔡军 夏晓彬 黄文博 李建伟 张志龙
5	一种银/氯化银参比电极及其制作方法	201410494891.0	2014/9/24	2017/6/13	发明	朱铁建 郑海洋 张国欣 黄卫龙德武 李晴暖
6	脉冲式指数衰减正弦信号发生器及其信号发生方法	201410674167.6	2014/11/21	2017/3/1	发明	冷用斌 赖龙伟 周伟民 阎映炳 袁任贤
7	一种同步辐射 X 射线 CT 校轴系统及方法	201410706151.9	2014/11/27	2017/1/11	发明	佟亚军 杜国浩 彭冠云 王玉丹 陈敏 肖体乔
8	一种原位测试样品平台	201410748771.9	2014/12/9	2017/10/31	发明	朱大明 李晓龙 刘春泽 顾月良 阴广志 高兴宇 黎忠
9	一种精确测量滤膜微小通量的装置	201410782451.5	2014/12/16	2017/1/11	发明	杨海军 侯铮迟 胡钧
10	载波抑制射频前端和方法、束流位置测量系统和方法	201410854329.4	2014/12/30	2017/9/15	发明	冷用斌 赖龙伟 阎映炳 袁任贤 周伟民
11	一种反射型光栅对脉宽展宽器	201510030106.0	2015/1/20	2017/7/18	发明	李宾 张文艳 刘波 刘晓庆
12	一种放射性气体和放射性气溶胶的在线监测系统及其方法	201510030680.6	2015/1/21	2017/10/27	发明	蔡军 夏晓彬 涂传火 陈明明 洪鹏飞 马英豪 张志龙 曾志强
13	一种放射性气溶胶的采样测量装置及其方法	201510030726.4	2015/1/21	2017/5/17	发明	涂传火 蔡军 夏晓彬 黄文博 陈明明 马英豪 张志龙
14	一种压弯装置	201510069683.0	2015/2/10	2017/9/26	发明	计展 薛松 祝万钱 王楠 陈家华 吴佳兴
15	一种用于同步辐射X射线衍射测试的联动装置	201510069762.1	2015/2/10	2017/11/28	发明	柳义 周平 阴广志 李丽 文闻 高兴宇

16	一种浊度仪	201510227951.7	2015/5/6	2017/8/1	发明	苏涛 汤睿 张鹏 谢雷东 侯惠奇
17	一种从含铀酰离子的水溶液中富集铀的方法	201510237626.9	2015/5/11	2017/11/17	发明	李景烨 张伯武 马红娟 刘西艳 凌长见 杨晓娟 虞鸣 张阔
18	一种吸收光谱仪	201510305564.0	2015/6/4	2017/12/22	发明	苏涛 张鹏 刘洪涛 程进辉 姚思德 谢雷乐 侯惠奇
19	炭/炭复合材料粘结剂、粘结方法及炭/炭复合材料构件	201510430307.X	2015/7/21	2017/6/16	发明	张东生 夏汇浩 周兴泰 杨新梅 宋金亮
20	一种复杂环境气体中不同形态氚的浓度监测装置	201510500470.9	2015/8/14	2017/3/22	发明	刘卫 王广华 钱楠 黄豫 钱渊 郭冰 魏永波 张宁 杜林 王玲 邓珂
21	一种透明毛细管内表面面型测试系统及测试方法	201510542214.6	2015/8/28	2017/9/5	发明	佟亚军 王玉丹 任玉琦 邓彪 陈敏 肖体乔
22	一种耐熔盐腐蚀镍基变形高温合金及其制备方法	201510612608.4	2015/9/23	2017/5/3	发明	叶祥熙 崔传勇 蒋力 李志军 艾华 孙晓峰 周兴泰
23	一种同步辐射X射线大面积干涉光刻系统	201510666500.3	2015/10/15	2017/11/28	发明	薛超凡 吴衍青 刘海岗 杨树敏 王连升 赵俊 邰仁忠
24	一种医用质子同步加速器的注入装置及注入方法	201510672967.9	2015/10/16	2017/9/15	发明	张满洲 李德明 唐靖宇 邱静 欧阳联华李浩虎 谢修璀
25	一种医用质子同步加速器	201510672823.3	2015/10/16	2017/10/31	发明	张满洲 赵振堂 方守贤 李德明 焦毅 李浩虎 谢修璀 王坤
26	一种分光光阑装置	201510673743.X	2015/10/16	2017/9/29	发明	张敏 李勇军 贾丹丹
27	一种燃料元件、其制备方法及其用途	201510853967.9	2015/11/27	2017/11/17	发明	林俊 仲亚娟 姜海涛 朱智勇
28	一种氟化锂的回收装置及其回收方法	201610012077.X	2016/1/8	2017/4/5	发明	宋昱龙 李峥 刘玉侠 张岚
29	一种快速温度跃升微流芯片系统	201610116013.4	2016/3/1	2017/11/10	发明	边风刚 李怡雯 洪春霞 王劼
30	一种放射性含氟废液水泥固化方法	201610192543.7	2016/3/30	2017/12/8	发明	钱正华 刘学阳 乔延波 马洪军 王帅 陈堃
31	抗熔盐腐蚀镍基高温合金焊接结构件的焊接后热处理方法	201610556346.9	2016/7/15	2017/6/16	发明	黎超文 李志军 陈双建 玉昆 李肖科 蒋力 王晚霞
32	带磁场生成机构的软X射线吸收谱测量装置	201620757123.4	2016/7/19	2017/3/29	实用新型	曹杰锋 王勇
33	一种原位X射线衍射测试样品平台	201620780020.X	2016/7/22	2017/3/1	实用新型	杨铁莹 李晓龙 高兴宇
34	炭/炭复合材料粘结剂、粘结方法及炭/炭复合材料构件	201510430307.X	2015/7/21	2017/6/16	发明	张东生 夏汇浩 周兴泰 杨新梅 宋金亮

35	薄膜X射线衍射原位测试装置	201621060031.7	2016/9/18	2017/4/5	实用新型	王瑞 刘春泽 朱大明 顾月良 阴广志 李晓龙
36	一种同步辐射原位测试装置	201621137968.X	2016/10/19	2017/4/26	实用新型	何燕 王娟 肖学章 李爱国
37	一种同步辐射软X射线无损实时位置分辨电离室	201621304472.7	2016/11/30	2017/5/24	实用新型	薛超凡 吴衍青 王勇 邰仁忠
38	一种钙钛矿太阳能电池的原位实时同步观测装置	201621409780.6	2016/12/21	2017/7/7	实用新型	杨迎国 阴广志 冯尚蕾 顾月良 季庚午 张晓楠 程振东 苏圳煌 高兴宇
39	一种用于掠入射X射线小角散射实验的真空冷热台	201720578463.5	2017/5/23	2017/12/19	实用新型	滑文强 杨春明 王玉柱 李秀宏 边风刚 王劼

2018

序号	专利名称	申请号	申请日	授权日	类型	发明人
1	一种平衡光学微波再生系统	201410455842.6	2014/9/9	2018/1/16	发明	张文艳 刘波 刘晓庆 王东
2	基于多通道电子倍增器件的电离吸收谱探测装置	201510305701.0	2015/6/4	2018/5/25	发明	李俊琴 邹鹰 陈振华 薛莲 王勇 邰仁忠
3	一种综合光谱仪	201510427484.2	2015/7/20	2018/1/19	发明	苏涛 葛敏 刘洪涛 张鹏 左勇 姚思德 谢雷东 侯惠奇
4	熔盐堆用碳素材料的熔盐浸渗实验装置	201510618392.2	2015/9/25	2018/1/19	发明	唐辉 夏汇浩 贺周同 高丽娜
5	一种基于静电收集法的氡和钍射气连续测量装置及方法	201510666644.9	2015/10/15	2018/5/25	发明	蔡军 夏晓彬 肖德涛 涂传火 吴喜军 黄文博 李志强 单健 赵桂芝 徐杰
6	一种氡和钍射气及其子体浓度的在线测量系统及方法	201510667018.1	2015/10/15	2018/1/30	发明	涂传火 蔡军 肖德涛 夏晓彬 单健 黄文博 李志强 吴喜军 谢贵英 赵桂芝
7	一种粘度仪	201510875579.0	2015/12/2	2018/3/30	发明	程进辉 张鹏 安学会 唐忠锋 黎忠 姚思德
8	一种基于硬件控制的辐照扫描装置及辐照扫描方法	201510947250.0	2015/12/16	2018/3/23	发明	舒航 殷重先 刘鸣 褚克成 赵黎颖 戴晓磊 苗春晖 赵斌清

9	一种测量粒子加速器束流流强的系统和方法	201610020937.4	2016/1/13	2018/7/13	发明	冷用斌 赖龙伟 阎映炳 袁任贤
10	一种测量粒子加速器束流到达时间的方法	201610066364.9	2016/1/29	2018/4/6	发明	冷用斌 赖龙伟 阎映炳
11	一种长程面形测量仪	201610100965.7	2016/2/24	2018/5/4	发明	彭川黔 何玉梅 王劼
12	一种长程光学表面面形检测系统	201610101562.4	2016/2/24	2018/3/30	发明	彭川黔 何玉梅 王劼
13	一种长程面形测量装置	201610101564.3	2016/2/24	2018/6/29	发明	彭川黔 何玉梅 王劼
14	一种长程光学表面面形检测仪	201610101533.8	2016/2/24	2018/6/19	发明	彭川黔 何玉梅 王劼
15	一种基于同步辐射的实时 X 射线立体成像系统及成像方法	201610118509.5	2016/3/2	2018/1/16	发明	邓彪 王玉丹 任玉琦 王飞翔 肖体乔
16	基于高分子预聚物前驱体的玻璃炭材料制备方法	201610141946.9	2016/3/14	2018/3/20	发明	张东生 夏汇浩 周兴泰 杨新梅 叶林凤 冯尚蕾
17	一种基于高分子预聚物前驱体的玻璃炭材料制备方法	201610141947.3	2016/3/14	2018/3/16	发明	张东生 夏汇浩 周兴泰 杨新梅 叶林凤 冯尚蕾
18	一种基于改性酚醛树脂前驱体的玻璃炭材料制备方法	201610142651.3	2016/3/14	2018/2/9	发明	张东生 夏汇浩 周兴泰 杨新梅 叶林凤 冯尚蕾
19	一种无机非金属包壳高温相变储热微胶囊及其制备方法	201610172155.2	2016/3/24	2018/1/19	发明	张锋 林俊 仲亚娟 李子威
20	一种交直流电流传感器的磁芯选择方法	201610171249.8	2016/3/24	2018/6/19	发明	朱燕燕 王东兴 李瑞 卢宋林
21	一种高温氟盐压力计	201610172143.X	2016/3/24	2018/11/27	发明	陈志军 张福春
22	一种卤化物放射性废物玻璃固化体及其制备方法	201610192527.8	2016/3/30	2018/3/13	发明	乔延波 马洪军 孙亚平 刘学阳 钱正华 王帅 陈堃
23	一种新型耐腐蚀防堵塞的超临界水氧化反应装置	201610192530.X	2016/3/30	2018/7/13	发明	王红玉 王帅 马洪军 秦强 乔延波 刘学阳 钱正华

24	含磷脂的微乳液及制备方法、在研究界面水性能中的应用	201610243873.4	2016/4/19	2018/12/4	发明	潘亚涛 吕军鸿
25	一种高性能钙钛矿太阳能电池及其制备方法	201610243807.7	2016/4/19	2018/1/12	发明	杨迎国 冯尚蕾 高兴宇
26	反应堆核测系统	201610256744.9	2016/4/22	2018/2/6	发明	黄国庆 赖伟 严慧娟 陈永忠
27	一种电流互感器跟踪精度的测量方法	201610288495.1	2016/5/4	2018/6/8	发明	王东兴 卢宋林 李瑞 朱燕燕 胡志敏
28	一种球形高温相变储热元件的组装方法和由此形成的储热元件	201610290089.9	2016/5/4	2018/3/6	发明	仲亚娟 林俊 张锋 姜海涛 李子威
29	冷却系统	201610316624.3	2016/5/12	2018/2/16	发明	黄国庆 赖伟 严慧娟 陈永忠
30	一种基于混合式行波加速结构的双能量电子直线加速器	201610504937.1	2016/6/30	2018/1/30	发明	赵振堂 方文程 赵明华 顾强
31	耐腐蚀高温合金管-管板连接方法及换热器	201610532317.9	2016/7/8	2018/3/30	发明	玉昆 邹文江 李志军 程耀永 黎超文 陈双建
32	用于抗熔盐腐蚀镍基高温合金焊接的实芯焊丝制备方法	201610556354.3	2016/7/15	2018/5/29	发明	黎超文 李志军 梁建平 玉昆 陈双建 蒋力
33	一种用于抗熔盐腐蚀镍基高温合金熔化焊的焊料	201610556350.5	2016/7/15	2018/2/9	发明	黎超文 李志军 蒋力 玉昆 陈双建 梁建平
34	C/C-SiC 复合材料部件的制造方法及 C/C?SiC 复合材料部件	201610561827.9	2016/7/18	2018/11/20	发明	张东生 夏汇浩 周兴泰 杨新梅 叶林凤 冯尚蕾
35	一种耐熔盐腐蚀镍钼铬合金无缝管的制备方法	201610850839.3	2016/9/26	2018/6/29	发明	梁建平 王宝顺 李志军 苏诚 李肖科 王曼
36	一种高温熔盐电池	201610361790.5	2016/5/26	2018/8/24	发明	彭程 肖国萍 关成志 王建强
37	真空密封容器及其真空密封方法、真空热处理方法	201610885108.2	2016/10/11	2018/4/17	发明	李志军 储祥伟 冷滨 贾彦彦 符彩涛 程宏伟
38	一种电流传感器的跟踪精度测量方法	201610926067.7	2016/10/24	2018/11/27	发明	王东兴 卢宋林 李瑞 朱燕燕 胡志敏
39	一种球形燃料元件的芯球定位装置及其制备方法	201611082015.2	2016/11/30	2018/6/19	发明	姜海涛 林俊 朱智勇 王鹏 仲亚娟

40	一种同步辐射软X射线无损实时位置分辨电离室	201611088759.5	2016/11/30	2018/8/24	发明	薛超凡 吴衍青 王勇 邰仁忠
41	一种合成气制备系统及其方法	201611224180.7	2016/12/27	2018/11/27	发明	关成志 彭程 陈新冰 肖国萍 王建强
42	基于高温电解水蒸气制氢技术的加氢站	201611224059.4	2016/12/27	2018/12/4	发明	关成志 肖国萍 陈新 冰彭程 侯权 杜贤龙 王建强
43	一种石墨中氢或其同位素解吸反应釜	201710083667.6	2017/2/16	2018/9/21	发明	刘卫 邓珂 王广华 黄豫 马玉华 秦来来 张钦 杨果 马兆伟 刘佳煜
44	高性能永磁体制备方法及含该永磁体的真空波荡器磁结构	201710025410.5	2017/1/13	2018/8/24	发明	何永周
45	一种医用超导质子同步加速器	201710134128.0	2017/3/8	2018/12/14	发明	张满洲 李德明 赵振堂
46	一种抗熔盐腐蚀高温复合材料及熔盐堆堆芯结构件	201710241930.X	2017/4/14	2018/11/27	发明	杨超 黄鹤飞 周兴泰
47	一种同步辐射用光学元件积碳清洗装置	201720619170.7	2017/5/31	2018/1/9	实用新型	张翼飞 罗红心 李中亮
48	一种紧凑型波荡器	201720874678.1	2017/7/18	2018/1/23	实用新型	邓海啸 宋明豪 蒋志强 刘波 王东
49	一种用于软X射线近边吸收谱测量的原位标样系统	201721313052.X	2017/10/12	2018/4/17	实用新型	曹杰峰 王勇 朱方园 孟祥雨 甄香君 邰仁忠
50	一种激光锁相装置	201721318568.3	2017/10/13	2018/4/17	实用新型	刘晓庆 刘波 张文艳
51	熔盐球床堆中燃料球的装料装置	201721328091.7	2017/10/16	2018/5/5	实用新型	陈兴伟 邹杨 曹云 孙雪静
52	一种气溶胶中金属元素的检测装置	201721732175.7	2017/12/13	2018/8/14	实用新型	刘艳成 崔荣荣 李晓云 韩玲 葛敏 刘洪涛 姚思德
53	熔盐蓄热储能发电系统及包含其的储能电站	201721684775.0	2017/12/6	2018/7/3	实用新型	袁晓凤 李启明 王建强 周翀
54	固体蓄热储能系统及包含其的储能电站	201721749466.7	2017/12/14	2018/9/14	实用新型	袁晓凤 陈兴伟 贾国斌 李明海 周翀 邹杨
55	用于熔盐体系铀氟化反应	201820061345.1	2018/1/15	2018/12/18	实用新型	孙理鑫 周金豪 牛永生 胡聪伟 窦强 李晴暖
56	一种环缝流道型熔盐加热器	201820105092.3	2018/1/22	2018/9/11	实用新型	李明海 邹杨 杨洋 孙慎德 王纳秀 严睿 阮见
57	一种治疗用质子同步加速器	201820123774.7	2018/1/25	2018/11/13	实用新型	张满洲 李德明 赵振堂 王坤 谢修璀
58	一种医用质子同步加速器	201820123775.1	2018/1/25	2018/11/13	实用新型	张满洲 李德明 赵振堂 王坤 谢修璀

59	一种采用组合型磁铁的质子同步加速器	201820123744.6	2018/1/25	2018/11/13	实用新型	张满洲 李德明 赵振堂 王坤 谢修璀
60	一种组合型磁铁构成的质子同步加速器	201820123773.2	2018/1/25	2018/11/13	实用新型	张满洲 李德明 赵振堂 王坤 谢修璀
61	熔盐堆堆芯、熔盐堆系统及燃料循环系统	201820215685.5	2018/2/7	2018/12/11	实用新型	伍建辉 刘亚芬 陈金根 邹杨
62	熔盐堆能量转换系统	201820294359.8	2018/3/2	2018/11/13	实用新型	张金红 邹杨 周翀 傅瑶 田健 朱贵凤 康旭忠

附录 4

2017-2018 年国际学术会议报告表

Presentations by SINAP Scientists at International Scientific Meetings in 2017-2018

2017

No.	会议全称	报告名称	报告人	报告类别	报告学科领域	时间	地点
1	参加第 24 届四代堆论坛熔盐堆核能系统执委会	China's thorium-fueled molten salt reactor program	李晴暖	分会报告	反应堆物理与技术	2017-09-27	奥地利
2	访问意大利米兰理工学院，参加技术交流会；参加 SINAP-JRC 合作会议；参加 GIF MSR 会议和第 22 届 PSSC 会议	Overview of SINAP R&D activities on MSRs	徐洪杰	大会报告	核技术及其应用	2017-01-16	瑞士
3	访问意大利米兰理工学院，参加技术交流会；参加 SINAP-JRC 合作会议；参加 GIF MSR 会议和第 22 届 PSSC 会议	TMSR program update	蔡翔舟	大会报告	核技术及其应用	2017-01-16	瑞士
4	参加第 8 届国际粒子加速器会议	Transverse beam instability observation and investigation using bunch by bunch on-line DAQ system	张宁	展板报告	束流物理与加速器技术	2017-05-13	丹麦
5	参加 RHIC-sPHENIX 合作组年会	The Opportunity and Plan for Chinese Collaboration to Join in sPHENIX"	陈金辉	大会报告	核物理	2017-12-06	美国
6	参加第 8 届国际粒子加速器会议	Proposal for the Generation of Terawatt, Attosecond X-Ray Pulse in Free Electron Lasers	相升旺	展板报告	束流物理与加速器技术	2017-05-13	丹麦
7	参加 2017 CLIC 研讨会	Progress in C and X-band technology	方文程	大会报告	束流物理与加速器技术	2017-03-05	瑞士

8	参加 2017 CLIC 研讨会	RF conditioning results of x-band deflecting structure	谭建豪	分会报告	束流物理与加速器技术	2017-03-05	瑞士
9	参加第 8 届国际粒子加速器会议	A New Femtosecond Timing System for Large Accelerator Facilities	王震	展板报告	束流物理与加速器技术	2017-05-13	丹麦
10	组织并参加 2017 年国际输运模型研讨会并进行国际核理论合作项目的合作研究	IBUU 输运模型计算结果探讨	徐骏	大会报告	核物理	2017-03-19	美国
11	参加第 8 届国际粒子加速器会议	Beam Stability Modeling and Jitter Control for Sxfel Linac	顾强	展板报告	束流物理与加速器技术	2017-05-13	丹麦
12	访问意大利米兰理工学院，参加技术交流会；参加 SINAP-JRC 合作会议；参加 GIF MSR 会议和第 22 届 PSSC 会议	China’s thorium-fueled molten salt reactor program	李晴暖	大会报告	核技术及其应用	2017-01-16	瑞士
13	第 25 届国际磁铁会议	Design and measurent of a 2.4 Tesla superbend magnet prototype at SSRF	钱茂飞	展板报告	同步辐射技术及其应用	2017-08-26	荷兰
14	第 25 届国际磁铁会议	Test results of the first superconducting undulator prototype at the SSRF	丁祎	展板报告	同步辐射技术及其应用	2017-08-26	荷兰
15	参加第 15 届国际先进材料大会	Unrevealing the catalyzed growth of freestanding graphene on SiC by Fe	宋飞	分会报告	凝聚态物理中的新效应及其他问题	2017-08-26	日本
16	参加 ASTM 人造碳和石墨生产的 DO2.F 小组委员会议	Chinese Nuclear Graphite Standard	曾广礼	大会报告	分析力学	2017-06-24	美国
17	参加英国物理学会-中国物理学会双边国际研讨会	中国同步辐射光源发展现状及发展规划	赵振堂	大会报告	基础物理学	2017-07-03	英国
18	参加第 24 届四代堆论坛熔盐堆核能系统执委会	Overview of SINAP R&D activities on MSRs	陈堃	分会报告	反应堆物理与技术	2017-09-27	奥地利

19	参加第 18 届国际核石墨专家会议	1）THE RELATIONSHIP BETWEEN POROSITY AND COEFFICIENT OF THERMAL EXPANSION IN NULCEAR GRAPHITES; 2) NUMERICAL STUDY OF DYNAMIC BEHAVIOUR FOR A TMSR GRAPHITE CORE; 3) GRAPHITES FOR LIQUID FUEL MOLTEN SALT REACTOR; 4) IMPREGNATION BEHAVIORS AND ION-IRRADIATED EFFECTS OF GRAPHITE MATRIX IN SPHERICAL FUEL ELEMENT FOR MOLTEN SALT REACTOR.	曾广礼	大会报告	分析力学	2017-09-16	美国
20	参加奇异夸克物质 2017 会议并与 AGH 科技大学开展合作研究	Resonance effect on chiral magnetic effect signal	马国亮	展板报告	核物理	2017-06-30	荷兰
21	参加第 24 届四代堆论坛熔盐堆核能系统执委会	TMSR program update	戴志敏	大会报告	反应堆物理与技术	2017-09-27	奥地利
22	参加第八届国际粒子加速器会议	A C-Band Spherical RF pulse Compressor for the SXFEL Linac Energy Upgrade	李宗斌	展板报告	束流物理与加速器技术	2017-05-13	丹麦
23	参加第六届国际加速器装置可靠性研讨会	The Administration’s Strategy for the Operational Reliability of the SSRF	何世江	展板报告	束流物理与加速器技术	2017-10-14	法国
24	参加日本辐射化学年会	Radiation grafting for preparation of fiber adsorbent of Au and U ions	吴国忠	大会报告	辐射化学	2017-09-25	日本
25	参加 MNE2017 国际会议	New developments in X-ray inteference Lithography and its applications	吴衍青	展板报告	同步辐射技术及其应用	2017-09-16	葡萄牙
26	参加 2017 年度低电平国际研讨会	SSRF Low Level RF Development	赵玉彬	大会报告	束流物理与加速器技术	2017-10-14	西班牙
27	参加美国核学会 2017 冬季年会	Progress of the Molten Salt Natural Circulation Experiment	陈堃	分会报告	反应堆物理与技术	2017-10-28	美国
28	参加第六届国际加速器装置可靠	Operation Reliability of SSRF in the Last Operation Season	孙启龙	大会报告	束流物理与加速器技术	2017-10-14	法国

	性研讨会	and upgrade plan at SSRF					
29	参加第六届国际加速器装置可靠性研讨会	Cryogenic System Operation and the Progress of SSRF II	徐俊杰	展板报告	束流物理与加速器技术	2017-10-14	法国
30	参加美国核学会 2017 冬季年会	The Thorium Molten Salt Reactor Program in China	徐洪杰	大会报告	反应堆物理与技术	2017-10-28	美国
31	参加 FEL2017 国际会议	Design of the beam switchyard of a soft X-ray FEL user facility	陈思	展板报告	束流物理与加速器技术	2017-08-19	美国
32	参加 FEL2017 国际会议	Suppression of microbunching instability in an electron laser with transverse - longitudinal couping	黄大章	展板报告	束流物理与加速器技术	2017-08-19	美国
33	参加 FEL2017 国际会议	Extending the photon energy coverage of an x-ray self-seeding FEL via the reverse taper enhanced harmonic generation technique	冯超	展板报告	束流物理与加速器技术	2017-08-19	美国
34	参加第 24 届 X 射线光学及微分析国际会议	Development of Kinoform Lenses for XPCS and other methods at SSRF	林鹤	展板报告	同步辐射技术及其应用	2017-09-23	意大利
35	参加 FEL2017 国际会议	Two-color soft x-ray generation based on the EEHG scheme	张文艳	展板报告	束流物理与加速器技术	2017-08-19	美国
36	参加第 25 届国际磁铁技术会议	THE SCANNING MAGNETS FOR PROTON THERAPY AT API	欧阳联华	展板报告	束流物理与加速器技术	2017-08-26	荷兰
37	参加 IBIC 2017 国际会议	IBIC2018 status	冷用斌	大会报告	核技术及其应用	2017-08-19	美国
38	参加第八届国际粒子加速器会议	POP experiment for the HB-HGHG scheme at SXFEL	周开尚	展板报告	束流物理与加速器技术	2017-05-13	丹麦
39	参加锕系元素 2017 国际会议	Probing the Influence of Acidity and Temperature to Th(IV) on Hydrolysis, Nucleation, and Structural Topology	林健	展板报告	核放射化学	2017-07-08	日本

40	参加第 66 届丹佛国际 X 射线会议	Multi-model X-ray Microtomography for in-situ Structure Quantification and Analysis	肖体乔	大会报告	同步辐射技术及其应用	2017-07-31	美国
41	参加“基础科学研究设施中的能效科技”研讨会	Energy issues at research infrastructures – a Chinese perspective”	冷用斌	大会报告	核技术及其应用	2017-11-21	罗马尼亚
42	参加第 26 届国际标准化组织表面化学分析技术委员会全体会议和第 17 届国际全反射 X 射线荧光分析大会	The development of TXRF method and its application on the study of trace elements in water at SSRF	黄宇营	大会报告	同步辐射技术及其应用	2017-09-16	英国
43	参加第 68 次国际电化学学会年会	In Operando Structure-property Studies of Bismuth Based Oxygen Ionic Conductors for Lithium Batteries Cathode Applications	文闻	分会报告	同步辐射技术及其应用	2017-08-26	美国
44	参加 ASME 2017 压力容器与管道会议	Evaluation on microstructure and mechanical properties of welded joints by GMAW in UNS N10003 alloy	玉昆	分会报告	金属结构材料	2017-07-15	美国
45	参加第 68 次国际电化学学会年会	In Operando Structure-property Studies of Bismuth Based Oxygen Ionic Conductors for Lithium Batteries Cathode Applications	姜政	分会报告	同步辐射技术及其应用	2017-08-26	美国
46	参加在快中子谱堆中冷却剂挑战的工作会议	compatibility research of fissionproduct tellurium and alloy N in molten salt reactor	李志军	分会报告	金属高温腐蚀与防护	2017-07-04	奥地利
47	参加熔盐堆技术状况的原子能机构技术文件编写工作顾问会议	Design and Construction of a High-Temperature Molten Salt Natural Circulation Test Loop	陈堃	大会报告	反应堆物理与技术	2017-09-24	奥地利
48	参加在快中子谱堆中冷却剂挑战的工作会议	Corrosion of metallic materials and carbide in molten fluoride salt	王建强	分会报告	金属高温腐蚀与防护	2017-07-04	奥地利

49	参加第 66 届丹佛国际 X 射线会议	X-ray Fluorescence Computed Tomography at SSRF	邓彪	展板报告	同步辐射技术及其应用	2017-07-31	美国
50	参加第 8 届生物医学 AFM 国际会议	Location Effect on Formation of Biotin–Streptavidin Complexes on DNA Origami Revealed by Time-Lapse Atomic Force Microscopy	李宾	展板报告	细胞、亚细胞、生物大分子力学	2017-09-03	波兰
51	参加 2017 年度低电平国际研讨会	A DDS-based method for tracking the resonance frequency of a RFQ cavity	郑湘	展板报告	束流物理与加速器技术	2017-10-14	西班牙
52	参加强子与核物理国际研讨会	Hypernuclear physics from view point of experiment	马余刚	大会报告	核物理	2017-12-17	日本
53	参加第 26 届国际标准化组织表面化学分析技术委员会全体会议和第 17 届国际全反射 X 射线荧光分析大会	The development of TXRF method and its application on the study of trace elements in water at SSRF	黄宇营	大会报告	同步辐射技术及其应用	2017-09-16	意大利
54	参加第 8 届生物医学 AFM 国际会议	Location Effect on Formation of Biotin–Streptavidin Complexes on DNA Origami Revealed by Time-Lapse Atomic Force Microscopy	张金金	展板报告	细胞、亚细胞、生物大分子力学	2017-09-03	波兰
55	参加 2017 年美国矿物、金属和材料协会国际会议	Nickel Ion Irradiation Damage In GH3535 Alloy Weld Metal and the Temperature Effect	黄鹤飞	展板报告	离子束与物质相互作用和辐照损伤	2017-02-25	美国
56	参加 2017 年度国际 X 射线自由电子激光五边会议	上海 X 射线自由电子激光项目情况介绍	赵振堂	大会报告	束流物理与加速器技术	2017-12-12	日本
57	参加第六届 MicroTCA 国际研讨会	MTCA.4-Based LLRF System is used at SINAP	张俊强	展板报告	射频技术与系统	2017-12-03	德国
58	参加第 10 届国际计算物理会议	The Structure and Morphology of Nanoparticles in Water Vapor Environment	高嶷	大会报告	量子计算中的凝聚态物理问题	2017-01-15	澳门
59	参加第 10 届国际计算物理会议	Ordered Water Monolayer That Does Not Completely Wet Water and Molecular-scale Hydrophilicity at Room	王春雷	大会报告	量子计算中的凝聚态物理问题	2017-01-15	澳门

		Temperature					
60	参加“关于核子与核的核反应”国际研讨会	Studies on the two-proton emission from the excited states of 23-Al and 22-Mg	方德清	大会报告	核物理	2017-10-21	意大利
61	参加第 7 届硬 X 射线光电子能谱国际会议	The ambient pressure XPS setup covering soft and hard x-ray (130 eV-10k eV) in SSRF	宋飞	展板报告	同步辐射技术及其应用	2017-09-09	美国
62	参加第 8 届生物医学 AFM 国际会议	Location Effect on Formation of Biotin–Streptavidin Complexes on DNA Origami Revealed by Time-Lapse Atomic Force Microscopy	张金金	展板报告	细胞、亚细胞、生物大分子力学	2017-09-03	德国
63	参加第八届同步辐射光源与放射性材料的分离、技术、设施研讨会	Recent progress of nuclear chemistry research in TMSR	王建强	分会报告	同步辐射技术及其应用	2017-04-10	英国
64	参加 2017 先进核电厂国际会议	Key Parameter Uncertainty and Sensitivity Analysis in the Nitrate Natural Circulation Loop	焦小伟	分会报告	核裂变、核聚变、核衰变	2017-04-24	日本
65	参加第 8 届生物医学 AFM 国际会议	Location Effect on Formation of Biotin–Streptavidin Complexes on DNA Origami Revealed by Time-Lapse Atomic Force Microscopy	李宾	展板报告	细胞、亚细胞、生物大分子力学	2017-09-03	德国
66	参加强子与核物理国际研讨会	Initial geometrical effect on collective flow	张松	分会报告	核物理	2017-12-17	日本
67	参加第五届国际多功能混合纳米材料会议	Macro–Mesoporous TiO2 Films by Polystyrene Array and Triblock Copolymer Bitemplate	付亚楠	展板报告	纳米复合	2017-03-05	葡萄牙
68	参加 2017 年度自由电子激光国际会议	Mechanical Engineering of SXFEL Project	殷立新	展板报告	束流物理与加速器技术	2017-08-19	美国
69	参加熔盐堆技术状况的原子能机构技术文件编写工作顾问会议	The status of TMSR project in China	戴志敏	大会报告	反应堆物理与技术	2017-09-24	奥地利
70	参加 DNA 纳米技术发展趋势研讨会并顺访 UCB 公	Smart DNA Nanomachines for Precise Electrochemical Detection	樊春海	大会报告	生物无机化学	2017-05-28	比利时

	司研究中心						
71	参加第 13 届中子和离子剂量国际研讨会	Neutron Dose and its Effect Factors in a Mixture Radiation Field	夏晓彬	展板报告	中子技术及其应用	2017-05-13	波兰
72	参加关于 DNA 纳米技术与智能传感器的应用重点项目专题讨论会	Highly sensitive detection of multiple biomarkers for cancer diagnostics	左小磊	分会报告	生物无机化学	2017-03-18	香港
73	参加 DNA 纳米技术发展趋势研讨会并顺访 UCB 公司研究中心	Smart DNA Nanomachines for Precise Electrochemical Detection	樊春海	大会报告	生物无机化学	2017-05-28	德国
74	参加原子能机构核石墨知识库现状技术会议	Nuclear Graphite for Molten Salt Reactor	曾广礼	大会报告	核技术及其应用	2017-10-31	奥地利
75	参加 2017 高登研究会议-团簇与纳米结构讨论会	Multiscale Structure Reconstruction Model for Nanoparticles under Real Conditions	朱倍恩	展板报告	高分子物理与高分子物理化学	2017-07-07	美国
76	参加 2017 年有关液体、化学与物理的高登研讨会	Ordered Water Monolayer That Does Not Completely Wet Water and molecular-scale hydrophilicity at Room Temperature	王春雷	展板报告	量子计算中的凝聚态物理问题	2017-08-05	美国
77	参加关于 DNA 纳米技术与智能传感器的应用重点项目专题讨论会	DNA nanostructure enabled organization for biosensors	樊春海	大会报告	生物无机化学	2017-03-18	香港
78	参加强子与核物理国际研讨会	Physics related to short lifetime of light hypernucleus	陈金辉	分会报告	核物理	2017-12-17	日本
79	参加国际原子能机构首届国际辐射科学与技术应用大会	Dyestuff Free: Coloring Fabrics by Graft Polymerization	李景烨	展板报告	新概念、新原理、新方法	2017-04-23	奥地利
80	参加德州农工大学回旋加速器实验室出束 50 年庆学术会议并进行学术交流	“Research progress on anti-matter in relativistic heavy-ion collisions”	马余刚	大会报告	核物理	2017-11-14	美国
81	参加第 62 届美国保健物理学会年会	Current Status and Challenges of Radiation Safety for Advanced Particle Accelerator	夏晓彬	大会报告	同步辐射光源原理和技术	2017-07-08	美国

		Facilities in China					
82	参加强子与核物理国际研讨会	Exotic radioactivity in proton-rich nuclei	方德清	分会报告	核物理	2017-12-17	日本
83	参加 2017 年度“SPIE 光学工程与应用”学术会议	Mutual optical intensity propagation through non-ideal optics	王勇	分会报告	束线光学技术和实验方法	2017-08-05	美国
84	参加第 25 届国际磁铁技术会议	Development of highly saturated dipole for SAPT booster	李德明	展板报告	束流物理与加速器技术	2017-08-26	荷兰
85	参加“关于核子与核的核反应”国际研讨会	Exploring Alpha-clustering of light nuclei in heavy-ion and photonuclear reactions	马余刚	大会报告	核物理	2017-10-21	意大利
86	参加第 25 届国际磁铁技术会议	Development of highly saturated dipole for SAPT booster	张淼	展板报告	束流物理与加速器技术	2017-08-26	荷兰
87	参加第 253 届美国化学会并赴劳伦斯伯克利国家实验室、弗吉尼亚大学开展合作研究	Recent progress on the development of pyroprocessing techniques for TMSR in SINAP	龚昱	分会报告	核放射化学	2017-03-23	美国
88	参加第 24 届国际光学组织大会	Multiple contrast mechanisms for material characterization with X-ray microtomography	肖体乔	分会报告	同步辐射技术及其应用	2017-08-20	日本
89	参加国际原子能机构首届国际辐射科学与技术应用大会	Radiation Induced oxidation, cross-linking and grafting of ultra-high molecular weight polyethylene	吴国忠	大会报告	新概念、新原理、新方法	2017-04-23	奥地利
90	参加第二届推动 XAFS 图谱质量的国际研讨会	Upgrade of XAFS Beamline at SSRF	顾颂琦	展板报告	同步辐射技术及其应用	2017-08-12	英国
91	参加国际化学生物工程 2017 年会	DNA-mediated metal nanoprobes with SERS-active nanogaps for multiplex biosensing	宋世平	分会报告	生物无机化学	2017-09-24	希腊
92	参加国际原子能机构研究核氢生产在氢经济背景	Research of nuclear hydrogen production by TMSR	王建强	分会报告	无机合成和制备化学	2017-07-16	奥地利

	下的作用技术会议						
93	参加第 24 届国际光学组织大会	Mapping volume-resolved nanostructure distribution in injection-molded poly(lactic acid) using SAXS-CT	郭瀚	展板报告	同步辐射技术及其应用	2017-08-20	日本
94	参加第 24 届国际光学组织大会	Non-destructive and Quantitative Analysis to Crystal Grains inside Bulk Polycrystalline Alloys	杜国浩	展板报告	同步辐射技术及其应用	2017-08-20	日本
95	参加 2017 年度“SPIE 光学工程与应用”学术会议	Progress of ptychography method at STXM beamline of SSRF	许子健	展板报告	束线光学技术和实验方法	2017-08-05	美国
96	第 18 届核石墨专家国际会议	Seismic Study on Multi-Body Structure in Reactor Core	蔡茂源	分会报告	多体系统动力学	2017-09-17	美国
97	参加 2017 国际光学工程学会会议	Research and Development of X-ray Optics at SSRF	王劼	分会报告	光学	2017-08-05	美国
98	参加 SPIE 国际会议	Finite element analysis for Bragg crystal of D-Line at SSRF	徐中民	分会报告	同步辐射技术及其应用	2017-08-05	美国
99	参加自由电子激光会议	Harmonic lasing & gain cascading: more efficicent X-ray free electron laser oscillators	邓海啸	大会报告	自由电子激光原理和技术	2017-08-16	美国
100	参加 2017 年夸克物质会议	Predictions for 5.02 TeV Pb + Pb collisions from a multiphase transport model	马国亮	大会报告	核物理	2017-02-04	美国
101	参加 2017 年矿物金属材料学会年会	Compatibility research of fission product Tellurium and Alloy N in molten salt reactor	李志军	分会报告	核技术及其应用	2017-02-25	美国
102	参加 2017 年度国际材料学会秋季会议	TMSR Materials Development-Carbide Dispersed Strengthening Nickel Based Alloys	黄鹤飞	分会报告	离子束与物质相互作用和辐照损伤	2017-11-25	美国

103	参加第 3 届“重离子碰撞中的手征、涡旋和磁场”国际会议	Isobar collision simulations using AMPT model	马国亮	大会报告	核物理	2017-03-26	美国
104	参加 2017 年国际对称能年度会议	“Spin dynamics within a BUU approach”	徐骏	大会报告	核物理	2017-09-03	法国
105	参加“2017 欧洲同位素研究学会”国际会议	Distribution of Organically Bound Tritium in Soil Around Nuclear Power Plant	杜林	展板报告	核技术及其应用	2017-06-24	罗马尼亚
106	开展纳米 X 射线荧光成像的学术交流并参加 2017 年度国际光电子学会光学工程和应用国际会议	Current status of the hard X-ray nanoprobe beamline at the SSRF	李爱国	分会报告	同步辐射技术及其应用	2017-08-01	美国
107	参加 2017 年夸克物质会议	Investigating the scaling of higher-order flows in relativistic heavy-ion collisions	张春健	展板报告	核物理	2017-02-04	美国
108	参加国际核物理会议	关于反物质研究	马余刚	大会报告	核物理	2017-05-13	斯洛伐克共和国
109	参加美国工程师协会-BPV 委员会会议	“Stress analysis result using new HHA-3217 standard”	曾广礼	大会报告	分析力学	2017-05-07	美国
110	参加第 253 届美国化学会议并访问劳伦斯伯克利国家实验室	Gas phase chemistry of the Ln(III)-TMGA/TMOGA complexes	陈秀婷	展板报告	配位化学	2017-03-28	美国
111	参加第 8 届国际粒子加速器会议	Commissioning Experience and Beam Optimization for DCLS Linac	张猛	展板报告	束流物理与加速器技术	2017-05-13	丹麦
112	参加国际核物理会议	Proton-proton correlations and two-proton emission mechanism in proton-rich nuclei	方德清	大会报告	核物理	2017-05-13	斯洛伐克共和国
113	参加第六次安大略与中国研究和创新合作论坛、2017 浦江创新论坛-加拿大论坛、2017 发现论坛	Hydrogen Production by High Temperature Steam Electrolysis	王建强	分会报告	固体无机化学	2017-05-13	加拿大

114	参加 ISWAMP-4 国际会议	Status of the SXFEL facility	冷用斌	大会报告	自由电子激光与 X 射线激光	2017-07-20	澳大利亚
115	参加矿物、金属和材料协会 2017 年年会	Shear-Coupled Grain Growth and Texture Development in a Nanocrystalline Ni-Fe Alloy during Cold Rolling	李丽	分会报告	同步辐射技术及其应用	2017-02-26	美国
116	2017 高登研究会议-无机反应机理	Theoretical prediction of Shape reconstruction of metal nanoparticles under reaction conditions	朱倍恩	展板报告	催化化学	2017-03-04	美国
117	参加第十三届亚洲生物技术大会	DNA nanotechnology-enabled organization for biosensors	樊春海	大会报告	生物无机化学	2017-07-22	泰国
118	访问意大利米兰理工学院，参加技术交流会；参加 SINAP-JRC 合作会议；参加 GIF MSR 会议和第 22 届 PSSC 会议	Overview of SINAP R&D activities on MSRs	徐洪杰	大会报告	核技术及其应用	2017-01-16	德国
119	参加自由电子激光会议	First lasing of SXFEL	刘波	大会报告	自由电子激光原理和技术	2017-08-16	美国
120	访问意大利米兰理工学院，参加技术交流会；参加 SINAP-JRC 合作会议；参加 GIF MSR 会议和第 22 届 PSSC 会议	TMSR program update	蔡翔舟	大会报告	核技术及其应用	2017-01-16	意大利
121	访问意大利米兰理工学院，参加技术交流会；参加 SINAP-JRC 合作会议；参加 GIF MSR 会议和第 22 届 PSSC 会议	China’s thorium-fueled molten salt reactor program	李晴暖	大会报告	核技术及其应用	2017-01-16	意大利

122	参加能量回收型直线加速器讨论会	Progress of SHLS VHF gun and electron source development	姜增公	分会报告	束流物理与加速器技术	2017-06-17	瑞士
123	访问意大利米兰理工学院，参加技术交流会；参加 SINAP-JRC 合作会议；参加 GIF MSR 会议和第 22 届 PSSC 会议	Overview of SINAP R&D activities on MSRs	徐洪杰	大会报告	核技术及其应用	2017-01-16	意大利
124	参加 2017 国际低温工程与超导材料大会	The Progress on 2K Cryogenic System for The Superconducing Cavity of SSRF II	许皆平	展板报告	束流物理与加速器技术	2017-07-08	美国
125	参加 2017 高梯度研讨会	Conditioning results of X-band deflecting structure	谭建豪	大会报告	束流物理与加速器技术	2017-06-12	西班牙
126	参加 2017 高梯度研讨会	Progress of C-band accelerating structure	方文程	大会报告	束流物理与加速器技术	2017-06-12	西班牙
127	参加 2017 高梯度研讨会	Progress of SXFEL of SINAP	顾强	大会报告	束流物理与加速器技术	2017-06-12	西班牙
128	参加亚洲原子能合作论坛-生物肥料与电子加速器应用项目 2017 年研讨会	The status of the electron accelerator applications in China	李景烨	大会报告	核技术及其应用	2017-11-12	日本
129	参加 2017 年度国际核石墨专家会议	离子辐照过程中石墨孔隙结构的演化	黄庆	分会报告	高性能碳素材料	2017-09-17	美国
130	访问意大利米兰理工学院，参加技术交流会；参加 SINAP-JRC 合作会议；参加 GIF	TMSR program update	蔡翔舟	大会报告	核技术及其应用	2017-01-16	德国

	MSR 会议和第 22 届 PSSC 会议						
131	参加新能源纳米材料、催化和表面国际专题研讨会	XAFS Technique：Application and Development on Catalysis at SSRF	黄宇营	大会报告	同步辐射技术及其应用	2017-10-27	日本
132	参加 SPIE 国际会议	1. X-ray multilayer mid-frequency characterizations using speckle scanning techniques	蒋晖	展板报告	同步辐射技术及其应用	2017-08-05	美国
133	参加 2017 年矿物金属材料学会年会	Bonding Characteristics and Site Occupancies of Si Atoms in M6C Carbides from First Principles and Experimental Study	蒋力	分会报告	核技术及其应用	2017-02-25	美国
134	讨论 SINAP-ORNL 的合作；参加 2017 年熔盐堆研讨会	The Thorium Molten Salt Reactor Program in China	戴志敏	大会报告	反应堆物理与技术	2017-10-01	美国
135	参加第五届大型真空系统运行国际会议	The Operation of vacuum system at SSRF	刘以勇	分会报告	核技术及其应用	2017-05-07	德国
136	参加第二届大强子对撞机上反物质、超核物质和奇特物质产生国际研讨会	Recent results from STAR (focus on p-Omega correlations)	陈金辉	大会报告	核物理	2017-11-05	意大利
137	访问意大利米兰理工学院，参加技术交流会；参加 SINAP-JRC 合作会议；参加 GIF MSR 会议和第 22 届 PSSC 会议	China’s thorium-fueled molten salt reactor program	李晴暖	大会报告	核技术及其应用	2017-01-16	德国
138	讨论 SINAP-ORNL 的合作；参加 2017 年熔盐堆研讨会	Progress of the Molten Salt Natural Circulation Experiment	陈堃	大会报告	反应堆物理与技术	2017-10-01	美国
139	2017 年国际束流诊断会议	The Application of Direct RF Sampling System on Cavity BPM Signal Processing	赖龙伟	展板报告	核技术及其应用	2017-08-19	美国

140	参加第二届中德先进核安全技术基础研讨会	Thermal hydraulic system analysis code development for the Thorium Molten Salt Reactor	刘桂民	大会报告	反应堆物理与技术	2017-09-12	德国
141	参加第二届中德先进核安全技术基础研讨会	Thermal hydraulic research progress of the Thorium Molten Salt Test Reactors in SINAP	周翀	大会报告	反应堆物理与技术	2017-09-12	德国
142	参加第 16 届加速器与大型实验物理控制系统国际会议	Design and prototyping of a new synchronization system with stability at femtoseconds	刘鸣	大会报告	核技术及其应用	2017-10-06	西班牙
143	参加欧洲材料学会 2017 年秋季会议	Nanoscale dielectric property characterizing based on surface adhesion mapping by atomic force microscopy	汪颖	展板报告	表面、薄膜和纳米结构的表征和分析	2017-09-17	波兰
144	参加欧洲材料学会 2017 年秋季会议	Charging and Charge Transfer between Individual rGO sheets on Insulating Substrates Studied with AFM	张益	展板报告	表面、薄膜和纳米结构的表征和分析	2017-09-17	波兰
145	参加第二届中德先进核安全技术基础研讨会	Design and Analysis of a Small Modular Thorium Molten Salt Reactor	邹杨	大会报告	反应堆物理与技术	2017-09-12	德国
146	参加第十届国际非弹性 X 射线散射（IXS）会议	A high resolution x-ray emission and Raman spectroscopy end-station at the Shanghai Synchrotron Radiation Facility	李炯	展板报告	光源、光学器件和光学系统中的物理问题	2017-08-22	德国
147	参加 2017 自由电子激光国际会议	XFEL study In hard X-ray spectrum	赵振堂	分会报告	束流物理与加速器技术	2017-08-19	美国
148	作为国际科学顾问参加第 16 届加速器及大型实验物理控制系统国际会议	The Control Systems of SXFEL and DCLS	阎映炳	分会报告	束流物理与加速器技术	2017-10-05	西班牙
149	参加 2017 年奇异性核物理国际大会	相对论重离子碰撞中的奇异粒子产生	马余刚	大会报告	核物理	2017-03-11	日本

150	参加第十届国际非弹性 X 射线散射（IXS）会议	A Three Crystal X-ray Spectrometer and its Application at SSRF	黄宇营	大会报告	光源、光学器件和光学系统中的物理问题	2017-08-22	德国
151	参加德州农工大学回旋加速器实验室出束 50 年庆学术会议	相对论重离子碰撞中的平均场势效应	徐骏	大会报告	核物理	2017-11-14	美国
152	参加 2017 年春季 EPICS 合作会议	The control system technological activities for five accelerator projects	米清茹	大会报告	核技术及其应用	2017-05-14	日本
153	访问 Cinel 科学仪器公司进行多层膜单色器交流并参加第 24 届 X 射线光学和显微分析国际会议	Monochromatic beam based quantitative dynamic micro computed tomography	陈荣昌	分会报告	同步辐射光源原理和技术	2017-09-23	意大利
154	访问加州大学伯克利分校并参加第二十三届 DNA 计算和分子编程国际会议	Programming Highly Knotted Molecular Topologies Using Single-stranded Nucleic Acids	樊春海	大会报告	生物无机化学	2017-09-19	美国
155	参加"FLASH 的未来科学-连续波极紫外与软 X 射线自由电子激光的机遇"国际会议	Data science and theoretical works in XFEL	怀平	分会报告	自由电子激光原理和技术	2017-09-24	德国
156	参加奇异夸克物质 2017 会议并与 AGH 科技大学开展合作研究	Resonance effect on chiral magnetic effect signal	马国亮	展板报告	核物理	2017-06-30	波兰
157	中德 X 射线自由电子激光科学与技术国际合作会议	Status of FEL-Facilities and future plans in China and Hamburg	赵振堂	大会报告	自由电子激光	2017/5/3	中国
158	中德 X 射线自由电子激光科学与技术国际合作会议	FEL developments in Shanghai	王东	大会报告	自由电子激光	2017/5/3	中国
159	中德 X 射线自由电子激光科学与技术国际合作会议	Coherent X-ray optics development @ SINAP	邰仁忠	大会报告	自由电子激光	2017/5/3	中国
160	中德 X 射线自由	DAQ, control and analysis	陈建辉	大会报告	自由电子激光	2017/5/3	中国

	电子激光科学与技术国际合作会议	system for SXFEL and SCLF					
161	中德 X 射线自由电子激光科学与技术国际合作会议	Photon science in China: Status and Plan	赵振堂	大会报告	自由电子激光	2017/5/3	中国
162	第十二届亚洲同步辐射医学成像会议	Invited: Current status of biomedical applications at SSRF	谢红兰	大会报告	生物成像	2017/7/21	中国
163	第十二届亚洲同步辐射医学成像会议	Grating-based and propagation-based X-ray phase contrast imaging at SSRF and their biological applications	任玉琦	分会报告	生物成像	2017/7/21	中国

2018

No.	会议全称	报告名称	报告人	报告类别	报告学科领域	时间	地点
1	全球功能材料与器件专题讨论会并访问新加坡南洋理工大学	Synchrotron based research of pervsokite solar cells	高兴宇	分会报告	有机无机复合功能材料	2018-01-10	新加坡
2	第七届低发射度储存环研讨会	the development of aluminum vacuum chamber with small aperture in SSRF	汤启升	展板报告	束流物理与加速器技术	2018-01-14	瑞士
3	第 7 届低发射度储存环国际研讨会	Using a bessel light beam as an ultra short period helical undulator	姜伯承	展板报告	束流物理与加速器技术	2018-01-14	瑞士
4	2018 年度紧凑型高梯度加速技术国际研讨会	The development of deflecting structure at SINAP	谭建豪	分会报告	束流物理与加速器技术	2018-01-21	瑞士
5	2018 年度紧凑型高梯度加速技术国际研讨会	The development of X-band Accelerating Structure at SINAP	黄晓霞	分会报告	束流物理与加速器技术	2018-01-21	瑞士
6	2018 年度紧凑型高梯度加速技术国际研讨会	C-band Accelerating Structure at SINAP	方文程	分会报告	束流物理与加速器技术	2018-01-21	瑞士
7	第 4 届国际能源转换和储存化学专题讨论会并访问德国 Fritz Haber 研究所	Synchrotron based research of pervsokite solar cells	高兴宇	分会报告	半导体光伏材料与太阳电池	2018-01-26	德国
8	第 4 届能源转换与存储化学论坛；	AP-XPS On Energy Materials	宋飞	分会报告	固体表面与界面化学	2018-01-27	德国

	开展 CO/TiO2 的近常压光电子能谱的实验合作研究						
9	第 4 届能源转换与存储化学论坛；开展 CO/TiO2 的近常压光电子能谱的实验合作研究	AP-XPS On Energy Materials	宋飞	分会报告	固体表面与界面化学	2018-01-27	荷兰
10	第 4 界国际化学能源转换与存储会议	能源材料的上海光源谱学分总体研究现状与展望	姜政	分会报告	催化表征方法与技术	2018-01-27	德国
11	亚洲加速器及探测论坛国际会议并进行高稳定性充电电源稳定性学术交流	Status of Free Electron Lasers in SINAP	刘波	分会报告	束流物理与加速器技术	2018-01-28	韩国
12	亚洲加速器及探测论坛国际会议并进行微波功率稳定性及高稳定性充电电源方面的学术交流	C-band high stability modulator design for SXFEL	谷鸣	展板报告	束流物理与加速器技术	2018-01-28	韩国
13	亚洲加速器及探测论坛国际会议并进行微波功率稳定性及高稳定性充电电源方面的学术交流	C-band high stability modulator design for SXFEL	吴勇华	展板报告	束流物理与加速器技术	2018-01-28	韩国
14	亚洲加速器及探测论坛国际会议并进行微波功率稳定性及高稳定性充电电源方面的学术交流	DEPU controller design based on beckhoff for SSRF 2nd Projec	袁启兵	展板报告	束流物理与加速器技术	2018-01-28	韩国
15	TESLA 射频超导技术研讨会	Developing 3.9GHz cavities for CW SCLF	陈锦芳	大会报告	束流物理与加速器技术	2018-02-03	意大利
16	2018 未来光源研讨会（fls2018）	Eliminating the microbunching-instability-induced sideband in asoft x-ray self-seeding free-electron laser:	张开庆	大会报告	自由电子激光原理和技术	2018/3/5	中国上海
17	2018 未来光源研	Injection Transient	陈汉娇	大会报告	自由电子激光	2018/3/5	中国上海

	讨会（fls2018）	Observationvia Bunch-by-Bunch Beam SizeMeasurement System			原理和技术		
18	2018 未来光源研讨会（fls2018）	Theoretical studies on XFELO	李凯	大会报告	自由电子激光原理和技术	2018/3/5	中国上海
19	2018 未来光源研讨会（fls2018）	The Shanghai Hard X-ray FreeElectron Laser Project	王东	大会报告	自由电子激光原理和技术	2018/3/5	中国上海
20	2018 未来光源研讨会（fls2018）	The development andapplications of the Digital BPMsignal processor at SINAP	赖龙伟	大会报告	自由电子激光原理和技术	2018/3/5	中国上海
21	2018 未来光源研讨会（fls2018）	The Feasibility of NeuronNetwork-Based Beam-BasedAlignment:	曾理	大会报告	自由电子激光原理和技术	2018/3/5	中国上海
22	第二届国际光子科学应用探测器国际论坛	Recent development of indirect X-ray detectors in SSRF	宋飞	展板报告	同步辐射光源原理和技术	2018-03-09	法国
23	第一届核物理与行星科学研讨会	“Deexcitation of excited nuclei in IQMD	方德清	大会报告	核物理	2018-03-10	澳门
24	第一届核物理与行星科学研讨会	Antimatter in relativistic heavy ion collisions	马余刚	大会报告	核物理	2018-03-10	澳门
25	访问加州大学伯克利分校，ACS 全国第 255 次会议暨展览会并访问德州大学圣安东尼奥分校	Shape dependent cell entry and intracellular transport of self-assembled DNA nanostructures；Application of DNA Interface Sensor in Early Diagnosis and Treatment of Prostate Cancer ；Designer DNA Architectures for Bionanotechnology	樊春海	分会报告	生物无机化学	2018-03-16	美国
26	第三届文物艺术品研究及新技术创新国际会议	THE MORPHOLOGY AND CRYSTAL STRUCTURES IN PURPLE-GOLD GLAZE OF QING DYNASTY EXCAVATED FROM THE FORBIDDEN CITY	魏向军	分会报告	同步辐射技术及其应用	2018-03-24	意大利
27	OSA 高亮度光源及光驱动作用大会	Generating intense coherent EUV radiation via three-dimensional manipulation of the electron beam in storage rings	赵振堂	大会报告	束流物理与加速器技术	2018-03-25	法国
28	“紧凑型 EUV 和 X 射线光源”研讨会	Generating intense coherent EUV radiation via	冯超	大会报告	自由电子激光原理和技术	2018-03-25	法国

		three-dimensional manipulation of the electron beam in storage rings					
29	第八届国际小型模块化与先进反应堆峰会	核反应堆的发展	陈堃	大会报告	核技术及其应用	2018-03-26	美国
30	第 11 届放射分析化学方法和应用国际会议	Coordination Structure of Uranium Complexes in disordered Systems using X-ray Absorption Fine Structure Spectroscopy	张林娟	分会报告	物理无机化学	2018-04-07	美国
31	第 11 届放射分析化学方法和应用国际会议	Research progress of Actinide Research in TMSR	王建强	分会报告	物理无机化学	2018-04-07	美国
32	访问法国国家科学研究院并“第一届中法核物理大会”	中国核物理科学发展现状与计划	马余刚	大会报告	核物理	2018-04-08	法国
33	第一届中法核物理大会	Studies on exotic structure and radioactivity in proton-rich nuclei	方德清	大会报告	核物理	2018-04-09	法国
34	“高效率自由电子激光物理及应用”研讨会并访问美国阿贡国家实验室	Generating isolated terawatt-attosecond x-ray pulses via a chirped-laser-enhanced high-gain free-electron laser	王震	大会报告	束流物理与加速器技术	2018-04-10	美国
35	“高效率自由电子激光物理及应用”研讨会并访问美国阿贡国家实验室	Reverse-taper enhanced pre-bunching for TW-FEL generation	冯超	大会报告	束流物理与加速器技术	2018-04-10	美国
36	“高效率自由电子激光物理及应用”研讨会并访问美国阿贡国家实验室	Seeding high-power free-electron laser with XFELO	邓海啸	大会报告	束流物理与加速器技术	2018-04-10	美国
37	第十八届纳米科学基础国际会议并访问斯坦福大学	DNA Origami Nanostructures Exhibit Predominant Renal Uptake and Alleviate Acute Kidney Injury。	葛志磊	分会报告	生物无机化学	2018-04-13	美国
38	第十八届纳米科学基础国际会议并访问斯坦福大学	Shape-dependent cell entry and intracellular transport of self-assembled DNA nanostructures	樊春海	大会报告	生物无机化学	2018-04-13	美国

39	RHIC-STAR 实验组重味径迹探测器物理分析进展研讨会	超氚核和反超氚核质量的精确测量	陈金辉	大会报告	核物理	2018-04-26	美国
40	Heavy Flavor Tracker(HFT) 会议	在相对论重离子对撞机上精确测量超氚与反超氚的寿命与质量	刘鹏	分会报告	核物理	2018/4/26	美国
41	第九届国际粒子加速器会议	A Proposal for Coherent Hard X-Ray Generation Based on Two-Stage EEHG	赵振堂	大会报告	束流物理与加速器技术	2018-04-28	加拿大
42	2018 年 IPAC 大会及 2019 年 IPAC 会议第二次国际组委会会议	Study of Transverse Instabilities via Bunch-by-Bunch Beam Size Measurement System at SSRF；Filling Pattern Measurement System Upgrade in SSRF；The Control System Design of SCLF	冷用斌	展板报告	束流物理与加速器技术	2018-04-28	加拿大
43	2018 年国际粒子加速器会议并赴耶鲁大学进行双频电子枪项目研讨	RF system for SXFEL: C-band, X-band and S-band	方文程	展板报告	核技术及其应用	2018-04-28	加拿大
44	2018 年粒子加速器国际会议并 BLAST 研讨会及开展自由电子激光物理方面的学术交流	产生超短 X 射线自由电子激光脉冲的新方法	黄大章	展板报告	束流物理与加速器技术	2018-04-28	加拿大
45	2018 年国际粒子加速器大会	Transverse Phase Space Reconstruction Study on Shanghai Soft X-Ray FEL Facility	赵明华	展板报告	束流物理与加速器技术	2018-04-28	加拿大
46	2018 年国际粒子加速器大会	Commissioning of the APPLE-Knot Undulator at SSRF	张文志	展板报告	束流物理与加速器技术	2018-04-28	加拿大
47	2018 年国际粒子加速器大会	The preliminary design of LLRF for Shanghai hard X FEL	赵玉彬	展板报告	束流物理与加速器技术	2018-04-28	加拿大
48	2018 年国际粒子加速器大会	Cryogenic permanent magnet undulator of SSRF	何永周	展板报告	束流物理与加速器技术	2018-04-28	加拿大
49	2018 年国际粒子加速器大会	Analysis and Design of High Power Pulse Transformer for	刘永芳	展板报告	束流物理与加速器技术	2018-04-28	加拿大

		C-Band Klystron Modulator，Precise Stability Control System for High Power Pulse Modulator					
50	2018 年国际粒子加速器大会	X-band RF system as linearizer for SXFEL	谭建豪	展板报告	束流物理与加速器技术	2018-04-28	加拿大
51	2018 年国际粒子加速器大会	The Magnetic Field Measurement Systems for a Cryogenic Undulator and a Superconducting Undulator at SSRF	王宏飞	展板报告	束流物理与加速器技术	2018-04-28	加拿大
52	2018 年国际粒子加速器大会	Design of the beam distribution system of a soft x-ray FEL user facility in Shanghai	刘波	展板报告	束流物理与加速器技术	2018-04-28	加拿大
53	2018 年国际粒子加速器大会	Multi FEL lines with compact undulator layout	王东	展板报告	束流物理与加速器技术	2018-04-28	加拿大
54	2018 年国际粒子加速器大会	Longitudinal Effects of Trapped Homs in Shanghai Coherent Light Facility	郭俊杰	展板报告	自由电子激光原理和技术	2018/4/28	加拿大
55	2018 年国际粒子加速器大会	PRELIMINARY RESULTS OF THE BUNCH ARRIVAL-TIME MONITOR AT SXFEL	汪金国	展板报告	自由电子激光原理和技术	2018/4/28	加拿大
56	2018 年国际粒子加速器大会	The soft x-ray self-seeding system design for preliminary experiment study of SCLF facility	张开庆	展板报告	自由电子激光原理和技术	2018/4/28	加拿大
57	2018 年国际粒子加速器大会	High-degree circular polarization at X-ray self-seeding FELs with crossed-planar undulators	李凯	展板报告	自由电子激光原理和技术	2018/4/28	加拿大
58	2018 年国际粒子加速器大会	LATTICE DESIGN FOR A 1.2GEV STORAGE RING	沈思淇	展板报告	自由电子激光原理和技术	2018/4/28	加拿大
59	2018 年国际粒子加速器大会	高带宽 X 波段腔式束流位置检测器研究	曹珊珊	展板报告	束流物理与加速器技术	2018/4/28	加拿大
60	2018 年国际粒子加速器大会	SXFEL Linac BPM System Development and Performance Evaluation	陈方舟	展板报告	束流物理与加速器技术	2018/4/28	加拿大
61	2018 年国际粒子加速器大会	A bean based method to optimize the SBPM system	陈健	展板报告	束流物理与加速器技术	2018/4/28	加拿大
62	美国机械工程协会委员会会议	Numerical study of new ASME graphite assessment	曾广礼	大会报告	分析力学	2018-05-05	美国

		method					
63	ASME 高温堆标准工作组委员会议	LF1 of TMSR at SINAP	张小春	分会报告	结构力学与结构优化	2018-05-05	美国
64	STAR Pre-QM 和 Quark Matter 2018 国际学术会议并作报告	precise measurement on (anti-)hypertriton mass with the Heavy Flavor Tracker and the production of triton in Au+Au collisions at STAR	刘鹏	分会报告	核物理	2018/5/6	波兰、意大利
65	STAR Pre-QM 会议和 Quark Matter 2018 国际学术会议	STAR 实验中手征磁波测量的最新进展	寿齐烨	分会报告	核物理	2018-05-07	波兰
66	夸克物质 2018 国际会议	Measurement of interaction between antiprotons	张正桥	展板报告	核物理	2018-05-12	意大利
67	“超相对论核核碰撞-夸克物质 2018 国际会议”	The sign change of the four-particle cumulant in small systems from hydrodynamics and momentum conservation	马国亮	展板报告	核物理	2018-05-13	意大利
68	Quark Matter 2018 国际学术会议	Impact of magnetic field fluctuations on the CME in small systems	赵新丽	展板报告	核物理	2018/5/16	意大利
69	第 5 届亚洲&海洋地区辐射防护国际会议	Shielding Design for the Target of an Accelerator-Based Neutron Source	张志宏	分会报告	辐射剂量学和辐射防护	2018-05-19	澳大利亚
70	第 5 届亚洲&海洋地区辐射防护国际会议	Development of Noble Gas-Monitor Based on the Coincidence Detectors	蔡军	展板报告	辐射剂量学和辐射防护	2018-05-19	澳大利亚
71	第 57 届 PTCOG 国际会议	Commissioning status of the first Chinese domestic proton facility in Shanghai	陈志凌	展板报告	核技术及其应用	2018-05-20	美国
72	第 57 届 PTCOG 国际会议	Design of electrostatic deflector in the Shanghai Advanced Proton Therapy facility	何子锋	展板报告	核技术及其应用	2018-05-20	美国
73	第 57 届粒子治疗合作组国际会议	Treatment control implementation and commissioning for spot scanning mode in Shanghai Proton Therapy Facility	刘鸣	大会报告	核技术在工、农业和医学中的应用	2018-05-20	美国
74	参加第 57 届 PTCOG 国际会议	Commissioning status of the first Chinese domestic protron	孔海云、严	展板报告	核技术	2018/5/20	美国

		facility in Shanghai	南				
75	2018 年美国书(刊)展及知识服务国际学术研讨会	Semantic publishing analysis of Nuclear Science and Techniques journal	徐冬梅	分会报告	图书情报档案管理	2018-05-28	美国
76	第 27 届希腊核物理学会研讨会并访问希腊雅典大学	Viscosity of Nuclear Matter	马余刚	大会报告	核物理	2018-06-04	希腊
77	第 11 届国际高梯度加速技术会议（hg2018）	.High gradient RF activities of projects at SINAP	方文程	大会报告	自由电子激光原理和技术	2018/6/5	中国上海
78	第 11 届国际高梯度加速技术会议（hg2018）	Progress of x-band high power test platform at SINAP	谭建豪	大会报告	自由电子激光原理和技术	2018/6/5	中国上海
79	第 11 届国际高梯度加速技术会议（hg2018）	Research on wakefield suppression of two bunch operation mode in X-band disk-loaded accelerating structure	黄晓霞	大会报告	自由电子激光原理和技术	2018/6/5	中国上海
80	第 11 届国际高梯度加速技术会议（hg2018）	A new spherical pulse compressor working with degenerated "Whispering Gallery" mode	李宗斌	大会报告	自由电子激光原理和技术	2018/6/5	中国上海
81	第 11 届国际高梯度加速技术会议（hg2018）	LLRF layout and design for X-band test setup at SINAP	肖诚诚	大会报告	自由电子激光原理和技术	2018/6/5	中国上海
82	第四届 3D 材料科学国际会议	3D investigation on colloidal crystals by synchrotron radiation phase-contrast computed tomography	付亚楠	展板报告	高分子材料结构与性能	2018-06-09	丹麦
83	第八届新材料国际研讨会	Pancake-like growth and coalescence of intergranular helium bubbles: in situ observation and analytical modelling	黄鹤飞	分会报告	离子束与物质相互作用和辐照损伤	2018-06-09	意大利
84	钍基熔盐堆研究进展技术研讨会	Preparations for Safety Review and Licensing for TMSR Project	夏晓彬	大会报告	反应堆物理与技术	2018-06-12	日本
85	钍基熔盐堆研究进展技术研讨会	Progress on Thorium Molten Salt Reactor Energy System (TMSR) in China	徐洪杰	大会报告	反应堆物理与技术	2018-06-12	日本
86	ICALEPCS 2019 国际科学顾问委	ICALEPCS-2021 准备情况	阎映炳	大会报告	束流物理与加速器技术	2018-06-16	美国

	员会会议						
87	首届XLS|CompactLight 中期评审会议并进行医用质子加速器方面的的学术交流	High gradient RF activities of projects at SINAP	方文程	分会报告	束流物理与加速器技术	2018-06-17	意大利
88	首届XLS|CompactLight 中期评审会议并进行医用质子加速器方面的的学术交流	Research on wakefield suppression of two bunch operation mode in X-band disk-loaded accelerating structure	黄晓霞	分会报告	束流物理与加速器技术	2018-06-17	意大利
89	“未来医学研究及质子治疗装置理念和技术研讨会”及“第二届中德双边自由电子激光技术研讨会”	Ion therapy in China	赵振堂	大会报告	束流物理与加速器技术	2018-06-17	法国
90	2018 年强相互作用前沿研讨会	Hadron-Hadron Correlations in heavy-ion experiments	陈金辉	大会报告	核物理	2018-06-17	日本
91	第二届中德 XFEL 科学与技术双边研讨会	Activities of XFEL-based structural biology studies in China	何建华	大会报告	同步辐射技术及其应用	2018-06-18	德国
92	第二届中德自由电子激光科学与技术双边研讨会并访问欧洲自由电子激光装置	Advanced FEL seeding techniques at SXFEL and SCLF	冯超	大会报告	自由电子激光原理和技术	2018-06-18	德国
93	第二届中德自由电子激光科学与技术双边研讨会	Theory and Data science applications in coherent X-ray source: material structural phase transition	怀平	分会报告	自由电子激光原理和技术	2018-06-19	德国
94	第二届中德自由电子激光科学与技术双边研讨会及第十届国际同步辐射装备和仪器机械工程设计大会	Hammerhead support design and application at SSRF	高飞	展板报告	束流物理与加速器技术	2018-06-20	德国
95	第二届中德自由电子激光科学与技术双边研讨会及第十届国际同	Design a vertical polarized undulator based on magnetic force compensation technology	张伟	展板报告	束流物理与加速器技术	2018-06-20	德国

	步辐射装备和仪器机械工程设计大会						
96	第二届中德自由电子激光科学与技术双边研讨会及第十届国际同步辐射装备和仪器机械工程设计大会	Study on cooling technology of the Superconducting Undulator at SSRF	刘以勇	展板报告	束流物理与加速器技术	2018-06-20	德国
97	第二届中德自由电子激光科学与技术双边研讨会及第十届国际同步辐射装备和仪器机械工程设计大会	Mechanical Engineering for SCLF Accelerator	殷立新	大会报告	束流物理与加速器技术	2018-06-20	德国
98	第二届中德自由电子激光科学与技术双边研讨会及第十届国际同步辐射装备和仪器机械工程设计大会	Hammerhead support design and application at SSRF	高飞	展板报告	束流物理与加速器技术	2018-06-20	法国
99	第二届中德自由电子激光科学与技术双边研讨会及第十届国际同步辐射装备和仪器机械工程设计大会	Design a vertical polarized undulator based on magnetic force compensation technology	张伟	展板报告	束流物理与加速器技术	2018-06-20	法国
100	第二届中德自由电子激光科学与技术双边研讨会及第十届国际同步辐射装备和仪器机械工程设计大会	Study on cooling technology of the Superconducting Undulator at SSRF	刘以勇	展板报告	束流物理与加速器技术	2018-06-20	法国
101	第二届中德自由电子激光科学与技术双边研讨会及第十届国际同步辐射装备和仪器机械工程设计	Mechanical Engineering for SCLF Accelerator	殷立新	大会报告	束流物理与加速器技术	2018-06-20	法国

	大会						
102	2018 年欧洲 X 射线光谱学国际会议并访问德国卡尔斯鲁厄大学	Potential Environmental Applications by Medium Energy Micro-probe Beamline Proposed in SSRF Phase-II Project	李丽娜	展板报告	同步辐射技术及其应用	2018-06-23	斯洛文尼亚共和国
103	2018 年欧洲 X 射线光谱学国际会议并访问德国卡尔斯鲁厄大学	The U-induced changes in crystal-field and covalency effects of Th4+ in Th1-xUxO2 mixed oxides probed by HERFD-XANES	黄宇营	展板报告	同步辐射技术及其应用	2018-06-23	斯洛文尼亚共和国
104	2018 年欧洲 X 射线光谱学国际会议并访问德国卡尔斯鲁厄大学	Potential Environmental Applications by Medium Energy Micro-probe Beamline Proposed in SSRF Phase-II Project	李丽娜	展板报告	同步辐射技术及其应用	2018-06-23	德国
105	2018 年欧洲 X 射线光谱学国际会议并访问德国卡尔斯鲁厄大学	The U-induced changes in crystal-field and covalency effects of Th4+ in Th1-xUxO2 mixed oxides probed by HERFD-XANES	黄宇营	展板报告	同步辐射技术及其应用	2018-06-23	德国
106	2018 年度纳米材料国际会议	Design of Energy Materials Beamline (E-line) for in-situ study at the Shanghai Synchrotron Radiation Facility	陈振华	展板报告	表面、薄膜和纳米结构的表征和分析	2018-06-23	香港
107	第十四届国际纳米结构材料会议	Designing nanomaterials for biosensors	樊春海	分会报告	生物无机化学	2018-06-23	香港
108	第十四届国际纳米结构材料会议	Graphene nanoprobes in high sensitive and selective biosensor	王丽华	分会报告	生物无机化学	2018-06-23	香港
109	ASTM 人造碳和石墨生产的 DO2.F 小组委员会议	The grain size effect on tensile strength measurement	曾广礼	大会报告	分析力学	2018-06-23	美国
110	第十三届国际超核物理和奇异粒子物理大会	Precise measurement on hypertriton and anti-hypertriton mass and lifetime with the STAR Heavy Flavor Tracker	陈金辉	大会报告	核物理	2018-06-24	美国
111	第十届国际同步辐射装备和仪器机械工程设计大会	Vibrational Stability of a Cryo-cooled Double Crystal Monochromator at SSRF	樊奕辰	展板报告	同步辐射技术及其应用	2018-06-24	法国

112	同步辐射和自由电子激光产生和应用国际会议	SSRF storage ring upgrade in the beam line phase II project	姜伯承	大会报告	核技术及其应用	2018-06-24	俄罗斯
113	2018 年 TESLA 技术的国际合作会议	上海光源超导三次谐波腔系统	侯洪涛	分会报告	束流物理与加速器技术	2018-06-25	日本
114	第 13 届欧洲 SOFC/SOEC 论坛	Molten salt synthesis of La0.6Sr0.4Co0.2Fe0.75Nb0.05O3-δ for symmetric solid oxide fuel cells	关成志	展板报告	燃料电池	2018-07-01	瑞士
115	第 13 届欧洲 SOFC/SOEC 论坛	High Temperature Steam/CO2 Co-electrolysis Using Solid Oxide Electrolyser Stack at Shanghai Institute of Applied Physics	肖国萍	分会报告	燃料电池	2018-07-01	瑞士
116	植物科学与生物安全学术年会	Structure and function relation on plants used for Chinese	薛艳玲	展板报告	同步辐射技术及其应用	2018-07-10	西班牙
117	植物科学与生物安全学术年会	Three-dimensional-microstructure characterization of plants with X-ray microtomography	肖体乔	大会报告	同步辐射技术及其应用	2018-07-10	西班牙
118	植物科学与生物安全学术年会	The three-dimensional network characterization of vascular bundles in the nodes of bamboo and rice	彭冠云	展板报告	同步辐射技术及其应用	2018-07-10	西班牙
119	植物科学与生物安全学术年会	A X-ray tube based phase-sensitive CT system for plant sicence research	陈荣昌	展板报告	同步辐射技术及其应用	2018-07-10	西班牙
120	第 16 届韩国国际纳米技术研讨会暨纳米博览会	DNA Nanotechnology and Biosensing	樊春海	大会报告	生物无机化学	2018-07-10	韩国
121	2018 年压力容器与管道会议	Effects of thermal aging on microstructure and hardness of Ni cladding on austenitic stainless steel by GTAW	玉昆	分会报告	金属结构材料	2018-07-15	捷克共和国
122	第十七届国际 X 射线吸收精细结构会议	HERFD-XANES study of crystal-field split of 6d orbits of ThO2	黄宇营	展板报告	同步辐射技术及其应用	2018-07-20	波兰
123	第十七届国际 X 射线吸收精细结构会议	Investigation of the fine structure around the copper site in CuZnSOD by XANES combined with ab initio calculations	王宇	展板报告	同步辐射技术及其应用	2018-07-20	波兰
124	第十七届国际 X	MoC-Mo2C/Co composites as	姜政	展板报告	同步辐射技术	2018-07-20	波兰

	射线吸收精细结构会议	efficient electrocatalysts for hydrogen evolution reaction			及其应用		
125	第 26 届国际核工程大会	Research of weld cladding of vessel in molten salt reactor	李志军	分会报告	反应堆物理与技术	2018-07-21	英国
126	第 26 届国际核工程大会	ELECTRIC FIELD SIMULATION OF IONIZATION CHAMBER USED IN TRITIUM MEASUREMENT IN TAIL GAS OF MOLTEN SALT REACTOR	钱楠	分会报告	反应堆物理与技术	2018-07-21	英国
127	第 26 届国际核工程大会	Design and Safety Features Analysis of the 2MW Chinese Thorium Molten Salt Test Reactor TMSR-LF1	周翀	分会报告	反应堆物理与技术	2018-07-21	英国
128	"Beta-decay studies of extremely proton-rich nuclei from Mg to S"研讨会并进行合作实验数据分析及相关合作讨论	“Two-proton emission from IAS of 22-Mg	方德清	大会报告	核物理	2018-07-21	香港
129	第二十六届国际核工程大会	THE COMPATIBILITY OF NUCLEAR GRAPHITE WITH MOLTEN SALT IN THEMOLTEN SALT REACTOR	贺周同	分会报告	核技术及其应用	2018-07-21	英国
130	“Beta-decay studies of extremely proton-rich nuclei from Mg to S”研讨会	beta-decay study of the T-z =-2 proton-rich nucleus Mg-20	马余刚	大会报告	核物理	2018-07-29	香港
131	2018 年度国际电化学能源科技大会	HIGHLY ACTIVE SURFACE STRUCTURE IN NANOSIZED SPINEL COBALT-BASED OXIDES FOR ELECTROCATALYTIC WATER SPLITTING	周靖	分会报告	电化学	2018-08-12	加拿大
132	2018 年度国际电化学能源科技大会	OPERANDO X-RAY ABSORPTION SPECTROSCOPY	张林娟	展板报告	电化学	2018-08-12	加拿大

		INVESTIGATION OF PEROVSKITE SYNTHESIZED BY MOLTEN-SALT METHOD AS EFFICIENT ELECTROCATALYSTS FOR OXYGEN EVOLUTION					
133	第 14 届 X 射线显微国际会议	Soft X-ray Spectro-Ptychography for Air Pollution Particulates	刘海岗	展板报告	同步辐射技术及其应用	2018-08-19	加拿大
134	第 14 届 X 射线显微国际会议	Automatic Calibrations of Sample Drift for Nanotomography at SSRF	张祥志	展板报告	同步辐射技术及其应用	2018-08-19	加拿大
135	第 14 届 X 射线显微国际会议	Eliminating Decoherence Effects and Improving Reconstructed Image Quality in Soft X-ray Ptychography	许子健	展板报告	同步辐射技术及其应用	2018-08-19	加拿大
136	第 14 届 X 射线显微国际会议	Designing of the SXFEL beamline for single pulse biological living cell imaging	郭智	展板报告	同步辐射技术及其应用	2018-08-19	加拿大
137	第 14 届 X 射线显微国际会议	The imaging quality improved significantly in a surface-modified scintillator X-ray imager	吴衍青	展板报告	同步辐射技术及其应用	2018-08-19	加拿大
138	第 14 届 X 射线显微国际会议	Single-bounce ellipsoidal capillary for X-ray microscopes: design and measurements	杜国浩	展板报告	同步辐射技术及其应用	2018-08-19	加拿大
139	第 14 届 X 射线显微国际会议	3D full-field transmission X-ray microscopy based on equally sloped tomography at Shanghai Synchrotron Radiation Facility	邓彪	展板报告	同步辐射技术及其应用	2018-08-19	加拿大
140	第 53 届 Zakopane 核物理国际会议	Studies on the two-proton emission from the IAS states of 22Mg	方德清	大会报告	核物理	2018-08-25	波兰
141	第 22 届欧洲裂纹大会	Investigation of heat-treatment-induced pore microstructural variations in cold sprayed titanium	肖体乔	大会报告	超常环境下材料和结构的力学行为	2018-08-26	塞尔维亚
142	BLTP/JINR-SKL TP/CAS 双边研讨会	“Photonuclear reaction as a tool to probe alpha-clustering structure”	马余刚	大会报告	核物理	2018-09-01	俄罗斯

143	第 19 届国际核石墨专家会议	Thorium Molten Salt Reactors and Their Nuclear Graphite	周兴泰	大会报告	核分析技术	2018/9/2	中国上海
144	第 19 届国际核石墨专家会议	Characterization of Gas-escape Pores of IG-110 Graphite before and after Irradiation	黄庆	大会报告	核分析技术	2018/9/2	中国上海
145	第 19 届国际核石墨专家会议	Experimental Study on Fluid-Structure Interaction of Graphite Core Components in Thorium-based Molten-Salt Reactor	黄超超	大会报告	核分析技术	2018/9/2	中国上海
146	第 19 届国际核石墨专家会议	Research and development of C/C composite used for TMSR	高彦涛	大会报告	核分析技术	2018/9/2	中国上海
147	第 19 届国际核石墨专家会议	Porosity Effect on CTE of Graphite	曾广礼	大会报告	核分析技术	2018/9/2	中国上海
148	钍熔盐堆发展方面的技术研讨会和日本原子力学会 2018 年会	Safety Licensing for TMSR Project	夏晓彬	大会报告	反应堆物理与技术	2018-09-03	日本
149	钍熔盐堆发展方面的技术研讨会和日本原子力学会 2018 年会	Progress on Thorium Molten Salt Reactor Energy System (TMSR) in China	徐洪杰	大会报告	反应堆物理与技术	2018-09-03	日本
150	第四届 X 射线掠入射散射会议	GISAXS study on Micro-Structure of Layer-by-Layer Self-Assembly multilayer	杨春明	展板报告	同步辐射技术及其应用	2018-09-03	韩国
151	第四届 X 射线掠入射散射会议	In-situ characterization of SAXS/WAXS in polymer processing	林金友	分会报告	同步辐射技术及其应用	2018-09-03	韩国
152	第七届同步辐射聚合物会议	Development of Small Angle X ray Scattering at Shanghai Synchrotron Radiation Facility	边风刚	大会报告	同步辐射技术及其应用	2018-09-03	韩国
153	2018 年度对称能国际研讨会及输运模拟研讨会	中低能重离子碰撞中的同位旋驰豫时间；pion production from transport simulations	徐骏	大会报告	核物理	2018-09-09	韩国
154	第 7 届国际束流诊断大会（IBIC2018）	Injection Transient Study Using 6-Dimensional Bunch-by-bunch Diagnostic System at SSRF	周逸媚	大会报告	加速器束流测量	2018/9/9	中国上海
155	第 7 届国际束流诊断大会	The Removal of Interference Noise of ICT using the PCA	陈健	大会报告	加速器束流测量	2018/9/9	中国上海

	（IBIC2018）	Method					
156	第 7 届国际束流诊断大会（IBIC2018）	The Application of Beam Arrival Time Measurement at SXFEL	曹姗姗	大会报告	加速器束流测量	2018/9/9	中国上海
157	第 7 届国际束流诊断大会（IBIC2018）	Identification of Faulty Beam Position Monitor Based Clustering by Fast Search and Find of Density Peaks	姜瑞涛	展板报告	加速器束流测量	2018/9/9	中国上海
158	第 7 届国际束流诊断大会（IBIC2018）	The Development and Applications of Digital BPM Signal Processor on SSRF	赖龙伟	展板报告	加速器束流测量	2018/9/9	中国上海
159	第 7 届国际束流诊断大会（IBIC2018）	On-line Crosstalk Measurement and Compensation Algorithm Study of SXFEL Digital BPM System	陈方舟	展板报告	加速器束流测量	2018/9/9	中国上海
160	第 7 届国际束流诊断大会（IBIC2018）	The Evaluation of Beam Inclination Angle on the Cavity BPM Position Measurement	陈健	展板报告	加速器束流测量	2018/9/9	中国上海
161	第 7 届国际束流诊断大会（IBIC2018）	Influence of Sampling Rate and Passband on the Performance of Stripline BPM	吴桐	展板报告	加速器束流测量	2018/9/9	中国上海
162	第 7 届国际束流诊断大会（IBIC2018）	EOM Based Beam Arrival Time Monitor for SXFEL	刘晓庆	展板报告	加速器束流测量	2018/9/9	中国上海
163	第 7 届国际束流诊断大会（IBIC2018）	Machine Learning Applied to Predict Transverse Oscillation at SSRF	高波	展板报告	加速器束流测量	2018/9/9	中国上海
164	第 7 届国际束流诊断大会（IBIC2018）	SSRF Beam Operation Stability Evaluation Using Bunch by Bunch Beam Position Method	张宁	展板报告	加速器束流测量	2018/9/9	中国上海
165	第 7 届国际束流诊断大会（IBIC2018）	Data Acquisition System for Beam Instrumentation of SXFEL and DCLS	阎映炳	展板报告	加速器束流测量与控制	2018/9/9	中国上海
166	“超快成像和粒子追踪仪器和方法”国际会议	The ultrafast X-ray imaging beamline at SSRF	陈荣昌	展板报告	同步辐射技术及其应用	2018-09-10	美国
167	“超快成像和粒子追踪仪器和方法”国际会议	Dynamic X-ray imaging at Shanghai Synchrotron Radia on Facility	肖体乔	大会报告	同步辐射技术及其应用	2018-09-10	美国
168	2018 年自由电子激光光子诊断国	Second Order Intensity Correlation Method to	李春雷	展板报告	自由电子激光原理和技术	2018-09-16	德国

	际会议	Characterize Spatial Coherence of Soft X-ray Free Electron Lasers					
169	第 20 届 21 世纪东亚地区核物理研讨会	Shear viscosity of nuclear matter from heavy-ion collision	马余刚	大会报告	核物理	2018-09-18	日本
170	第 27 届国际标准化组织表面化学分析技术委员会全体会议和第 11 届国际表面、材料和真空大会	Study of the nanostructure catalyst by XAFS technique at SSRF	黄宇营	大会报告	同步辐射技术及其应用	2018-09-19	墨西哥
171	第 62 届 ICFA 先进束流动力学研讨会	Summary from IBIC2018 in Shanghai	冷用斌	大会报告	束流物理与加速器技术	2018-09-23	香港
172	第七届有机氚专题研讨会	Preliminary Study on the Source of NE-OBT in the Soil around the Qinshan Nuclear Power Plant	刘卫	分会报告	核技术及其应用	2018-09-23	加拿大
173	21 世纪太平洋地区核能大会	Progress of TMSR Project in China	戴志敏	大会报告	反应堆物理与技术	2018-09-29	美国
174	第十一届加速器运行研讨会	Operation Reliability of SSRF in Last Operation Season and upgrade plan at SSRF	孙启龙	展板报告	束流物理与加速器技术	2018-09-29	美国
175	第十一届加速器运行研讨会	Main Tools in one System Operation	赵申杰	展板报告	束流物理与加速器技术	2018-09-29	美国
176	第六届核能和可再生能源国际会议	Progress of High Temperature Steam Electrolysis with Molten Salt Reactor	王建强	分会报告	核技术及其应用	2018-09-29	韩国
177	21 世纪太平洋地区核能大会	overview of TMSR-LF1 design	邹杨	分会报告	反应堆物理与技术	2018-09-29	美国
178	第十届国际镅和锎科学和应用研讨会	Immobilization of ReO_4^- by a family of rare-earth plumbite perchlorates based on single crystal-to-single crystal transformation	林健	分会报告	核放射化学	2018-10-02	俄罗斯
179	第十七届国际小角散射会议	Development of Automation technology with Small Angel X-ray Scattering at Shanghai Synchrotron Radiation Facility	周平	展板报告	同步辐射技术及其应用	2018-10-06	美国
180	第十七届国际小角散射会议	PROBING MICRO-STRUCTURE OF LAYER-BY-LAYER	杨春明	展板报告	同步辐射技术及其应用	2018-10-06	美国

181	第十七届国际小角散射会议	SELF-ASSEMBLY CHITOSAN/POLY(？-GLUTAMIC ACID) MULTILAYER USING GISAXS MULTI-TECHNIQUES IN SITU WITH SMALL ANGLE X RAY SCATTERING AT SHANGHAI SYNCHROTRON RADIATION FACILITY	王玉柱	分会报告	同步辐射技术及其应用	2018-10-06	美国
182	第十七届国际小角散射会议	DEVELOPMENT OF SAXS/WAXS/RAMAN COMBINED TEST METHODOLOGY AT SHANGHAI SYNCHROTRON RADIATION FACILITY	缪夏然	展板报告	同步辐射技术及其应用	2018-10-06	美国
183	2018 年度亚洲核合作论坛- 辐射技术在高分子改性在农业、环境和医学上在应用研讨会	Radiation Processing and Polymer Modification for Environmental Applications	马红娟	大会报告	核技术在环境科学、地学和考古中的应用	2018-10-07	哈萨克斯坦
184	2018 年国际粒子加速器准直测量会议	上海光源超长线准直测量方法研究	张翼飞	展板报告	同步辐射光源原理和技术	2018-10-07	美国
185	第 5 届光注入器中的光阴极物理国际会议	Study on the K-Cs-Sb photocathode preparation based on the co-evaporation K and Cs source	顾强	展板报告	束流物理与加速器技术	2018-10-13	美国
186	2018 纳米气泡/纳米液滴国际会议	Nanobubbles and Applications	胡钧	大会报告	核分析	2018/10/16	中国苏州
187	2018 纳米气泡/纳米液滴国际会议	Biological Effect of Inert Gas/Nanobubbles	方海平	大会报告	核分析	2018/10/16	中国苏州
188	2018 纳米气泡/纳米液滴国际会议	The Chemical Information of Nanobubbles Inside Explored by Synchrotron Based STXM	周利民	大会报告	核分析	2018/10/16	中国苏州
189	2018 纳米气泡/纳米液滴国际会议	Effects of nanobubbles on peptide self-assembly	张益	大会报告	核分析	2018/10/16	中国苏州
190	2018 纳米气泡/纳米液滴国际会议	Bubble Formation Behavior From Vertical Wall Orifice of Venturi-type Bubble	马兆伟	大会报告	核分析	2018/10/16	中国苏州

		Generator					
191	新能源和环境相关的低温和同位素技术国际会议	Fabrication and hydrogen permeation of Al2O3/Er2O3 coating by MOD method	张东勋	分会报告	核技术及其应用	2018-10-22	罗马尼亚
192	2018 年国际核燃料干法技术研讨会	Separation of rare earth，thorium fluoride using precipitation-distillation coupled method in FLiNaK melts.	付海英	分会报告	核化学与核燃料化学	2018-10-23	日本
193	2018 年国际核燃料干法技术研讨会	Application of electrochemical technology in TMSR	黄卫	分会报告	核化学与核燃料化学	2018-10-23	日本
194	2018 年国际核燃料干法技术研讨会	Pyroprocessing technologies dedicated to nuclear fuel cycle in Thorium-based Molten Salt Reactor.	李晴暖	分会报告	核化学与核燃料化学	2018-10-23	日本
195	2018 年国际核燃料干法技术研讨会	Study on Fluoride Volatility and Low Pressure Distillation Technology in TMSR.	窦强	分会报告	核化学与核燃料化学	2018-10-23	日本
196	2018 年度应用超导大会	Hall probe measurement scheme for a long planner superconducting undulator	钱茂飞	展板报告	束流物理与加速器技术	2018-10-27	美国
197	2018 年度美国应用超导学大会	Test result of the 50-period superconducting undulator prototype at SSRF	许皆平	展板报告	同步辐射光源原理和技术	2018-10-27	美国
198	2018 年度美国应用超导学大会	Quench Simulation of REBCO Undulator Magnet	丁祎	展板报告	同步辐射光源原理和技术	2018-10-27	美国
199	第一届四代小模堆国际会议	Hydrogen production by molten salt reactor	王建强	大会报告	反应堆物理与技术	2018-11-04	加拿大
200	第一届四代小模堆国际会议	Progress of small modular TMSR design	邹杨	大会报告	反应堆物理与技术	2018-11-04	加拿大
201	第一届四代小模堆国际会议	Progress of TMSR Project in China	徐洪杰	大会报告	反应堆物理与技术	2018-11-04	加拿大
202	第七届亚太地区辐射化学国际会议	Radiation functionalized polymer material for possible sensing and environment preservation	吴国忠	大会报告	核分析技术	2018/11/4	中国上海
203	第七届亚太地区辐射化学国际会议	Amidoxime-based Fiber Adsorbents in the Application of Uranium Extraction from Seawater	马红娟	大会报告	核分析技术	2018/11/4	中国上海
204	第一届先进材料研讨会	Introduction of Shanghai Synchrotron Radiation Facility	文闻	大会报告	同步辐射技术及其应用	2018-11-21	韩国

205	2018 年亚洲晶体学国际会议	Acquirement and measurement of Micro-focused beam for MX at SSRF	刘科	展板报告	同步辐射技术及其应用	2018-12-01	新西兰
206	2018 年亚洲晶体学国际会议	Crystal Structure and Enantioselectivity of Terpene Cyclization in SAM Dependent Methyltransferase TleD	郁峰	展板报告	同步辐射技术及其应用	2018-12-01	新西兰
207	研究核氢生产在氢经济背景下的作用技术会议并访问丹麦托普索公司和丹麦技术大学	Nuclear Hydrogen Research in TMSR	王建强	分会报告	应用无机化学	2018-12-02	奥地利
208	2018 年度国际核-核碰撞大会	Mechanism of two-proton emission from the IAS of 22Mg	方德清	大会报告	核物理	2018-12-03	日本
209	原子能机构核石墨知识库现状技术会议	Graphite oxidation	曾广礼	大会报告	核技术及其应用	2018-12-11	奥地利
210	全球功能材料与器件专题讨论会并访问新加坡南洋理工大学	Synchrotron based research of pervsokite solar cells	高兴宇	分会报告	有机无机复合功能材料	2018-01-10	新加坡