ICM-CN 2021

2021 International Conference on Materials: Advanced and Emerging Materials

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中国科学院深圳理工大学
SHENZHEN INSTITUTE OF ADVANCED TECHNOLOGY
CHINESE ACADEMY OF SCIENCES

中国科学院深圳先进技术研究院
SHENZHEN INSTITUTE OF ADVANCED TECHNOLOGY
CHINESE ACADEMY OF SCIENCES

Orginazer

中国科学院深圳先进技术研究院
SHENZHEN INSTITUTES OF ADVANCED TECHNOLOGY
CHINESE ACADEMY OF SCIENCES

中国科学院深圳理工大学
SHENZHEN INSTITUTE OF ADVANCED TECHNOLOGY
CHINESE ACADEMY OF SCIENCES

Shenzhen Institutes of Advanced Technology, Chinese Academy of Sciences

The Shenzhen Institutes of Advanced Technology (SIAT) of the Chinese Academy of Science (CAS) was jointly established by CAS, the Shenzhen municipal government and the Chinese University of Hong Kong in February 2006. SIAT aims to enhance the innovative capacity of the equipment manufacturing and service industries in the Guangdong-Hong Kong region, promote the development of emerging industries possessing their own proprietary intellectual property, and become a world-class industrial research institute.

SIAT focuses on the multi-disciplinary integration development of Information Technology and Biotechnology. It mainly includes 8 affiliated institutes(51 research centers): Shenzhen Institute of Advanced Integration Technology (SIAIT); Institute of Biomedical and Health Engineering (IBHE); Institute of Advanced Computing and Digital Engineering (IACDE); Institute of Biomedicine and Biotechnology (IBB); Guangzhou Institute of Advanced Technology (GIAT); Brain Cognition and Brain Disease Institute (BCBDI), collaborated with MIT McGovern Institute; Institute of Synthetic Biology; Institute of Advanced Electronic Materials (IAEM); Institute of Carbon Neutral (under construction).

It is also home to 9 national innovation labs, 33 key labs and platforms at the provincial level and 63 key labs and platforms at the municipal level.

Affiliated Institutes:

- Institute of Advanced Integration Technology
- Institute of Biomedical and Health Engineering
- Institute of Advanced Computing and Digital Engineering
- Institute of Biomedicine and Biotechnology
- Guangzhou Institute of Advanced Technology
- Brain Cognition and Brain Disease Institute
- Institute of Synthetic Biology
- Institute of Advanced Electronic Materials

SIAT has a broad cooperation with overseas partners covering 38 countries and districts, more than 200 programs 98 institutions like MIT, Stanford University, UCL, UBC, UCLA, EPFL, HU Berlin etc. 48% of annual publication are international cooperated papers.

SIAT is already a leading research institute in the south of China and innovative reforming model in China, as is reflected by the consistency with our high-quality papers and contribution to industries. However, we still have a long way to go for our ultimate goal as the top-tier ‘ E(Engineering) - T(Technology) - S(Science)’ institute around the world.

http://english.siat.cas.cn/

MDPI

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MDPI is committed to open access publishing services and currently publishes 374 academic journals in English, including 93 SCIE journals. The journals cover biology, chemistry, medicine, machinery, energy, environment and other disciplines, Including Materials, Molecules, Sensors, International Journal of Molecular Sciences, Marine Drugs, Energies, International Journal of Environmental Research and Public Health and so on. https://www.mdpi.com/

Materials

Materials (ISSN 1996-1944) is a peer-reviewed, open access journal of materials science and engineering published semimonthly online by MDPI. Prof. Dr. Maryam Tabrizian from McGill University serves as the Editor-in-Chief. The Portuguese Materials Society (SPM), Spanish Materials Society (SOCIEMAT) and Manufacturing Engineering Society (MES) are affiliated with Materials and their members receive a discount on the article processing charges.

Materials indexed within Scopus, SCIE (Web of Science), PubMed, PMC, Ei Compendex, CaPlus / SciFinder, Inspec, Astrophysics Data System, and many other databases.。Impact Factor is 3.623 (2020) and 5-Year Impact Factor: 3.920 (2020), Citescore 4.2, ranking JCR - Q1 (Metallurgy & Metallurgical Engineering) / CiteScore - Q2 (Condensed Matter Physics). Materials provides a forum for publishing papers which advance the in-depth understanding of the relationship between the structure, the properties or the functions of all kinds of materials. Chemical syntheses, chemical structures and mechanical, chemical, electronic, magnetic and optical properties and various applications will be considered.

Manuscripts in *Materials* are peer-reviewed and a first decision provided to authors approximately 13.6 days after submission; acceptance to publication is undertaken in 3.6 days (median values for papers published in this journal in the first half of 2021).

https://www.mdpi.com/journal/materials

Co-organizers and Cooperations

Rare Earth Crystal Committee of Chinese Rare Earth Society

The Chinese Society of Rare Earths(CSRE), founded in 1979, is the first national society on rare earth science, technology and applications in the world. Rare Earth Crystal Committee of CSRE was established in May 2019. As a branch of The Chinese Society of Rare Earth, it is an important organizational foundation of the Society

Chemical Engineering Department, Tsinghua University

The Department of Chemical Engineering was founded in 1946. The department currently has more than 60 faculty members of whom 34 are professors. Among the faculty, one is an academician of the Chinese Academy of Sciences, two are academicians of the Chinese Academy of Engineering, three are Ministry of Education's Chang Jiang Scholar Chair Professors.

Shenzhen International Graduate School of Tsinghua University

Tsinghua and Shenzhen's joint venture into graduate education and scientific innovation began with the creation of the Graduate School at Shenzhen, Tsinghua University (GSST) in 2001. An important part of Tsinghua's commitment to becoming a leading global university and revolutionizing higher education, GSST adopted a globalized, comprehensive, and innovative approach to graduate education

Chinese Chemical Society

The Chinese Chemical Society (CCS) is an academic organization formed by Chinese chemists of their own accord with the purpose of uniting Chinese chemists at home and abroad to promote the development of chemistry in China. The CCS was founded on August 4, 1932. It currently has more than 85,000 individual members and 166 organizational members.

Shenzhen Modern Material Association

Shenzhen New Materials Industry Association was established in 2010 to promote the revitalization and development of new materials industry as its mission, to build a comprehensive association integrating industrial chain, industry-university-research and capital promotion.

Media Partners

Applied Sciences, founded in 2011, is an international, peer-reviewed, open access journal on all aspects of applied natural sciences published semimonthly online by MDPI. Indexed within Scopus, SCIE (Web of Science), Inspec, CAPlus/SciFinder, and many other databases. IF 2.679, ranking JCR-Q2 (*Engineering, Multidisciplinary*)/ CiteScore-Q2 (*General Engineering*)

https://www.mdpi.com/journal/applsci

Nanomaterials founded in 2010, it publishes reviews, regular research papers, communications, and short notes that relevant to any field of study that involves nanomaterials. IF 5.076, ranking JCR-Q1 (*Physics, Applied*)/ CiteScore-Q1 (*General Chemical Engineering*)

https://www.mdpi.com/journal/nanomaterials

Electronic Materials is an international, peer-reviewed, open access journal on fundamental science, engineering, and practical applications of electronic materials published quarterly online. There is no restriction on the length of the papers. The full experimental details must be provided so that the results can be reproduced.

https://www.mdpi.com/journal/electronicmat

Coatings founded in 2011, is a peer-reviewed journal of coatings and surface engineering published monthly. Manuscripts are peer-reviewed and a first decision provided to authors approximately 11.4 days after submission; acceptance to publication is undertaken in 3.4 days. IF 2.881

https://www.mdpi.com/journal/coatings

Journal of Functional Biomaterials is an international, interdisciplinary, peer-reviewed, open access journal on materials for biomedical use and is published quarterly online. The publications are all free to readers. CiteScore-Q1 (*Biomedical Engineering*)

https://www.mdpi.com/journal/jfb

Catalysts (IF: 4.146, CiteScore: 4.5) is a peer-reviewed open access journal of catalysts and catalyzed reactions published monthly online. The Romanian Catalysis Society (RCS) are partners of Catalysts journal. Catalysts ranking JCR-Q2 (*Chemistry, Physical*) / CiteScore-Q2 (*Physical and Theoretical Chemistry*)

https://www.mdpi.com/journal/catalysts

Electronics (ISSN 2079-9292，IF 2.397) is an international, peer-reviewed, open access journal on the science of electronics and its applications published semimonthly online. It indexed within Scopus, SCIE (Web of Science), CAPlus / SciFinder, Inspec, and many other databases, ranking CiteScore - Q2 (*Electrical and Electronic Engineering*)

https://www.mdpi.com/journal/electronics

Metals (ISSN: 2075-4701, IF 2.351) is an international, peer-reviewed, open access journal published monthly online. *Metals* provides a forum for publishing papers which advance the in-depth understanding of the relationship between the structure, the properties or the functions of all kinds of metals.

https://www.mdpi.com/journal/metals

Energies (ISSN 1996-1073) is an open access journal and publishes papers on scientific research, technology development, engineering policy and management studies related to the general field of energy, from technologies of energy supply, conversion, dispatch and final use to the physical and chemical processes behind such technologies.

https://www.mdpi.com/journal/energies

Polymers (ISSN 2073-4360, IF 4.329) provides an interdisciplinary forum for publishing papers which advance the fields of (i) polymerization methods, (ii) theory, simulation, and modeling, (iii) understanding of new physical phenomena, (iv) advances in characterization techniques, and (v) harnessing of self-assembly and biological strategies for producing complex multifunctional structures.

https://www.mdpi.com/journal/polymers

Membranes (ISSN 2077-0375) is an international, peer-reviewed, open access journal. The journal covers broad science- and technology-related aspects of both biological and non-biological membranes. IF 4.106, ranking JCR - Q1 (*Polymer Science*), CiteScore - Q2 (*Chemical Engineering, miscellaneous*)

https://www.mdpi.com/journal/membranes

Sponsor

Mikrouna

Mikrouna took the lead in R&D, production and sales of glove box equipment in China in 2000. It is the third R&D and production company after VAC and MBRAUN in the world, and it is a domestic initiative.

As a high-tech company integrating R&D, production and service, Mikrouna has always been committed to providing high-end technology products and services to customers around the world. Mikrouna has more than 90 engineers and technicians. Among them, there are 2 researchers (professor-level senior engineers), 8 senior engineers, and more than 80 engineers.

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Mikrouna's production equipment is advanced and complete, with 73 patented technologies, 1 national major special research and development project, and 2 high-tech achievement transformations.

https://www.mikrouna.com/index/Start

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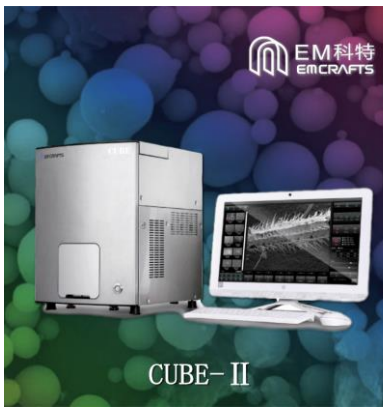

ICM-CN 2021 Organizing Committee

Conference Chair:

Dongfeng Xue

Shenzhen Institutes of Advanced Technology, Chinese Academy of Sciences, China

Research Area: Crystallization Physics and Chemistry of Inorganic Materials; Materials Design and Simulation; Novel Synthesis Strategies of Inorganic Compounds

Session Chair:

Session 1: Electronic Materials

Huixia Luo

Sun Yat-Sen University, China

Research Area: New superconductors, Topological insulators

Guangyu Zhang

Beijing National Laboratory for Condensed Matter Physics & Institute of Physics, Chinese Academy of Sciences, Beijing, China

Research Area: Nanoscience and Nanotechnology

Bilu Liu

Tsinghua-Berkeley Shenzhen Institute (TBSI), Tsinghua University, China

Research Area: electronics of low-dimensional materials with an emphasis on carbon nanotubes, graphene, and two-dimensional semiconductors

Hong Meng

Peking University Shenzhen Graduate School (PKU Shenzhen), China

Research Area: Synthesis of conductive polymer and conductive materials

Gongbin Tang

Shandong University, China

Research Area: Study on high performance piezoelectric thin film acoustic devices

Session 2: Biomaterials and Smart Materials

Weiqiu Chen

Zhejiang University

Research Area: Flexible electronics, Mechanics of soft matter, Tunable phononics

Zhou Li

Beijing Institute of Nanoenergy and Nanosystems, Chinese Academy of Sciences, China

Research Area: Nanoenergy and Nanosystems, Single cell force sensor

Huaiyu Wang

Shenzhen Institutes of Advanced Technology, Chinese Academy of Sciences, China

Research Area: Bone-related Biomaterials, Nanoscale Biomaterials, Surface Modifications

Huacheng Zhang

School of Chemical Engineering and Technology, Xi'an Jiaotong Univeristy, Xi'an China

Research Area: Functional materials for environmental and energy applications

Tianyu Ma

Xi'an Jiaotong Univeristy, Xi'an China

Research Area: Solid state phase transition in magnetic alloys and compounds

Session 3：Energy Materials

Kai Yan

Sun Yat-sen University, China

Research Area: renewable energy, engineering strain, hydrogen, biomass conversion

Feng Liang

Kunming University of Science and Technology, China

Research Area: Electrochemical Energy Storage and Conversion Devices, Solid Electrolyte

Xin Wang

Shenzhen Institutes of Advanced Technology, Chinese Academy of Sciences, China

Research Area: Band gap regulation of two-dimensional layered materials

Session 4：Functional Ceramics, Thin Films and Crystalline Materials

Yanlin Song

Key Laboratory of Green Printing, Institute of Chemistry, CAS, China

Research Area: information function materials, application of polymers photonic crystals

Wei Pan

State Key Laboratory of New Ceramics and Fine Processing, School of Materials Science & Engineering, Tsinghua University, China

Research Area: Advanced ceramics processing, Nanofibers and devices

Kunfeng Chen

Shandong University, China

Research Area: Novel electrochemical energy storage materials and devices

Session 5: Rare Earth Materials and Optics and Photonics

Jianggao Mao

Fujian Institute of Research on the Structure of Matter, Chinese Academy of Sciences, China

Research Area: Syntheses, properties and structures of inorganic solid materials, especially inorganic nonlinear optical crystal materials

Lili Hu

Shanghai Institute of Optics and Fine Mechanics, Chinese Academy of Sciences, China

Research Area: Relationship between composition, structure and properties of laser glass

Yaping Du

Nankai University, China

Research Area: rare-earth functional materials, colloidal inorganic nanocrystals, and energy storage and conversion materials

Yibo Zhang

Changchun Istitute of Applied Chemistry, Chinese Academy of Sciences, China

Research Area: Graphene derivatives, polymer luminescent materials

Session 6: Advanced Nanomaterials and Nanotechnology

Xuming Xie

Department of Chemical Engineering, Tsinghua University, China

Research Area: Modification and assembly of nanomaterials and their nanocomposites

Guangming Chen

College of Materials Science and Engineering, Shenzhen University, Shenzhen, China

Research Area: Organic/inorganic thermoelectric composites

Junqing Hu
Shenzhen Technology University
Research Area: Synthesis and basic application of nano-photothermal/photoelectric materials

Session 7: Structure Materials and Application

Jinshu Wang
Beijing University of Technology, China
Research Area: Refractory metal-based electronic emission materials

Shouke Yan
Beijing University of Chemical Technology, China
Research Area: surface-induced polymer crystallization, orientation-induced polymer crystallization

Dianzhong Li
Institute of Metal Research, Chinese Academy of Sciences, Shenyang, China
Research Area: Key material composition optimization and metallographic control of large castings and forgings

Session 8: Materials Simulation and Design

Chunxu Pan
School of Physics and Technology, Wuhan University, Wuhan, China
Research Area: Materials Physics, Nanomaterials

Chao Peng
Shenzhen Institutes of Advanced Technology, Chinese Academy of Sciences, China
Research Area: First-principles research on surface interface of electrochemical energy storage materials and solid optoelectronic materials

Guilin Zhuang
Zhejiang University of Technology, China
Research Area: Establishment and application of intelligent simulation method for cluster structure-effect relationship (magnetic structure, accelerant)

Jun Liu
South China University of Technology, China

Research Area: High energy density lithium ion batteries, sodium ion batteries, lithium sulfur batteries and other new energy storage materials and devices

Session 9: Multiscale Analysis and Characterization of Materials

Yanfeng Zhang
Peking University, China
Research Area: Material Science, Physical chemistry, Nanoscience and Nanotechnology, Surface Science

Yunlong Li
Shenzhen Institutes of Advanced Technology, Chinese Academy of Sciences, China
Research Area: Optoelectronic materials and devices

Feng Yang
Southern University of Science and Technology
Research Area: chirality controlled growth of carbon nanotubes and mechanism

Zhengyang Zhou
Shanghai Institute of Ceramics, Chinese Academy of Sciences, China
Research Area: Chemical; Materials Science; Inorganic chemical

Session 10: Manufacturing Processes and Systems

Yulin Hao
Institute of Metal Research, Chinese Academy of Sciences, Shenyang, China
Research Area: Properties of polymer composites

Changshun Ruan
Shenzhen Institutes of Advanced Technology, Chinese Academy of Sciences, China
Research Area: 3D-Bioprinting; Biodegradable Polymeric Biomaterials

Jian Yuan
Wuhan University of Technology, China
Research Area: Glasses and special glasses, energy and environmental catalytic materials

Advisory Committee Members:

Qikun Xue	**Huiming Cheng**	**Weihua Wang**
Qingjie Zhang	**Nobuhito Imanaka**	**Sridhar Komarneni**
Xueliang Sun	**Jinzhong Zhang**	**Kexin Chen**

Conference Schedule：

Date	Time	Program	Channel
22 November	8:30-10:00	Open Ceremony Plenary Speech	Main
22-23 November	9:00-18:00	Session Report	Sessions
24 November	9:00-12:00	Poster Award Ceremony	Main

Link：https://www.koushare.com/topicLive/i/icm-cn

code：

Full Schedule

Open Ceremony, Plenary Speech, Poster & Award Ceremony (Main)

22 November	
Open Speech (Video)	
8:30-8:33	Conference Chair: Prof. Dr. Dongfeng Xue
8:33-8:36	MDPI Managing Director China: Mr. Leo Jiang
Plenary Speech	
8:36-9:06	Prof. Jinzhong Zhang Shed Light on Metal Halide Perovskites: Insight into Their Novel Properties and Functionalities
9:06-9:36	Prof. Sridhar Komarnei Designer Micro-meso-macro-porous Materials
9:36-10:06	Prof. Nobuhito Imanaka Rare Earths Oxides, How They Contribute as Environmental Catalysts
10:06-10:15 Break	
24 November	
9:00-12:00: Poster & Award Ceremony	

Session Reports

Session 1：Electronic Materials

Session Chairs： Huixia Luo, Guangyu Zhang, Bilu Liu, Hong Meng, Gongbin Tang

22 November				
10:15-12:05 Host:【Zhu-An Xu, Hao Zheng】				
Time	Type	Report Title	Speaker	Affiliation
10:15-10:45	Keynote	Giant Anomalous Nernst Effect in Kagome Lattice Semimetals	Zhu-An Xu	Zhejiang University
10:45-11:05	Invited	Towards Novel Quantum Materials: Design, Synthesis and Characterizations	Ruidan Zhong	Shanghai Jiaotong University
11:05-11:25	Invited	Discovery of Segmented Fermi Surface Induced by Cooper Pair Momentum	Hao Zheng	Shanghai Jiaotong University
11:25-11:45	Invited	Quantum Oscillations and A Nontrivial Berry Phase of Non-Fermi Surfaces	Liyuan Zhang	Southern University of Science and Technology
11:45-12:05	Invited	Topology, Correlation and Superconductivity in Kagome Metals	Hechang Lei	Renmin University of China
12:05-14:00 Break				
14:00-16:55 Host:【Haizhou Lu, Dong Qian】				
14:00-14:30	Keynote	3D Quantum Hall Effect	Haizhou Lu	Southern University of Science and Technology
14:30-15:00	Keynote	Study on the Coexistence of Ferroelectric-Like Polarization and Dirac-Like Surface State	Dong Qian	Shanghai Jiaotong University
15:00-15:20	Invited	High-Power, Solid-State, Deep Ultraviolet Laser Generation	Hongwen Xuan	Institute of Aerospace Information, Chinese Academy of Sciences
15:20-15:40	Invited	Optoelectronic and Electronic Devices Based on Wide Bandgap Amorphous Ga2O3	Zengxia Mei	Songshan Lake Materials Laboratory

15:40-16:00	Invited	Superconducting and topological properties of ternary transition metal tellurides	Wenhe Jiao	Zhejiang University of Technology
16:00-16:20	Invited	Substrate Guided Controlled Growth of 2D Transition Metal Dichalcogenides	Jingwei Wang	Tsinghua Shenzhen International Graduate School, Tsinghua University
16:20-16:35	Oral	A U-Shaped Dual-Frequency Reconfigurable Monopole Antenna Based on Liquid Metal	Peng Qin	CAS Key Laboratory of Cryogenics

Session 2：Biomaterials and Smart Materials

Session Chairs： Weiqiu Chen, Zhou Li, Huaiyu Wang, Huacheng Zhang, Tianyu Ma

22 November				
10:15-12:05 Host:【Huaiyu Wang】				
Time	Type	Report Title	Speaker	Affiliation
10:15-10:45	Keynote	Translational formulations for precise anti-leukemia therapy	Wei Wei	Institute of Process Engineering, Chinese Academy of Sciences, China
10:45-11:05	Invited	Multifunctional hydrogels for rapid hemostasis and tissue repair	Baolin Guo	Xi'an Jiaotong University
11:05-11:25	Invited	Research on composite tissue engineering scaffolds containing black phosphorus and their functions	Liping Tong	Shenzhen Institute of Advanced Technology, Chinese Academy of Sciences, China
11:25-11:45	Invited	Facile and versatile surface functional polyetheretherketone with enhanced bacteriostasis	Dechun Geng	Suzhou University
11:45-12:05	Invited	Delivery Strategies of Nucleic Acid Molecules for The Treatment of Diverse Diseases	Yuanyu Huang	Beijing Institute of Technology
12:05-14:00 Break				
14:00-16:05 Host:【Guozheng Kang, Jinjin Zhao】				
14:00-14:30	Keynote	Research on Low Cycle Fatigue Performance and Damage Mechanism of Extruded AZ31 Magnesium Alloy	Guozheng Kang	Southwest Jiaotong University
14:30-14:50	Invited	High-throughput Screening and Rational Design of Multi-Biofunctionalized Antimicrobial Implant	Lin Wang	South China University of Technology

14:50-15:10	Invited	Cell Mechanotransduction	Qiang Wei	Sichuan University
15:10-15:30	Invited	Biofilm Elimination by Synergistic Physical-Chemical Multi-Mechanism on Titanium Implant	Xiangyu Zhang	Taiyuan University of Technology
15:30-15:50	Invited	Resolving Organometal Halide Perovskite Structural Symmetry	Jinjin Zhao	Shijiazhuang Tiedao University
15:50-16:05	Oral	Tuning the Surface Immunomodulatory Functions of Polyetheretherketone for Enhanced Osseointegration	Ang Gao	Shenzhen Institute of Advanced Technology, Chinese Academy of Sciences
16:05-16:15 Break				
16:15-18:15 Host:【Junhong Guo, Weijian Zhou】				
16:15-16:45	Keynote	Materials under the tip: Quantitative Imaging of Localized Functionalities at the Nanoscale	Jiangyu Li	Southern University of Science and Technology
16:45-17:05	Invited	Mechanically Control of Piezotronic Effects in Piezoelectric Semiconductor Structures	Chunli Zhang	Zhejiang University
17:05-17:25	Invited	Static deformation and dynamic response of multilayered magnetoelectroelastic nano-plates	Junhong Guo	Inner Mongol University of Technology
17:25-17:45	Invited	Smart Topological Elastic Metamaterials with Tunable Spin Hall Effect	Weijian Zhou	Nanyang Technological University
17:45-18:00	Oral	Construction of Bioactive Micro/Nano Arrays on the Surface of Polyetheretherketone	Shi Mo	Shenzhen Institute of Advanced Technology, Chinese Academy of Sciences

		(PEEK) for Antibacterial Research		
18:00-18:15	Oral	Dual Bioactive Peptides Functionalized Visible Light Curable Hydrogel Accelerates Bone Regeneration	Ning Yuan	Peking University
23 November				
9:00-10:30 Host:【Zhou Li】				
9:00-9:30	Keynote	Transscale mechanics of soft matter "condensed matter"	Haibao Lv	Harbin Institute of Technology
9:30-9:50	Invited	Research on activities with recreational regeneration and repair functions	Zhilu Yang	Dongguan Hospital affiliated to Southern Medical University
9:50-10:10	Invited	Electroactive Biomaterials and Systems and Biomedical Applications	Linlin Li	Beijing Institute of Nanoenergy and Systems
10:10-10:30	Invited	Sensitive magnetoelasticity from nanoprecipitates-bearing ferromagnet	Tianyu Ma	Xi'an Jiaotong University
10:30-10:40 Break				
10:40-12:10 Host:【Tianyu Ma】				
10:40-11:10	Keynote	Contact mechanics of functionally graded piezoelectric materials	Liaoliang Ke	Tianjin University
11:10-11:30	Invited	Learning from Superelasticity Data to Search for Ti-Ni Alloys with Large Elastocaloric Effect	Dezhen Xue	Xi'an Jiaotong University
11:30-11:50	Invited	Design and properties of novel intelligent glass based on one-dimensional magnetic nanomaterials	Yin Zhang	Xi'an Jiaotong University
11:50-12:10	Invited	Anisotropy engineering of metallic magnetic composites for	Chen Wu	Zhejiang University

		electromagnetic energy conversion		

Session 3：Energy Materials

Session Chairs： Kai Yan, Feng Liang, Xin Wang

22 November				
10:15-11:55 Host:【Kai Yan】				
Time	Type	Report Title	Speaker	Affiliation
10:15-10:45	Keynote	Preliminary Study on the Photoelectric Catalytic Performance of Several Types of Two-dimensional Micro/Nano Structures	Dongpeng Yan	Beijing Normal University
10:45-11:15	Keynote	Structural evolution of copper-based electrocatalysts for carbon dioxide reduction	Zhe Weng	Tianjin University
11:15-11:35	Invited	The Atomic Arrangement Regulations of Electrocatalysts	An-Liang Wang	Shandong University
11:35-11:55	Invited	Construction of Stable Surface Interface of High-Voltage Nickel-Rich Ternary Cathode Material	Ding Wang	Kunming University of Science and Technology
11:55-14:00 Break				
14:00-15:40 Host:【Feng Liang】				
14:00-14:30	Keynote	Photocatalytic Conversion of Biomass to Hydrogen and Low Carbon Molecules	Feng Wang	Dalian Institute of Chemical Physics, Chinese Academy of Sciences
14:30-15:00	Keynote	Study on the Mechanism of Cu-based CO2 Electrocatalytic Reduction Reaction	Zhijian Zhao	Tianjin University
15:00-15:20	Invited	In situ Fabrication of Gel Electrolyte and Its Utilization in Metal-Air Batteries	Xizheng Liu	Tianjin University of Technology
15:20-15:40	Invited	Defect chemical engineering improves oxygen precipitation performance of hydrotalcite structure	Yao Kang	Kunming University of Science and Technology

15:40-15:50 Break				
15:50-17:05 Host:【Xin Wang】				
15:50-16:05	Oral	Electrocatalytic reductive amination and simultaneous oxidation of 5-hydroxymethylfurfural on nanomaterials	Man Zhang	Sun Yat-sen University
16:05-16:20	Oral	Design and preparation of polymeric carbon nitride-based photocatalysts for CO2 reduction	Keyan Li	Dalian University of Technology
16:20-16:35	Oral	Study on the application of pyrolysis carbon black in supercapacitor	Shengping Hou	Kunming University of Science and Technology
16:35-16:50	Oral	Insight into the Stabilized OER Performance on Highly Active Manganese Nickel Oxide	Fengling Zhou	Dongguan University of Technology
16:50-17:05	Oral	An efficient and non-precious anode electrocatalyst of NiO-modified carbon nanofibers towards electrochemical urea oxidation in alkaline media	Ibrahim M. A. Mohamed	Sohag University

Session 4：Functional Ceramics, Thin Films and Crystalline Materials

Session Chairs： Yanlin Song, Wei Pan, Kunfeng Chen

22 November				
10:15-12:05 Host:【Kunfeng Chen, Jun Jiang】				
Time	Type	Report Title	Speaker	Affiliation
10:15-10:45	Keynote	Green Printed Photonic Crystals and Devices	Yanlin Song	Key Laboratory of Green Printing, Institute of Chemistry, CAS
10:45-11:15	Keynote	Scandium-Based Nano Luminescent Materials	Ling Huang	Xinjiang University
11:05-11:25	Invited	Single-Crystal Lithium Niobate Thin Films	Hui Hu	Shandong University
11:25-11:45	Invited	Metal nitrides from structural design to sensor applications	Minghui Yang	Ningbo Institute of Materials, Chinese Academy of Sciences
11:45-12:05	Invited	Using X-ray Absorption Fine Structure Spectroscopy to Study Supported Small-Size Catalysts	Rui Si	Sun Yat-Sen University
12:05-14:00 Break				
14:00-16:10 Host:【Wei Pan, Jiehua Liu】				
14:00-14:30	Keynote	-	Guangshe Li	Jilin University
14:30-14:50	Invited	GGAG Scintillation Ceramic and CT Detector	Jun Jiang	Ningbo Institute of Materials, Chinese Academy of Sciences
14:50-15:10	Invited	Piezoelectric Single Crystals for High Temperature Sensing: Recent Development	Fapeng Yu	Shandong University
15:10-15:30	Invited	Luminescence Dynamics of Inorganic Perovskite CsPbX3 Nanoparticles and Thin Films	Bingqiang Cao	Jinan University
15:30-15:40	Corporate Report	Mikrouna Promotion Video	Mikrouna	
15:40-16:10 Break				

16:10-17:35 Host:【Guangshe Li, Fapeng Yu】				
16:10-16:40	Keynote	Design and Performance of High Temperature and Low Thermal Conductivity Ceramic Coating Materials for Gas Turbines	Wei Pan	Tsinghua University
16:40-17:00	Invited	Study on the Controllable Structure of Perovskite Single Crystal and Its Optical and Electrical Properties	Jiehua Liu	Hefei University of Technology
17:00-17:20	Invited	Growth and Characterization of Novel Mid-IR Laser Crystals	Peixiong Zhang	Ji'nan University
17:20-17:35	Oral	Research on the component design, fabrication and performance control of terbium oxide magneto-optical transparent ceramics	Yue Wu	Dalian University of Technology
23 November				
9:00-10:20 Host:【Fangfang Zhang, Mengye Wang】				
9:00-9:20	Invited	Active Manipulation of Metamaterials and Plasmonics with Thin-film IGZO Schottky Diodes	Yifei Zhang	Shandong University
9:20-9:40	Invited	Semiconductor Device Based on Gallium Nitride Single Crystal Substrate	Xinke Liu	Shenzhen University
9:40-10:00	Invited	High-performanced piezoelectric energy harvester based on PIN-PMN-PT crystals	Xiangyu Gao	Xi'an Jiaotong University
10:00-10:20	Invited	Silver Cluster Chemistry	Di Sun	Shandong University
10:20-10:30 Break				
10:30-11:50 Host:【Di Sun, Xinke Liu】				
10:30-10:50	Invited	Study on the Stability of Semiconductor Photocatalyst	Mengye Wang	Sun Yat-Sen University
10:50-11:10	Invited	Study on Growth of Aluminum Nitride Crystal by PVT Method	Lei Zhang	Shandong University

11:10-11:30	Invited	Design and Synthesis of Deep-Ultraviolet Optoelectronic Crystals Based on Borates	Fangfang Zhang	Xinjiang Technical Institute of Physics and Chemistry, CAS
11:30-11:45	Oral	Research on the component design, fabrication and performance control of terbium oxide magneto-optical transparent	Ding Zhou	Shanghai Institute of Technology
11:45-12:00	Oral	Effect of hexamethylenetetramine on enhanced corrosion resistance of AZ31B magnesium alloys by micro-arc oxidation	Xi Miao	Jiangxi Science and Technology Normal University
12:00-14:00 Break				
14:00-16:00 Host:【Jiaming Zhu, Kunfeng Chen】				
14:00-14:20	Invited	Minimally Invasive Brain Intervention Technology and Device Based on Microhole Craniotomy	Zhe Li	Sun Yat-Sen University
14:20-14:40	Invited	Novel Structural Topotactic Transformation Synthetic Strategy for Lanthnide-based Micro/Nanocrystals with Multicolor Emissions	Baiqi Shao	Wenzhou Research Institute, University of Chinese Academy of Sciences
16:00-16:20	Invited	Exploration and Properties of Topological Materials with ZrSiS-Type Structure	Gang Wang	Institute of Physics, Chinese Academy of Sciences
15:00-15:15	Oral	Fabrication of Monodispersed core-shell Co3O4@C and Co@C nanocomposites with enhanced electromagnetic performance	Jiahang Qiu	Northeastern University
15:15-15:20 Break				
15:20-16:30 Host:【Gang Wang, Zhe Li】				
15:20-15:40	Invited	Multi-Scale Crystal Growth and Performance Research	Kunfeng Chen	Shandong University

15:40-16:00	Invited	High-Performance Design of Shape Memory Alloy Based on "Concentration Gradient Engineering"	Jiaming Zhu	Shandong University
16:00-16:15	Oral	Self-aligned suture growth of centimeter-level quasi-single crystal hexagonal boron nitride monolayer on liquid copper	Huixin Chen	Zhengzhou University
16:15-16:30	Oral	Graphene-like wide-gap two-dimensional semiconductors and graphene surface functionalization	Guoqiang Shi	
16::30-16:35	Oral	Pulsed Laser Deposited Bi-Phasic Calcium Phosphate Implant Coatings Fabricated from Fish Bones	Gianina Popescu-Pelin	National Institute for Lasers, Plasma and Radiation Physics, Romania

Session 5：Rare Earth Materials and Optics and Photonics

Session Chairs： Jianggao Mao, Lili Hu, Yaping Du, Yibo Zhang

22 November				
10:15-12:05 Host:【Yaping Du】				
Time	Type	Report Title	Speaker	Affiliation
10:15-10:45	Keynote	Ultrathin metallic gap-enabled extreme nanophotonics	Pan Wang	Zhejiang University
10:45-11:05	Invited	Luminescent Nanocrystal-Doped Glass and Fiber	Guoping Dong	South China University of Technology
11:05-11:25	Invited	Development and Fabrication of Multispectral Chalcogenide Glasses	Changgui Lin	Ningbo University
11:25-11:45	Invited	Development of glass film highly doped with rare earth ions and its application in optical fiber preparation	Chunlei Yu	Shanghai Institute of Optics and Fine Mechanics, Chinese Academy of Sciences
11:45-12:05	Invited	Upconversion emission properties and applications of RE3+:YnOn-1Fn+2 nanocrystals embedded glass-ceramics	Chao Liu	State Key Laboratory of Silicate Materials for Architectures, Wuhan University of Technology
12:05-14:00 Break				
14:00-15:50 Host:【Yaping Du】				
14:00-14:30	Keynote	Theory-guided design and synthesis of emerging luminescent materials	Hongtao Sun	National Institute for Material Science (NIMS), Japan
14:30-14:50	Invited	Rare earth doped upconversion luminescent oxyfluoride glass ceramics: microstructure study using advanced solid-state NMR spectroscopy	Jinjun Ren	Shanghai Institute of Optics and Fine Mechanics, Chinese Academy of Sciences
14:50-15:10	Invited	Luminescence control and detection device application	Gongxun Bai	China Jiliang University

		of rare earth doped optoelectronic materials		
15:10-15:30	Invited	Confined Electrocatalysis of Nanoporous Materials	Cuiling Li	School of Chemistry and Chemical Engineering, Beijing Institute of Technology
15:30-15:50	Invited	Thermal-induced Ion Migration in Solids: An optical Perspective with Rare-Earth Luminescence	Shi Ye	South China University of Technology
15:50-16:00 Break				
16:00-17:50 Host:【Yibo Zhang】				
16:00-16:30	Keynote	Rare Earth Long Afterglow Luminescent Materials	Weisheng Liu	Colleague of Chemistry and Chemical Engineering, Lanzhou University
16:30-16:50	Invited	CeO2-Based Low Temperature Denitration Catalyst	Changjin Tang	School of Environment, Nanjing Normal University
16:50-17:10	Invited	Study on the Controlled Synthesis and Electrocatalytic Properties of Copper-Based Nanomaterials	Zhenxing Li	College of New Energy and Materials, China University of Petroleum (Beijing)
17:10-17:30	Invited	Controlled Synthesis of CeO2-Based Catalytic Materials and Catalytic Purification Performance of VOCs	Wangcheng Zhan	School of Chemistry and Molecular Engineering, East China University of Science and Technology
17:30-17:50	Invited	Study on Hydrogen Production from Water Gas Shift with Monoatomic Pt Metal Catalysts	Jian Lin	Dalian Institute of Chemical Physics, Chinese Academy of Sciences
23 November				
9:00-11:05 Host:【Junjiang Zhan】				

9:00-9:30	Keynote	Multi-Material Optical Fiber and Device	Shifeng Zhou	State Key Laboratory of Luminescent Materials and Devices, South China University of Techonology
9:30-9:50	Invited	Status of Rare earth industry in China and its application in medical field	Yongqing Wen	Baotou Rare Earth Research Institute
9:50-10:10	Invited	Construction of High Performance Rare Earth Perovskite Oxide Catalyst and Its Catalytic Performance	Junjiang Zhu	School of Chemistry and Chemical Engineering, Wuhan Textile University
10:10-10:30	Invited	The Design of New Biosensors and Applications	Ren Cai	Hunan University
10:30-10:50	Invited	Design and Biological Application of Photofunctional Nanocomposites	Chunxia Li	Shandong University
10:50-11:05	Oral	Rare Earth Doped Solid Materials for Optical Quantum Technologies	Shuping Liu	Southern University of Science and Technology

Session 6: Advanced Nanomaterials and Nanotechnology

Session Chairs： Xuming Xie, Guangming Chen, Junqing Hu

22 November				
10:15-12:05 Host:【Jin Zhu】				
Time	Type	Report Title	Speaker	Affiliation
9:30-9:55	Keynote	Organic/Inorganic Thermoelectric Nanocomposites and Flexible Devices	Guangming Chen	Shenzhen University
9:55-10:15	Invited	Investigation on the Stability of Liquid-Like Thermoelectric Materials and Modules	Pengfei Qiu	Shanghai Institute of Ceramics, Chinese Academy of Sciences
10:15-10:35	Invited	Structure and Properties of Biodegradable Polymer Based Multicomponent Materials	Zhaobin Qiu	Beijing University of Chemical Technology
10:35-10:55	Invited	Hybrid Organic/Inorganic Chalcogenides Based Conductive Materials: Synthesis, Characterizations and Performances	Wei Xu	Institute of Chemistry, Chinese Academy of Sciences
10:55-11:05 Break				
11:05-12:10 Host:【Guangming Chen】				
11:05-11:30	Keynote	Observations and Hypotheses: A Journey in Expanding the Structural, Functional, and Mechanistic Scope of Synthesis	Jin Zhu	Nanjing University
11:30-11:50	Invited	Molecular Engineering and Application Exploration of Antiadhesion Coating Surfaces and Interfaces	Xu Wu	Guangzhou University
11:50-12:10	Invited	Interfacial Architecting with Anion Treatment for Enhanced Thermoelectric	Zhuoxin Liu	Shenzhen University

		Power of Flexible Ternary Polymer Nanocomposites		
12:10-14:00 Break				
14:00-15:25 Host:【Zhongren Chen】				
14:00-14:25	Keynote	Super Tough and Intelligent Multi-bond Network (MBN) Physical Hydrogels Facilitated by MXene Nanosheets	Xuming Xie	Tsinghua University
14:25-14:45	Invited	Rapid and Sensitive Aging Evaluation of Polyolefin Nanocomposites and Correlation to Natural Aging	Rui Yang	Tsinghua University
14:45-15:05	Invited	PSS/Xuan Paper Composites for Thermoelectric Applications	Liang Deng	Shenzhen University
15:05-15:25	Invited	Ionic Liquid-Modulated PEDOT:PSS-based Thermoelectric Composites	Yichuan Zhang	Shenzhen University
15:25-15:35 Break				
15:35-17:30 Host:【Xuming Xie】				
15:35-16:00	Keynote	Nano-sized Polymer Supports Immobilizing Mono(phenoxy-imine) Metal Complexes for Ethylene Polymerization	Zhongren Chen	Southern University of Science and Technology
16:00-16:20	Invited	Biological and Artificial Nanoionics: Lons Transport Based Energy and Sensory Systems	Kai Xiao	Southern University of Science and Technology
16:20-16:40	Invited	Construction of High-Performance Electromagnetic Shielding Materials Based on Nano-Carbon Fillers and Silicone Rubber	Yehai Yan	Qingdao University of Science and Technology

16:40-17:00	Invited	Ultralong Carbon Nanotubes: Controlled Synthesis and Applications	Rufan Zhang	Tsinghua University
17:00-17:15	Oral	Ultrafast, High-Resolution and Large-Size Three-Dimensional Structure Manufacturing Through High-Efficiency Two-Photon Polymerization	Shanggeng Li	University of Science and Technology of China
17:15-17:30	Oral	Antimicrobial Biodegradable Polymeric Implants	Anita Ioana Visan	National Institute for Lasers, Plasma and Radiation Physics, Romania
23 November				
9:00-10:25 Host:【Jun Fu】				
9:00-9:25	Keynote	Development of New Sulfur Compounds and Exploration of Their Application in Cancer Diagnosis and Treatment	Junqing Hu	Shenzhen Technology University
9:25-9:45	Invited	Conducting Polymer/Carbon Nanotube Thermoelectric Composites	Cunyue Guo	University of Chinese Academy of Sciences
9:45-10:05	Invited	Modification of the self-assembly morphology of nanoparticle and polymer composites	Minna Sun	Beijing Information Science and Technology University
10:05-10:25	Invited	Combined Defect, Interface and Structure Engineering in Nanofibrous Catalysts for High-Efficiency Electroreduction of N2	Yitao Liu	Donghua University
10:25-10:35 Break				
10:35-12:30 Host:【Junqing Hu】				

10:35-11:00	Keynote	High Performance Conductive Nanocomposite Hydrogels for Monitoring Organ Motions	Jun Fu	Sun Yat-Sen University
11:00-11:20	Invited	Organic Thin Film Thermoelectric Material and Device	Weishu Liu	Southern University of Science and Technology
11:20-11:40	Invited	Intrinsic Nanostructure Induced Ultralow Thermal Conductivity in Eu2ZnSb2 Zintl Phase Thermoelectric Materials	Qian Zhang	Harbin Institute of Technology, Shenzhen
11:40-12:00	Oral	Graphene / Gold Nanoparticles Electrochemical Enzyme Biosensor	Jianfang Wang	National University of Defense Technology
12:00-12:15	Oral	Highly Flexible and Stretchable Quasi-Solid-State Thermoelectrochemical Cells for Self-Powered Strain Sensors	Lirong Liang	University of Macau
12:15-12:30	Oral	N Doped Fluorescent Carbon Dots for Sensing,Bioimaging and Light-Emitting Diodes	Yawen Zhou	Research Center of Laser Fusion, China Academy of Engineering Physics

Session 7: Structure Materials and Application

Session Chairs： Jinshu Wang, Shouke Yan, Dianzhong Li

23 November				
14:00-16:00 Host:【Yunbo Zhong, Yunzhu Ma】				
Time	Type	Report Title	Speaker	Affiliation
14:00-14:30	Keynote	High Static Magnetic Metallurgy and Processing of Metallic Alloys	Yunbo Zhang	Shanghai University
14:30-14:50	Invited	Atomic Scale Study of Compositional and Structural Evolution of Early-Stage Grain Boundary Precipitation in Al-Cu Alloys Through Phase-Field Crystal	Yunzhu Ma	Central South University
14:50-15:10	Invited	Mechanism and microstructure regulation of deformation induced ferrite transformation in 3Mn medium manganese steel	Chengwu Zheng	Institute of Metal Research Chinese Academy of Sciences
15:10-15:30	Invited	Process and application of ultrasonic composite brazing/diffusion welding of non-ferrous metals	Qian Wang	Jiangxi Rare Earth Research Institute
15:30-15:45	Oral	Superlubricity of Fullerene Derivatives Induced by Host-guest Assembly	Shanchao Tan	Tsinghua University
15:45-16:00	Oral	Metal-Organic Frameworks (MOFs) for Superlubricity	Lei Liu	Tsinghua University

16:00-16:15	Oral	Numerical Study on UnequalLlateral Impact Behavior of CFRP Reinforced Concrete Square Members	KHALIL AL-BUKHAITI	Southwest Jiaotong University

Session 8: Materials Simulation and Design

Session Chairs： Chunxu Pan, Chao Peng, Guilin Zhuang, Jun Liu

22 November				
10:15-11:55 Host:【Jun Liu, Chao Peng】				
Time	Type	Report Title	Speaker	Affiliation
10:15-10:35	Invited	Next Generation Batteries System: Low Cost and In-situ Recycling	Yuxiang Hu	Beijing University of Technology
10:35-10:55	Invited	Interface regulation of high voltage lithium metal battery based on fluorinated electrolyte	Long Chen	East China University Of Science and Technology
10:55-11:15	Invited	A Multiscale-Simulation and Data-Driven Study of Lithium Battery Electrolytes	Xiang Chen	Tsinghua University
11:15-11:35	Invited	Finding Li-ion Solid-State Electrolytes with First-Principles Calculations	Bingkai Zhang	Guangdong University of Technology
11:35-11:55	Invited	Interface Regulation for High-Performance Sodium Metal Batteries	Chao Wu	Shanghai University
11:55-14:00 Break				
14:00-15:40 Host:【Yuxiang Hu, Guilin Zhuang】				
14:00-14:20	Invited	Calculation and design of electrochemical energy storage materials	Siqi Shi	Shanghai University
14:20-14:40	Invited	Computational electrochemistry and structural design of electrochemical energy storage materials	Jianjun Liu	Shanghai Institute of Ceramics, CAS

14:40-15:00	Invited	Theoretical Studies of Photocatalysis with Metal–Organic Frameworks	Xinping Wu	East China University Of Science and Technology
15:00-15:20	Invited	Design Pinciples and High-Throughput Screening of Supports Boosting the Stability of Metal Nanocatalysts	Sulei Hu	University of Science and Technology of China
15:20-15:40	Invited	Theoretical Design and Simulation of Acidic Water Electrolysis Catalyst	Ziqi Tian	Ningbo Institute of Materials, CAS
15:40-15:50 Break				
15:50-17:40 Host:【Chunxu Pan, Siqi Shi】				
15:50-16:20	Keynote	On the Application of Time-Temperature Equivalent Formulation for the Description of Thermorheologically Complex Material Behaviour	Linan Qiao	Germany
16:20-16:40	Invited	Decarbonising Data Science to Reveal the Dependency between Material Formulation and Battery Property	Kailong Liu	University of Warwick
16:40-17:00	Invited	Recent Progress on the Modelling of Creep Cavitation and Rupture, and Creep Damage Constitutive Equations	Qiang Xu	University of Huddersfield
17:00-17:20	Invited	Phase Field Simulations Accelerated Heterogeneous Microstructure Design and Mechanical Properties Optimization in Titanium Alloys	Dong Wang	Xi'an Jiaotong University

17:20-17:40	Invited	Quantitative Insights into the Reaction Mechanism for the Direct Synthesis of H2O2 over Transition Metals: Coverage-Dependent Microkinetic Modeling	Zihao Yao	Zhejiang University of Technology
23 November				
9:00-10:20 Host:【Xinping Wu, Sulei Hu】				
9:00-9:20	Invited	A Rational Design for the Separation of Metallic and Semiconducting Single-Walled Carbon Nanotubes Using a Magnetic Field	Chunxu Pan	Wuhan University
9:20-9:40	Invited	Simulations of Plasmonic Nanoparticles and Molecular Response	Xing Chen	Tianjin University
9:40-10:00	Invited	Point Defect-Induced Dielectric Response Mechanism of RECOB Crystals	Yanlu Li	Shandong University
10:00-10:20	Invited	Theoretical Study on Degradation Mechanism of Hybrid Perovskite	Xiao Wang	Shenzhen Institute of Advanced Technology, CAS
10:20-10:30 Break				
10:30-12:20 Host:【Yanlu Li, Xiao Wang】				
10:30-10:50	Invited	Theoretical path of discovering novel stackings of MXenes	Weiwei Sun	Southeast University
10:50-11:10	Invited	DFT Guided Catalyst Design for Photocatalytic HER	Dong Wang	East China University Of Science and Technology
11:10-11:30	Invited	Recycling of Solid Wastes(Low-Grade Diatomite, Steel Slag) for Water-Cleaning	Junshu Wu	Beijing University of Technology

11:30-11:45	Oral	Understanding the effect of water molecule on Electrocatalytic Hydrogen Peroxide Synthesis	Yongyong Cao	Jiaxing University
11:45-12:00	Oral	Extended Electric Double Layer Model and the Surface Charge of Alkali Halides	Feng Liu	Shenzhen Institutes of Advanced Technology, CAS

Session 9: Multiscale Analysis and Characterization of Materials

Session Chairs：Yanfeng Zhang, Yunlong Li, Feng Yang, Zhengyang Zhou

22 November				
9:00-10:30 Host:【 Pinxian Xi, Feng Yang】				
Time	Type	Report Title	Speaker	Affiliation
09:00- 9:30	Keynote	Structure Analysis of Porous Materials by 3D Electron Diffraction	Junliang Sun	Peking University
9:30-9:50	Invited	Crystal Grwoth and Characterization of Several NLO and Laser Crystals	Kunpeng Wang	Zaozhuang University
9:50-10:10	Invited	Line-Rotated Remapping for High-Resolution Electron Backscatter Diffraction	Yongzhe Wang	Shanghai Institute of Ceramics, CAS
10:10-10:30	Invited	Probing the Optoelectronic Properties of Semiconductors via Time-Resolved Microwave Conductivity (TRMC)	Qianqian Lin	Wuhan University
10:30-10:40 Break				
10:40-12:00 Host:【Junliang Sun, Yongzhe Wang】				
10:40-11:00	Invited	Synthesis and Application of Chalcogenide Nanostructures	Pinxian Xi	Lanzhou University
11:00-11:20	Invited	Synthesis of Active Bimetal Oxide by Calcination Followed by Alkaline Activation and Its Application for Chloride Adsorption from Simulated Concrete Pore Solution	Ji-Hua Zhu	Shenzhen University
11：20-11:40	Invited	In-Situ Environmental TEM for Probing the Dynamic of Catalysts at High Temperature	Feng Yang	China University of Petroleum
11：40-12:00	Invited	Crystal Phase-Controlled Synthesis of Noble Metal Nanocrystals for Electrocatalytic Applications	Qipeng Wu	University of Science and Technology Beijing
12:00-14:00 Break				
14:00-15:50 Host:【Changjian Li, Xiaohui Wu】				
14:00-14:30	Keynote	Studies on the Smart Luminescent Materials Based on Rare Earth Complexes	Yu Tang	Lanzhou University

14:30 - 14:50	Invited	I Ligand Engineering of Nanocrystal Assembly Advanced by In Situ Liquid-Cell TEM	Yu Wang	South China University of Technology
14:50-15:10	Invited	In-situ Study of Structure-Activity Relationship of Molybdenum Carbide-Based Methanol Hydrogen Production Catalyst	Lili Lin	Zhejiang University of Technology
15:10 - 15:30	Invited	Probing and Modulating the Interactions of the Dnazyme with DNA-Functionalized Nanoparticles	Tongbo Wu	Huazhong University of Science and Technology
15:30-15:50	Invited	Study of the Synthesis Mechanism of Heterogeneous Catalytic Materials at the Atomic Level by In-situ Characterization	Siyu Yao	Zhejiang University
15:50-16:00 Break				
16:00-17:00 Host:【Yu Tang, Lili Lin】				
16:00-16:20	Invited	Multiple Length Scale Investigations on Multifunctional Oxides for Electronic Device Applications	Changjian Li	Southern University of Science and Technology
16:20-16:40	Invited	The Origin of the Forbidden Reflection in Black Phosphorus	Jian Mao	McGill University
16:40-17:00	Invited	Boosting Lithium-ion Storage of Misfit-Layered Sulfide by Pre-lithiation as Free-standing Anode	Xiaohui Wu	Fujian Normal University
23 November				
9:00-10:30 Host:【Jun Ming, Xiaodong Hao】				
9:00- 9:30	Keynote	Green Printing Technology for Manufacturing Functional Devices	Yanlin Song	Key Laboratory of Green Printing, Institute of Chemistry, CAS
9:30- 9:50	Invited	Organic Cation Intercalation in Reduced-Dimensional Perovskites: The Influences on the Crystal Orientation and the Bandedge Integrity	Zhenyu Yang	Sun Yat-Sen University

9:50- 10:10	Invited	Mechanism and Control of Negative Thermal Expansion in Metal-Based Magnetic Materials	Yuzhu Song	University of Science and Technology Beijing
10:10- 10:30	Invited	Defect Structures and Ionic Transporting Mechanisms in Two New Families of Oxide Ion Conductors: Melilite La1+xCa1-xAl3O7-0.5x and Ruddlesden-Popper Perovskite La2-x(Ca/Sr/Ba)xBaIn2O7-0.5x	Jungu Xu	Guilin University of Technology
10:30- 10:40 Break				
10:40-12:00 Host:【Yanlin Song, Yuzhu Song】				
10:40- 11:00	Invited	Electrolyte and Interfacial Model	Jun Ming	Changchun Istitute of Applied Chemistry, CAS
11:00-11:20	Invited	Host-Guest Complexation for Efficient Formamidinium-Based Perovskite Solar Cells	Hong Zhang	Ecole Polytechnique Federale de Lausanne, Switzerland
11:20-11:40	Invited	Atomic Insights Into the Growth and Self-Assembly of Ultrafine Cerium Oxides Nanocatalysts	Xiaodong Hao	Shaanxi University of Science and Technology
11:40-12:00	Invited	Experimental Determination of Magnetic Anisotropy in Lanthanide Metallocene Single-Molecule Magnet	Yinshan Meng	Dalian University of Technology
12:00-14:00 Break				
14:00-16:10 Host:【Yanfeng Zhang, Zhengyang Zhou】				
14:00-14 :30	Keynote	Application of Synchrotron X-Ray Spectroscopy in Characterization of Energy Materials From Monatomic to Cluster	Zheng Jiang	Shanghai Advanced Research Institute, CAS
14:30-14:50	Invited	Interfacial van der Waals Engineering and Atomic-Scale Characterization of Low Dimensional Materials	Shaochun Li	Nanjing University
14:50 - 15:10	Invited	Highly Stable and Efficient Copper-Based Perovskite Scintillators	Yuntao Wu	Shanghai Institute of Ceramics, CAS

15:10 - 15:30	Invited	Diffraction Grating and Its Application in Spectral Measurement	Xiaotian Li	Changchun Institute of Optics, Fine Mechanics and Physics, CAS
15:30 - 15:50	Invited	The Borate Optical Crystals with Anomalous Thermal/Mechanical Properties	Xingxing Jiang	Technical Institute of Physics and Chemistry, CAS
15:50-16:10	Invited	Realization of Quasi-1D Materials via Chemical Strategy	Shu Guo	Southern University of Science and Technology
16:10-16:15 Break				
16:15-18:00 Host:【Zheng Jiang, Yunlong Li】				
16:15-16:30	Oral	Synthesis, Crystal Growth and Morphologies of the Co-Doping NH4VO3	Qilin Cui	Zaozhuang University
16:30-16:45	Oral	Thermoelectric Properties of Nano-grained Mooihoekite Cu9Fe9S16	Xianxiu Qiu	University of Chinese Academy of Sciences
16:45-17:00	Oral	Crystal Growth, Morphologies, Optical and Thermal Properties of Co-Doping Sulfamic Acid	Hongbin Chen	Zaozhuang University
17:00-17:15	Oral	Progress of Nonlinear Optical Materials with NH2SO3H Structure	Xuejiao Wang	Zaozhuang University
17:15-17:30	Oral	Single Crystal Growth and Characterization of the Nickel Doped Thiourea CH4N2S	Longyu Cao	Zaozhuang University
17:30-17:45	Oral	A Novel Antiferroelectric Dipoles Configuration	Botao Gao	University of Science and Technology Beijing
17:45-18:00	Oral	Partial Lattice Ions Substituted by Aluminum Ions in Sepiolite	Huiwen Chen	Shenzhen Institute of Advanced Technology, CAS

Session 10: Manufacturing Processes and Systems

Session Chairs： Yulin Hao, Changshun Ruan, Jian Yuan

22 November				
10:15-11:45 Host:【Yulin Hao, Limin Ma】				
Time	Type	Report Title	Speaker	Affiliation
10:15-10:45	Keynote	Processing Optimization, Mechanical Properties, Corrosion Behavior and Cytocompatibility of Additively Manufactured Zn-0.7Li Biodegradable	Peng Wen	Tsinghua University
10:45-11:05	Invited	Intelligent Polymers and Shape-Adaptable Bioelectronics	Xuemin Du	Shenzhen Institute of Advanced Technology, CAS
11:05-11:25	Invited	Design and Additive Manufacturing of High Performance Porous Ceramics	Zhangwei Chen	Shenzhen University
11:25-11:45	Invited	Construction of 3D Printed Hydrogel and Its Application in Tissue Regeneration	Xiaodong Cao	South China University of Technology
12:05-14：00 Break				
14:00-15:50 Host:【Changshun Ruan, Guocheng Wang】				
14:00-14:30	Keynote	Research and Evaluation of Laser Additive Manufacturing Ti3Zr2Sn3Mo25Nb Medical Titanium Alloy	Sen Yu	Northwest Institute for Non-ferrous Metal Research
14:30-14:50	Invited	Digital Organ Manufacturing Technology System and Its Application Progress	Xiongfei Zheng	Shenyang Institute of Automation Chinese Academy of Sciences
14:50-15:10	Invited	Functionalized Biofabrication Technologies for Tissue Regeneration	Yang Wu	Harbin Institute of Technology, Shenzhen
15:10-15:30	Invited	Bone Material Design based on Bioactive Ceramics/Glasses	Guocheng Wang	Shenzhen Institute of Advanced Technology, Chinese

				Academy of Sciences
15:30-15:50	Invited	3D Printed Scaffolds with Tubular Structures for Tissue Engineering Application	Yongxiang Luo	Shenzhen University
15:50-16:00 Break				
16:00-17:30 Host:【Yuxiao Lai, Dechun Ren】				
16:00-16:30	Keynote	Borosilicate Regulates the Mechanism of Soft and Hard Tissue Regeneration	Haobo Pan	Shenzhen Institute of Advanced Technology, Chinese Academy of Sciences
16:30-16:50	Invited	Study on the Forming and Properties of Ti-Ni Based Alloy with Porous Structure Additive Manufacturing	Dechun Ren	Institute of Metals, Chinese Academy of Sciences
16:50-17:10	Invited	Porous Ta Implant Fabricated by EB-PBF	Jian Wang	Northwest Insititute For Non-Ferrous Metal Research
17:10-17:30	Invited	3D printing of bone repair materials	Yuxiao Lai	Shenzhen Institute of Advanced Technology, CAS
23 November				
9:00-10:30 Host:【Jian Yuan, Bin Han】				
9:00-9:30	Keynote	High-Precision Glass Manufacturing	Shibin Jiang	Zhejiang University; Nankai University; Shanghai Institute of Optics and Fine Mechanics, Chinese Academy of Sciences
9:30-9:50	Invited	Study on Preparation Technology of Large Size Optical Quartz Glass	Zaikui Xiang	Quartz and Special Glass Research Institute, China General Research

				Institute of Building Materials science
9:50-10:10	Invited	Oxide High-Entropy Glass with Ultra-High Hardness and Modulus	Jianqiang Li	Institute of Process, Chinese Academy of Sciences; University of Science and Technology Beijing
10:10-10:30	Invited	From R&D to Mass Production - VON ARDENNE's PVD Solutions for Emerging Technologies	Bin Han	VON ARDENNE GmbH
10:30-10:50	Invited	Development and Manufacture of High Strength Glass Ceramics for Mobile Terminal	Jian Yuan	Wuhan University of Technology
10:50-11:00 Break				
11:00-12:20 Host:【Xi Yang, Ji Liu】				
11:00-11:20	Invited	3d Bioprinting and Application in Regenerative Medicine	Xi Yang	Novaprint, Suzhou
11:20-11:40	Invited	Design and Fabrication of Soft Materials with Unprecedented Mechanics	Ji Liu	Southern University of Science and Technology
11:40-12:00	Invited	Microstructure and Mechanical Properties of Beta-Type Ti-24Nb-4Zr-8Sn Cellular Structures Fabricated by Electron Beam Melting	Shujun Li	Institute of Metal Research, Chinese Academy of Sciences
12:00-12:20	Invited	Study on the Mechanism of Porous Titanium Alloy/GelMA Bionic Composite Scaffold for Repair of Large Segmental Bone Defects	Limin Ma	Guangdong Provincial People's Hospital

Abstract Book

Session 1: Electronic Materials

Rational Electrode-Electrolyte Design for Long-Life Rechargeable Aqueous Zinc-Ion Batteries

Wen Liu

Guangxi University

Abstract: Due to its high theoretical energy density, better safety and availability as well as lower prices, the rechargeable aqueous zinc ion battery is considered as one of the most promising systems for the next generation of energy storage devices. However, due to the strong electrostatic interaction between Zn^{2+} and host and the proton/Zn^{2+} co-intercalation in aqueous media, the development of zinc ion battery with high capacity and long lifetime remains an uphill task. In this work, a novel electrode-electrolyte design has been employed by using a Zn/ZIF heterostructure as a microporous host matrix and an organic zinc trifluoromethanesulfonate as the constituent of the electrolyte. A zinc ion battery based on the Zn/ZIF heterostructure anode delivers a specific capacity of 149 mAh g^{-1} and remains the retention as high as 80% after 330 cycles at 1 A g^{-1}. The synergistic effect of microstructural ZIF and hydrophobic trifluoromethanesulfonate anions creates a unique electrode-electrolyte interface, which suppresses the formation of Zn dendrites and self-discharge of Zn anode, resulting in a long cycling stability of the aqueous zinc ion batteries.

A Degradable NFC Label Antenna Based on Gallium-Based Liquid Metal and PVA Substrate

Li Chunwei, Qin Peng, Deng Zhong-Shan

Technical Institute of Physics and Chemistry CAS

Abstract: Near-field communication (NFC) technology is developing towards portable, flexible, wearable, and even recyclable. In this study, a degradable NFC label antenna was designed and fabricated, using gallium-based liquid metal (GBLM) and water-soluble polyvinyl alcohol (PVA) substrate. The GBLM was printed as the NFC induction coil on the PVA substrate. The good conductivity and flexibility of GBLM make the label antenna have sensitive response characteristics and a certain degree of deformability and stretchability. The label antenna can keep the inductance change and resonance offset small in the process of proper deformation and stretching. The PVA substrate dissolved in water gives the NFC label the advantage of recycling. The GBLM can realize the self-healing of the induction coil under a magnetic field control. It is also more affordable than the silver pulp that current widely used and conducts wireless communication at 13.56 MHz. Thus, this degradable recycling NFC label antenna based on GBLM can fit to the surface of commodity packaging and human skin, applied in environmental protection, information exchange, personal health testing, wearable biosensing and other fields.

A U-Shaped Dual-Frequency Reconfigurable Monopole Antenna Based on Liquid Metal

Peng Qin, Zhong-Shan Deng

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Abstract: This study presents a U-shaped dual-frequency reconfigurable monopole antenna based on liquid metal. EGaIn was used as a conductive fluid and was filled in the two branches of the U-shaped glass tube. A precision syringe pump was connected to one of the branches of the U-shaped tube by a silicone tube to drive EGaIn to form a height difference between the two liquid levels. The results indicated that the two branches respectively obtained two different working bandwidths of 2.39–4.98 GHz and 3.42–8.39 GHz, if the liquid-column heights of liquid metals met the initial condition of L1 = L2 = 10 mm while L1 increased from 10 mm to 18 mm. The maximum peak gain was 4.00 dBi. The initial amount of EGaIn also affected the available operating bandwidth. When L1 was adjusted within the range of 12–20 mm with the initial condition of L1 = L2 = 12 mm, the two corresponding working bandwidths were respectively 2.18–4.32 GHz and 3.13–9.09 GHz, and the measured maximum peak gain was 3.72 dBi. The simulation results corresponded well with the measurement data. A series of dual-frequency reconfigurable antennas can be obtained by changing the initial amount of EGaIn. The merits showed in the above antennas could allow for application in the fields of base stations or navigation. This article shows that liquid metal as an electronic material has good application prospects in radio frequency fields such as antennas.

Calculation of the Superconducting Transition Temperature of Elements with the Roeser-Huber Formalism

Michael Rudolf Koblischka, Anjela Koblischka-Veneva

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Abstract: The superconducting transition temperature, T_c, is calculated for practically all superconducting elements using the Roeser-Huber formalism. Superconductivity is treated as a resonance effect between the charge carrier wave, i.e., the Cooper pairs, and a characteristic distance, x, in the crystal structure. To calculate T_c, only these distances, where for complicated crystal structures several ones are possible, and informations on the electronic configuration are required. Here, we lay out the required principles to find this characteristic length x, which requires to build sums of several possible paths for more complicated crystal structures. In this way, we establish a non-trivial relation between superconductivity and the respective crystal structure. The model enables a detailed study of elements showing superconductivity in different types of crystal structures, like e.g., lanthanum (La) which superconducts at T_c = 4.8 K when it is double hexagonal closed packed (dhcp-structure) as compared to T_c = 6 K when being face-centered cubic (fcc-structure). Similar cases are observed for superconducting Hg as well as for Ga. Using the Roeser-Huber approach, the structure-dependent different Tc's of these materials can nicely be reproduced, demonstrating the usefulness of this approach offering an easy and relatively simple calculation procedure, which can be straightforwardly incorporated in machine-learning approaches.

Fabrication of A Silicone-Based Double-Network Ionogel with High Mechanical Strength

Jingxian Sun

China Tobacco Shandong Industrial Co. Ltd

Abstract: To date, ionogels have aroused the extensive interest, as they are ideal materials for the preparation of many electronics. However, the poor mechanical properties of some ionogels greatly limit their applications in flexible electronics. In this work, a double-network ionogel (DN ionogel) with high mechanical strength was successfully synthesized. The brittle first network was fabricated by a non-hydrolytic sol-gel route: tetramethoxysilane (TMOS) was induced by formic acid (FA) to react to form a silicone network in ionic liquid 1-butyl-3-methylimidazolium hexafluorophosphate ([BMIM]PF_6). Then, hydroxyethyl acrylate (HEA) and methyl methacrylate (MMA) were photopolymerized with the addition of a crosslinker poly (ethylene glycol) diacrylate (PEGDA) to form the soft second network. In addition to the energy dissipation effect of the double-network, the hydrogen bonds among hydroxyl groups or between hydroxyl groups and Si–O–Si bonds also greatly improves the mechanical strength of the ionogel. The obtained ionogel also possessed high conductivity, good transparency and extreme temperature tolerance. Therefore, it is believed that this high-performance DN ionogel offers a promising prospect in flexible electronics.

Making High Thermal Conductivity BN-Epoxy Composite Material by Urea Melting Pore Preparation Method

Shanzhi Wei

Abstract: With the increasing demand of miniaturization and high power of electronic equipment, heat dissipation has become a key problem to be solved. It is still a challenge to maintain the advantages of polymer electrical insulation and good mechanical properties and further improve the thermal conductivity. In this paper, BN was selected as the thermal conductive filler and epoxy resin as the polymer matrix. The three-dimensional BN skeleton with smooth surface, low interfacial thermal resistance and good mechanical and thermal conductivity was prepared by urea melting pore preparation method (MPPM). Further, BN / epoxy resin composites with high thermal conductivity were obtained by filling epoxy resin into BN skeleton with vacuum assistance. When the volume ratio of BN is 80%, The thermal conductivity can reach 13.65 $W \cdot M^{-1} \cdot K^{-1}$, which is 68 times as compared with that of a pure epoxy matrix. Its thermal conductivity is higher than that of BN skeleton based epoxy composites reported previously. The traditional thermal conductive skeleton is bonded by polymer materials with low thermal conductivity .In this work the strength of the skeleton comes from the bonding of urea with high thermal conductivity，which bonded BN tightly and effectively reduced the interfacial thermal resistance. This strategy provides a new idea for the design and manufacture of three-dimensional networks in polymer matrix.

Optoelectronic and Electronic Devices Based on Wide Bandgap Amorphous Ga_2O_3

Zengxia Mei [1,2]

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[2] Songshan Lake Materials Laboratory

Abstract: As building blocks, scalable, cost-effective, and lightweight optoelectronic and electronic devices become increasingly important for IoT platforms. Amorphous Ga_2O_3 (a-Ga_2O_3), a new emerging oxide semiconductor, owns decent merits of wide bandgap (~4.9 eV), high absorption coefficient ($>10^5$ cm^{-1}), moderate permittivity (~12), perfect anti-radiation performance, and low growth temperature etc. These versatile features enable a-Ga_2O_3 possibly applied in advanced devices. It is widely accepted that oxygen vacancy (V_O) defects play a key role in oxide semiconductor device performance, such as the long persistent photoconductivity (PPC) phenomenon in PDs and gate bias stress instability in TFTs. In present work, a fine-oxygen-flux controlling approach was adopted during the room-temperature sputtering process of a-Ga_2O_3 films and flexibly utilized in different device architectures, according to the specific requirements on V_O concentrations and material's optical and electric properties. We will give some application examples to illustrate the success of the technique in fabricating high-performance solar-blind UV photodetector (PD), X-ray detector, thin-film transistor (TFT), and optoelectronic synapse etc. All the work suggests the appealing prospects of cost-effective a-Ga_2O_3 thin films in the development of scalable optoelectronics.

Stress/Strain Analysis by Electron Backscatter Diffraction (EBSD) in Superconducting Materials

Anjela Koblischka-Veneva, Michael Rudolf Koblischka

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Abstract: We have recently applied the electron backscatter diffraction (EBSD) technique to determine residual strains/stresses in bulk $YBa_2Cu_3O_7$ (YBCO) and MgB_2 superconducting materials. The stresses/strains are very important to the performance of the superconductors as they determine (a) possible cracking due to magnetostriction effects when applying strong magnetic fields (e.g., for charging up a bulk sample to be used as superconducting trapped field magnet), (b) possible additional flux pinning due to the interaction of the vortices with the stress/strain field and (c) even the superconducting transition temperature of the samples may be influenced. Thus, it is very important to have a high spatially resolved analysis method fur this purposes, as e.g., nanoparticles embedded within the superconducting matrix may introduce such stresses/strains due to the misfitting of the unit cell parameters. In the present contribution, we apply the analysis of the kernel average orientation (KAM) mappings to various superconducting materials and discuss the effects of the detected stress/strain distributions on the resulting flux pinning properties.

This work is part of the SUPERFOAM international project funded by ANR and DFG under the references ANR-17-CE05-0030 and DFG-ANR Ko2323-10, which is gratefully acknowledged.

Study on the Stability and Electronic Properties of 2D Layered Phosphorus

Shenghuang Lin

Songshan Lake Materials Laboratory

Abstract: Two-dimensional (2D) layered phosphorus (including black phosphorus and violet phosphorus, with excellent physical and chemical properties, has shown great potential for next generation electronics and optoelectronics. However, 2D materials always show different thermal properties when compared to its bulk counterpart. Therefore, it is necessary to understand the thermal process of 2D layered P to reveal its natural physical properties. Herein, an atomic-scale microscopic and spectroscopic study is performed to characterize the thermal degradation of solution-exfoliated layered P. The in situ decomposition temperature of the BP and VP is observed to be greater than 300 °C and 340 °C respectively. Moreover, the thickness of the BP flakes can be moderately controlled through thermal thinning process. The obtained highest carrier mobility of BP through thermal annealing can be up to ~358 $cm^2 V^{-1} S^{-1}$. Our study provides an insight into the thermal stability of 2D layered P in vacuum and opens an avenue in fabricating large-area ultra-thin layered P films.

Towards Novel Quantum Materials: Design, Synthesis and Characterizations

Ruidan Zhong

Abstract: Quantum materials are materials where the extraordinary effects of quantum mechanics give rise to exotic and often incredible properties. To understand their basic behavior if we are to enable optimization for a specific purpose, discovering novel quantum materials is a primary task for scientists in the field of condensed matter physics and materials science. In this talk, research strategies toward novel quantum materials in experiment will be introduced from the perspective of chemistry, materials science and physics. Such research process leads to fruitful results, and two recent discovered candidates of quantum spin liquid (QSL) will be briefly presented as an example. The first candidate is a geometric frustrated magnet, $Na_2BaCo(PO_4)_2$, which is structurally perfect without intrinsic disorder. Experimental results, including magnetization, specific heat, and neutron scattering, have indicated that this compound is an ideal QSL candidate. The second compound, $BaCo_2(AsO_4)_2$, are believed to be a Kitaev QSL candidate. This is the first time that Kitaev physics are proposed to be realized in 3*d*-transition-metal honeycomb in experiment. Non-Kitaev interactions can be fully suppressed by low field, yielding nonmagnetic ground state and many other similarities with the well-studied Kitaev QSL α-$RuCl_3$.

Substrate Guided Controlled Growth of 2D Transition Metal Dichalcogenides

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Abstract: Two-dimensional (2D) transition metal dichalcogenides (TMDCs) have attracted great research interest due to their potential applications in electronics, optoelectronics, catalysis, *etc*. To satisfy these expectations, controlled growth of 2D TMDCs with designed structure and properties is highly desired. During vapor phase synthesis, the substrate plays a crucial role as it not only provides the growth platform but also affects the nucleation and surface diffusion, eliciting epitaxial products with various structures, morphologies, and defect types. In this report, the merit of substrate pretreatments will be demonstrated for tailoring the morphology of monolayer MoS_2 from compact polygon to fractal dendrite, which is derived from different nucleation modes. Besides, the facile modulation of band structure, orientation, and dimension of epitaxial monolayer WS_2 will be presented via exploiting the unique physicochemical properties of the *m*-plane quartz substrate. Finally, the potential approaches of manipulating proper substrate to preparing 2D TMDCs with desired structure and properties will be proposed.

Keywords: Two-dimensional materials, chemical vapor deposition, substrate, strain engineering

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Bio: Jingwei Wang is currently a Post-doc in Prof. Bilu Liu's group at Tsinghua-Berkeley Shenzhen Institute (TBSI), Tsinghua University, China. He received his bachelor's degree in Materials Science and Engineering from the Jinan University (JNU), Guangzhou, China in 2012, Master degree in Crystalline Materials in 2015 from Albert Ludwig University of Freiburg (UFR), Germany, and Ph.D. degree in Nano Science and Technology from the Hong Kong University of Science and Technology (HKUST) in 2020. He was a research assistant and joint training student at the Southern University of Science and Technology (SUSTech) from 2015 to 2020. His research interests include the growth mechanism of two-dimensional materials and their potential applications in electronics, optoelectronics, and catalysis. He has published more than 40 papers in peer-reviewed journals such as *ACS Nano, Nano Lett., Adv. Funct. Mater.*

Session 2: Biomaterials and Smart Materials

Materials under the Tip: Quantitative Imaging of Localized Functionalities at the Nanoscale

Jiangyu Li

Southern University of Science and Technology

Abstract: In the last two decades, nanostructured materials have revolutionized information technology, energy systems, and medicines. With the advances in microscopy and analytical tools, we can now image compositions, phases, and structures with atomic and sub-atomic resolution. The length scales upon which physical properties can be quantitatively measured, however, largely lag behind, making it difficult to directly connect compositions, structures and properties of nanostructured materials and systems. In this talk, I will briefly review our efforts using scanning probe microscopy to address this challenge in the past a few years, with particular emphasis on mechanistic understanding regarding competing microscopic mechanisms and data analytic approaches with machine learning and artificial intelligence. Cases studies on polar order in organic-inorganic solar cells, and flexoelectricity in two-dimensional heterostructures, and heat conduction in nanostructured thermoelectrics will be given, and future challenges and opportunities will be highlighted.

Jiangyu Li recently joins Southern University of Science and Technology, and serves as the Chair in the Department of Materials and Science and Engineering. Prior that, he was a Research Scientist at Shenzhen Institutes of Advanced Technology, Chinese Academy of Sciences, and a Professor in the Department of Mechanical Engineering, University of Washington. Li works in the general field of mechanics and physics of materials, focusing on advanced scanning probe microscopy and its applications in functional materials. He has published over 200 journal articles, and has been recognized by Sia Nemat-Nasser Medal from ASEM, Young Investigator Award from ICCES, and Microscopy Today Innovation Award from Microscopy Society of America. He currently serves as Associate Editor for Journal of Applied Physics and Science Bulletin, and serves on the Editorial Board of npj Computational Materials and Theoretical and Applied Mechanics Letters.

Preparation and Formation Mechanism of Ga-Containing Coatings Developed on Ti-6Al-4V Alloys by Micro-Arc Oxidation

Sheng Zhong, Rongfa Zhang, Rongfang Zhao, Jin Qin

Jiangxi Science and Technology Normal University

Abstract: Medical titanium (Ti) alloys do not possess antibacterial ability, which restricts their clinical applications. In this study, gallium (Ga) element, known to be effective against both bacteria and cancer, was doped into anodic coatings on Ti-6Al-4V alloys by micro-arc oxidation (MAO) technology. In a solution composed of 5 g/L Na_3PO_4, the influences of $Ga(NO_3)_3$ concentration, Na_2SiO_3 concentration, Na_2SO_4 concentration and treatment time on coating properties were studied by using an orthogonal experiment. In addition, the roles of each electrolyte on coating formation were clarified by using signal factor experiments. The results show that MAO coatings containing 3.13 to 13.50 wt.% Ga were successfully fabricated. The raised $Ga(NO_3)_3$ concentration and current density continually increase the Ga content, showing that the Ga element enters into MAO coatings by both diffusion and electromigration. For Ti alloys, $Ga(NO_3)_3$ is a strong corrosive agent, while Na_2SO_4, Na_2SiO_3 and Na_3PO_4 act as film-forming agents. The Si content is negatively related to the P content resulted from the competition between Na_2SiO_3 and Na_3PO_4 to take part in the coating formation, while the P content is positively related to the Ga content attributed to the main existence form of Ga element in MAO coatings as Ga_2O_3 and $GaPO_4$.

Sorption of Heavy Metal ions by Composite Cryogels Based on Bentonite Clay with Ionic and Nonionic Polymer

Gulfairuz Zhumabaevna Kairalapova, Rizvangul Sinyasulkyzy Iminova, Perizat Baimyrza

Al-Farabi Kazakh National University

Abstract: One of the most important problems of today is the protection of water resources from depletion and pollution, including industrial wastewater treatment. Thus it is essential to synthesize more affordable sorbents for toxic metals removal with increased physico-chemical, sorption-desorption and mechanical properties. In this regard, our research work aimed at the development of new composite materials based on polymers and domestic clay minerals from East Kazakhstan for use as sorbents of heavy metal ions from wastewater. Composite cryosorbent based on bentonite clay (BC) and ionic polymer–polyacrylamide (PAA), nonionic polyacrylamide (PAAm) was synthesized and characterized physico-chemical properties, sorption capacity in relation to cadmium and lead metals using the individual and model aqueous solution with the two metal ions mixture. The synthesis of PAA, PAAm cryogel was carried out by radical polymerization methods at −20°C for 8 hours. The composite polymer/clay cryogel was obtained with the ratio 1:1, 1:5 and 1:10. The structure and morphology of composite cryogels were investigated using FTIR, SEM and AFM. The BC content was determined and found that the clay consists of mineral montmorillonite with high dispersion. The SEM and AFM images show the high porosity of polymer/clay composite cryogels compare to pure cryogels. PAA/BC sorption capacity for [Pb^{2+}] was 97% and for [Cd^{2+}] was 98%, and as for PAAm/BC for [Pb^{2+}] was 88% and for [Cd^{2+}] was 89%. Overall, the sorption capacity of PAA/BC was higher than PAAm/BC composite cryogels. During the evaluation of sorption capacity of cryogels using the model solution, the value of both PAA/BC and PAAm/BC composites for [Cd^{2+}] (97% and 93%, respectively) was higher than that of [Pb^{2+}] (90% and 85%, respectively). This is predicted by their differences in coordination number, atomic mass, and radius. Thus, our cryogel might be beneficial for wastewater treatment and further can be set as a heavy metal filter.

An Aptamer Based Fiber Optic Sensor for Rapid Peanut Allergen Detection

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Abstract: In the last decade, food allergies have become an important food safety issue and health concern worldwide. One of the most life-threatening food sensitivities is the peanut allergy, because it triggers the highest frequency of severe and fatal reactions. Ara h 1 is considered one of the major peanut allergens. This trimeric protein is also resistant to heat and food processing, therefore it is widely accepted as the most common biomarker of the peanut presence in food. Because there is no medical prophylactic treatment so far, the European food labelling legislation should become stricter, as accurate product information is essential for allergic persons. Consequently, the food market is facing an urgent need for sensitive biosensors that can rapidly detect very low quantities of allergens in complex food matrices, to be easily employed within food quality and safety sector. Herein, we use an in-house developed point-of-care diagnostic tool based on fiber optic – surface plasmon resonance (FO-SPR) technology for rapid and sensitive detection of Ara h 1 allergen. An aptamer-based bioassay against the major peanut allergen Ara h 1 was design and implemented on the FO-SPR sensor. This research outcome will open the door to automated, on-site and throughput allergen detection, aiming at providing the end-consumer safer food.

This work was financially supported by the Executive Agency for Higher Education, Research, Development and Innovation (UEFISCDI) funding, Project PD 195/2020 (PN-III-P1-1.1-PD-2019-0466).

Anisotropy Engineering of Metallic Magnetic Composites for Electromagnetic Energy Conversion

Chen Wu, Chenhui Zhou, Guang Liu, Mi Yan

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Abstract: Metallic magnetic materials with simultaneous dielectric and magnetic loss are technologically important for electromagnetic wave absorption. Their applications however, are restrained by the Snoek Limit, poor impedance match and large density. Here we took three strategies including hetero-nucleation, confined and templated growth, to tune the surface and planar anisotropy for enhanced magnetic loss. Meanwhile, dielectric components have been introduced with designed microstructures for optimized impedance and density. For the hetero-nucleation, MoS_2 nanoflowers with numerous nucleation sites allow dispersive growth of FeCo nanoparticles close to single domain size for enhanced natural resonance over a wide frequency range. For confined growth, porous FeCo/ZnO nanosheets are resulted for further increased bandwidth and decreased density. For templated growth, hierarchical MOFs constructed with 2D nanoflakes have been synthesized, which derive into Co/C composites with maintained architectures. The anisotropy of such assemblies has been evaluated based on shape, flatness and angle in-between the constituent nanoflakes, and correlations between the assembled anisotropy with the magnetic loss have been established.

Co-Assembled Supramolecular Structures of A Pair of Enantiomeric Peptides

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[2] University of Chinese Academy of Sciences, Beijing, China
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Abstract: As a universal phenomenon in biological systems, chirality of biomolecules especially peptides and proteins played an important role in the biometabolic processes and biological activities. The structural difference between self-assembly and co-assembly of enantiomeric peptides was helpful in material research and biological application. However, there is still a lack of the co-assembly behaviors of chiral peptides with different proportions, which may adjust the properties of the corresponding materials. Here, two chiral pentapeptides, ^{L}E-^{L}C-^{L}A-^{L}F-^{L}F (ECF-5) and ^{D}E-^{D}C-^{D}A-^{D}F-^{D}F (ecf-5) composed of entirely either L- or D-amino acids, were designed and obtained to study the supramolecular structural characteristics co-assembled at different ratios. Results showed that smooth and continuous fibers were observed under non-equal co-assembly conditions (1:9, 1:3, 1:2, 2:1, 3:1and 9:1), while discontinuous fibers were formed under proportional co-assembly conditions. Both circular dichroism and Fourier transform infrared spectra indicated that the secondary structures changed when the ratio between L- and D-peptides ranged from 1:2 to 1:1 and 2:1. MTT study showed that structures formed by co-assembly and self-assembly were biocompatible. All the results shed light on the co-assembly of chiral peptides into supramolecular structures and broadened application fields.

Co-Delivery of PTH and VEGF Mimetic Peptide by Covalent Immobilization within Blue Light-Curable Hydrogel Synergisticly Accelerates Bone Regeneration

Ning Yuan [1], Suwei Dong [2]

[1] State Key Laboratory of Natural and Biomimetic Drugs, and Department of Chemical Biology at School of Pharmaceutical Sciences, Peking University
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Abstract: Bone regeneration is one of the most challenging tasks in the tissue engineering area. In recent years, biomaterials carrying growth factors such as bone morphogenetic proteins (BMPs) and vascular endothelial growth factor (VEGF) have arose a lot of research interests for their high biocompatibility, biodegradability and excellent angiogenic and osteogenic effects. However, the utilization of protein growth factors has been greatly hindered by the difficulties of expression preparation and high costs. Compared to proteins, bioactive peptides are ideal alternatives for their low cost by large-amount chemical synthesis as well as comparable activity to proteins. What's more, by chemical synthesis it's more easy for the incorporation of unnatural modifications into peptides, which could significantly improve the affinity to biomaterial scaffolds and tune their releasing properties. Parathyroid hormone (PTH) is a single chain polypeptide hormone released by parathyroid gland, which has been approved by FDA to treat osteoporosis. Its N-terminal peptide PTH1-34, also called Teriparatide, has also been developed into drug for the activation of the receptor PTHR1 is mainly mediated by PTH's N-terminal α-helix. Nevertheless, the half-life of Teriparatide is very short and small doses of intermittent administration are used in clinical leading to poor compliance. Besides, high dose systematic administration of Teriparatide might lead to many side effects such as osteosarcoma and hypercalcemia. As a result, the application of Teriparatide for the treatment of local bone defects has not been achieved up to now. In this work, based on a blue light curable gelatin hydrogel system we developed a versatile platform for the covalent delivery of peptides for bone regeneration. We chemically synthesized modified PTH1-34 peptide with higher stability and installed a handle for covalent linkage to the scaffold, which could be *in situ* interpreted into the hydrogel by a photo-induced pre-immobilization method we developed. What's more, angiogenesis has thought to be the key challenge in bone regeneration process. To improve the angiogenic effect of our hydrogel system, we explored the combinational use of Teriparatide and a VEGF mimetic peptide, which has not been reported to our knowledge. Next, we thoroughly characterized our hydrogel system by swelling, compression, in vitro degradation, rheological tests and SEM analysis. In vitro experiments proved that the combinational use of Teriparatide and VEGF mimetic peptide could significantly increase the angiogenic and osteogenic abilities of cells. What's more, in vivo mice cranial bone defects regeneration tests showed our hydrogels loaded with individual Teriparatide or VEGF mimetic peptide promoted more than 60% defect regeneration. The combinational application of two peptides had the best result promoting closely to 80% defect regeneration.

Construction of Bioactive Micro/Nano Arrays on the Surface of Polyetheretherketone (PEEK) for Antibacterial Research

Shi Mo, Liping Tong, Huaiyu Wang

Center for Human Tissues and Organs Degeneration, Shenzhen Institute of Advanced Technology, Chinese Academy of Sciences, Shenzhen, China

Abstract: Bacterial infection may lead to implant failure of orthopedics after surgeries, such as polyetheretherketone (PEEK), which is biocompatible but with poor antibacterial and bioactive properties. Nanostructural construction on the surface of implants is proved to be a promising way to solve these problems. However, many aspects may affect the biological properties of nanostructures including the geometrical parameters. Herein, the pillar-like and cone-like mirco/nano-arrays were constructed on the surface of PEEK using colloidal lithography to analyze the effect of the geometrical parameters. The size of polystyrene spheres and the type of plasma were applied to adjust the shape and the dimension of arrays. The nanoarrays with sharp tips penetrated and killed *E. coli* cells like cicada wings. However, the microarrays utilized the hybrid micro-submicron structure and the increased surface energy to stretch, distort, and, killed the bacteria, demonstrating a different antibacterial mechanism. Taken the improved bioactivity for osteoblast proliferation together, the findings may shed light on the design of surface engineered biomaterials.

Effect of the Constant Anodizing Potential on the Surface Morphology of AZ31B Magnesium Alloys

Muhammad Zain Azeem, Muhammad Umar Manzoor, Muhammad Kamran, Faraz Hussain, Hamza Hasnain

Institute of Metallurgy and Materials Engineering, University of The Punjab, Lahore, Pakistan

Abstract: Recently, magnesium alloys have attracted the attention of researchers in the field of biomedical application because of their close density near to the human bone, non-toxic nature, excellent biocompatibility, and biodegradation properties. Furthermore, a major disadvantage of magnesium alloys as biomaterials is their high rate of corrosion in the physiological environment. To overcome this problem various surface modification techniques are used. Among them, the most widely used technique is the anodizing treatment which is based on electrolytic oxidation. In this process, metal is converted to its oxide form and deposited onto the surface of the metallic substrate. However, numerous studies are available in the literature concerning the effect of electrolyte composition and electrical parameters on anodizing, but little work has been done over anodization time to a constant potential. In this study, the effect of constant anodizing potential on the ground AZ31B substrate was investigated for understanding the surface morphology at different anodizing times. The anodizing treatment was performed at the potential of 20 V for the time interval of 30 and 40 minutes in two different electrolyte solutions. The surface chemistry and morphology of the anodized sample were observed by using energy dispersive spectroscopy (EDS) and scanning electron microscopy (SEM).

Entrance Mechanism of Calcium and Magnesium into Anodic Coatings on Ti-6Al-4V Alloys in Solutions with Calcium and Magnesium Gluconates

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Abstract: Due to its excellent biocompatibility, good mechanical properties and reasonable price, Ti-6Al-4V is widely used in biomaterials. However, as bioinert materials, titanium alloys cannot chemically bond with bone tissue. Calcium (Ca) and magnesium (Mg) are the main elements comprising human bone. It is desirable to fabricate Ca-containing and Mg-containing coatings on titanium alloys by micro-arc oxidation (MAO). Because the waste solution after MAO treatment may cause pollution to the environment, it is very important to simultaneously consider coating property and environmental amity of MAO electrolytes. As organic calcium and magnesium salts, calcium and magnesium gluconates not only are nontoxic and soluble in water solution, but also can ionize gluconic acid, which is an important nutritive component for animals. However, calcium and magnesium gluconates have been rarely used as Ca- or Mg-containing MAO electrolytes. In this study, calcium gluconate ($Ca(C_6H_{11}O_7)_2$), magnesium gluconate ($Mg(C_6H_{11}O_7)_2$), calcium glycerophosphate ($C_3H_7CaO_6P$) and phytic acid were selected as the electrolyte, and Mg-Ca coatings were obtained by MAO treatment. The influences of sodium glycerophosphate and calcium glycerophosphate concentrations on coating surface characteristics were investigated by SEM, EDS, XRD and XPS. The results show that at the same processing condition, the Ca amount in MAO coatings is higher than the Mg amount. $C_3H_7CaO_6P$ can improve both Ca and Mg amounts in MAO coatings, indicating that electromigration plays an important role for Ca and Mg ions into anodic coatings.

Gram-Selective Antibacterial Peptide Hydrogel

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Abstract: Microbial resistance to antibiotics posed a growing threat to global medical health. The balance of microorganisms in the human body would be disrupted by broad-spectrum antibiotics, and eventually caused the production of resistant bacteria. Specific targeting antimicrobial peptides (STAMP) were urgently needed, bacterial cell membranes were destroyed by STAMP, bacterial drug resistance was reduced, and the stability of the microbiota would not be destroyed. Here, the antibacterial activity, Gram selectivity and biocompatibility of the amphiphilic antimicrobial peptides were optimized by us and further made them form hydrogels. Five AMPs (IK1, IK2, IK3, IK4 and IK5) were designed and synthesized by us. Among them, IK1, IK3 and IK4 can self-assemble into hydrogels in PBS. IK1 and IK4 were antimicrobial peptide gels targeted at Gram-positive bacteria and Gram-negative bacteria, respectively, while IK3 was a broad-spectrum antibacterial gel. At present, no targeted antibacterial hydrogel has been reported. In addition, cell viability assays showed that the three peptides have very good biocompatibility. Wound healing experiments in a mouse bacterial infection model are underway. Compared with other peptide hydrogels, these new peptide hydrogel materials have enhanced antibacterial activity and have Gram selectivity. It may have great potential in wound healing and tissue engineering.

Liquid Metal-Enabled Hydrogel for Light-Responsive Actuation

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Abstract: The development of smart soft materials, which feature shape-morphing abilities towards specific stimuli, is playing a crucial role in the endeavor of soft robots. The light-responsive strategy is an attractive option, for it can promise untethered actuation with ease of manipulation and light sources. As for preparation, incorporating photoactive molecular into blank materials is a popular way, which will depend on specific couples of raw materials. Current studies about liquid metal (LM) to serve soft robots are mostly based on characteristics in macroscale, while LM nanoparticles (LMNPs) with NIR photothermal sensitivity can offer some other possible routes. In this research, we applied LMNPs in dual crosslinked polymer of Poly(N-isopropylacrylamide) (PNIPAm) and Poly(Acrylamide) (PAm) hydrogel, to build a new type of composite (PNA/LM) for light-responsive actuation. The embedded LMNPs can catalyze racial initiators to enable a rapid in situ polymerization, and its oxide layer can provide anchoring for monomers to ensure stability of composites. Its photothermal response can efficiently transfer heat to thermal-sensitive PNIPAm to trigger volume changes. Based on this PNA/LM composite, we further exhibited the design of light-driven actuators, which showed flexible responsiveness and good deformation. A positive trial toward the wish of exploiting LM's robotic potentials is represented.

Mechanically Control of Piezotronic Effects in Piezoelectric Semiconductor Fibers

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Abstract: Piezoelectric semiconductors (PSs) simultaneously exhibit piezoelectricity and semiconductor properties, and have an important application in smart and functional devices. Under the mechanical force, the induced piezoelectric potential due to piezoelectricity in piezoelectric semiconductors can effectively tune the semiconductor properties in piezoelectric semiconductors. This is named as piezotronic effects by Prof. Z.L. Wang. The physical mechanism of piezotronics is that the piezoelectric potential, induced by the external force due to piezoelectricity, shifts band structures of the semiconductors and affects transport behaviors of holes and electrons. This makes PS structures a promising building block in novel semiconductor devices. Compared to the traditional semiconductor devices, piezoelectric semiconductor devices can be controlled by the mechanical force rather than the bias voltage. This is an extremely advantage to not need the extra electrodes. From the view of device's application, it is important to investigate the electromechanical behavior or performance of PS devices under the applied force. For example, how does the applied force change transport properties and distribution of carriers and built-in electric field in a PS PN junction? Hence, we aim to develop theoretical model and study the electro-mechanical and semiconducting behaviors of PS structures using the developed model. The basic behaviors of piezoelectric semiconductors can be described by the conventional phenomenological theory consisting of the equations of linear piezoelectricity and the equations of the conservations of charge of electrons and holes. We employ the linearization method for the mathematical simplification with the assumption of small carrier concentration perturbations from the reference state. Under the linearization assumption, we present one-dimensional model for PS fibers with extensional and flexural deformations. The tuning effects of the applied force on the electromechanical fields and distributions of carriers are studied for different PS fibers. The obtained results are helpful for better understanding the piezotronic effect and developing piezotronic devices with high performance.

Multifunctional Hydrogels for Rapid Hemostasis and Tissue Repair

Baolin Guo

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Abstract: Uncontrolled bleeding results in more than 30% of traumatic deaths. Although currently used hemostatic agents exhibit excellent performance in hemostasis of limb surface wounds, they generally have a poor hemostatic effect on deep un-compressible wound bleeding. We prepared chitosan derivatives and carbon nanotube materials based injectable shape memory nanocomposite porous hemostatic materials. Chitosan derivatives can provide good hemostatic properties, promote wound healing and blood-triggered shape memory recovery. Due to the rapid blood absorption, blood concentration and rapid blood-triggered shape recovery of the composite gel, as a physical filling barrier with sufficient mechanical properties, it exhibits excellent performance in rabbit liver volume loss, incompressible hemorrhage death model and lethal non-compressible swine subclavian artery and vein transection model. After the bleeding stops, the severe skin defect is a serious threat to people's health and life. At present, most of the injectable hydrogel dressings have a single biological activity, which limits their multiple promoting effects on wound healing. We have reported an injectable hydrogel dressing that has multi-functionality, including conductivity, anti-oxidation, self-healing and high adhesion. The in-situ gelation and tissue adhesion properties of the hydrogel can quickly seal any shape of the wound to provide a physical barrier, while the hemostatic and antibacterial properties of the gel can allow the wound to stop bleeding quickly and prevent wound infection. The conductivity and anti-oxidation of the hydrogel can significantly promote the wound healing process. Thus, the hydrogel has great potential as a multi-functional dressing in wound healing applications.

Resolving Organometal Halide Perovskite Structural Symmetry

Jinjin Zhao

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Abstract: The photoelectric conversion efficiency (PCE) of metal halide perovskites (MHPs) based solar cells have reached to 25.5% during the past decade. Photovoltaic properties of MHPs based devices have been extensively investigated in terms of their microstructure, environmental characteristics, carrier dynamics etc. The room temperature tetragonal $MAPbI_3$ has two space group: polar I4cm and non-polar I4/mcm. Significant amounts of efforts have been devoted to proven the I4cm MHPs are ferroelectric and I4/mcm MHPs are antiferroelectric. In the meanwhile, both structures belonging to ferroelastic point group torched hot debate whether domain structures observed on MHPs are ferroelectric or ferroelastic. The relationship between ferroelectricity and ferroelasticity of MHPs are scarcely discussed as these two properties were regarded mutually exclusive. In this presentation, a brief description of the basic concepts of structural symmetry, such as ferroelectricity and ferroelasticity, have been given. The connection of ferroelectricity and ferroelasticity of MHPs have been proposed.

Sensitive Magnetoelasticity from Nanoprecipitates-Bearing Ferromagnet

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Abstract: Magnetoelasticity of ferromagnetic materials refers to their deformation under external magnetic fields, making them useful for smart devices, such as actuators, transducers, sensors and energy harvesting systems. For most applications, it is highly desired to have a combination of large magnetostriction and small switching field, i.e. sensitive magnetoelasticity. However, simultaneously achieving large magnetostriction and small switching field is challenging because the magnetostriction and switching field are both proportional to the magnetocrystalline anisotropy (MCA). In this talk, we shall present the achievement of sensitive magnetoelasticity by a novel nanoprecipitation strategy. As exhibited in cubic alloy iron-gallium, introducing coherent tetragonal nanoprecipitates can simultaneously enhance the magnetostriction and reduce the switching field, giving rise to five-fold enhancement in the figure of merit, defined by saturation magnetostriction over MCA constant. The mutual elastic interactions between the coherent tetragonal nanoprecipitates and the soft cubic matrix can result in an average tetragonal symmetry, i.e. substantially enlarge the saturation magnetostriction constant (c/a-1). The random magnetic interactions between the matrix and the dispersive nanoprecipitates can also result in the collapse of net MCA as well as the switching field. By co-engineering the nanoprecipitates and grain/magnetic domain orientations, the magnetoelasticity can be further enhanced. The feasibility of obtaining such two-phase nanostructure by aging a supersaturated solid solution then allows one to develop high-performance magnetostrictive materials from a large class of ferromagnetic alloys.

Smart Topological Elastic Metamaterials with Tunable Valley Hall Effect

Weijian Zhou

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Abstract: Recently, valley Hall effect have been observed in mechanical systems. It has attracted enormous attention from researchers due to its exceptional capacity in inducing topologically protected interface modes, which have shown high robustness against structural defects. However, most of current topological metamaterials suffer from narrow working frequency ranges. A feasible approach to broaden the frequency range is using modern control techniques to tune the behaviors of metamaterials to match the needs, so that the narrow working frequency range can be changed in a wide range. Furthermore, control techniques can make topological metamaterials intelligent. Their functions can be changed or even switched at will. In this work, we start from the analysis of a theoretical model and find a suitable way to design tunable topological plate-type metamaterial by using piezo-patching techniques. Finite element simulations show the existence of topologically protected interface mode, whose working frequency can be tuned by changing the capacitances in the electric circuits. The tunable topological metamaterial proposed in this work may guide the design of intelligent acoustic devices with robust wave guiding performances.

Study the Effect of laundry on the Electrical Resistance of Silver Coated Vectran Conductive Yarn for the Application of E-Textile

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Abstract: Electronic textiles are an early developing hybrid system and require new standards of reliability and permanence for the application of smart wearable textile. The washing durability of the e-textiles is one of the most important aspects for their reliability and maintenance. The standards must meet the requirements for both textile and electronic components of e-textile products. In these paper, the effects of laundry washing on the electrical resistance of silver-coated Vectran (SCV) conductive yarns which are used for the application of wearable e-textile products is studied. Several factors, such as mechanical, thermal, chemical, and other stress was damage to the tiny coated silver particles on the surfaces of SCV conductive yarn during the washing process. The Structural changes of SCV conductive yarns were investigated and analyzed by using FTIR and DSC machines. Various peaks observed before and after washing in the SCV conductive yarn were analyzed. The analytical finding shows that the electrical conductivity of SCV conductive yarns were severely affected by repetitive and cyclic laundry washing, having an increased electrical resistance from 0.84 Ω to 1.9 Ω per 0.3 m gauge length after 25 washing cycles.

The Effect of Tungsten Addition on the Co-Cr Dental Alloys

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Abstract: The variety of alloys for prosthetic restorations has increased rapidly over the last twenty-five years, which makes their selection for a given clinical situation very difficult. A series of properties - such as elastic modulus, microstructural phases, grain size, corrosion resistance, coefficient of thermal expansion, oxide and color, strength, hardness, - are of relevance when it comes to the correct selection of an alloy. The most important factor in such a choice is patient biosafety. The alloy selection decision has profound financial, legal, technical, practitioner satisfaction, and patient health consequences. The analyzed dental materials are Co-Cr alloys used for the fabrication of ceramic or composite coated crowns and bridges. Due to their coefficients of thermal expansion they are suitable for the most common metal veneering ceramics on the market. In this study, 3 Co-Cr alloys with increasing tungsten content have been analyzed. Corrosion potential, corrosion rate and pitting potential measurements have been carried out. The behavior under service conditions has been evaluated by means of electrochemical impedance spectroscopy whose spectra have been fitted to an equivalent circuit which has allowed to determine the characteristic parameters of the taking place process. The composition of the corrosion products has been analyzed by scanning electron microscopy and EDAX. As the tungsten content increases, the properties of the alloy improve: it acquires optimum casting qualities and an extra fine molecular structure resulting in smooth and compact surfaces for easy and simple processing.

Thin Films Based on Isoflavonoids and Antibiotics against Major Bacterial infections

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Abstract: Because their widespread distribution, opportunistic behavior, and drug resistance, *Staphylococcus aureus* (Gram-positive) and *Pseudomonas aeruginosa* (Gram-negative) bacteria represent major infectious concerns in the hospital settings. In our present study we report on polyvinylpyrrolidone/antibiotic/isoflavonoid thin films obtained by the matrix-assisted pulsed laser evaporation (MAPLE) technique for improved resistance to microbial colonization. The thin films were characterized by Fourier transform infrared spectroscopy, infrared microscopy, and scanning electron microscopy. *In vitro* biological assays were made in order to evaluate the thin films impact on the development of *Staphylococcus aureus* and *Pseudomonas aeruginosa* biofilms. *In vitro* biocompatibility tests on human endothelial cells were performed for up to five days of incubation, by qualitative and quantitative methods. The results of our study revealed that the laser-fabricated coatings are biocompatible and resistant to microbial colonization and biofilm formation. The polyvinylpyrrolidone/antibiotic/isoflavonoid thin films can be considered as viable candidates for biomedical devices and contact surfaces that would otherwise be amenable to contact transmission.

Tuning the Surface Immunomodulatory Functions of Polyetheretherketone for Enhanced Osseointegration

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Abstract: The adverse macrophage-mediated immune response elicited by the surface of polyetheretherketone (PEEK) is responsible for the formation of fibrous encapsulation and resulting inferior osseointegration of PEEK implants in the dental and orthopedic fields. Therefore, endowing the PEEK surface with immunomodulatory ability is an appealing strategy to enhance implant-bone integration. Herein, a reliable and cost-effective method to construct adherent films with tunable nanoporous structures on PEEK is described. The functionalized surface not only suppresses the acute inflammatory response of macrophages, but also provides a favorable milieu for osteogenic differentiation of human bone marrow mesenchymal stem cells (hBMSCs). Whole genome expression analysis reveals that the suppression effect arises from synergistic inhibition of focal adhesion, Toll-like receptor, and NOD-like receptor signaling pathways, as well as the attenuating loop through the JAK-STAT and TNF signaling pathways in macrophages. Further in vivo studies confirm that the functionalized surface induces less fibrous capsule formation and an improved bone regeneration. The nanoporous films fabricated on PEEK harmonize the early macrophage-mediated inflammatory response and subsequent hBMSCs-centered osteogenic functions consequently yielding superior osseointegration.

Learning from Superelasticity Data to Search for Ti-Ni Alloys with Large Elastocaloric Effect

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Abstract: The reversible adiabatic temperature change (ΔT_{ad}) of shape memory alloys is shown to be proportional to the mechanical work released by the reverse martensitic transformation during unloading (ΔW_u). As there exists a considerable amount of data (ΔW_u) on superelastic stress-strain measurements in shape memory alloys, the proposed relationship allows us to predict ΔTad without caloric measurements. The estimated ΔT_{ad} from the ΔW_u of different Ti-Ni alloys shows good linear relationship with the directly measured values. Moreover, following such a design criterion and by tuning of composition and thermo-mechanical treatment, a group of Ti-Ni binary shape memory alloys with directly measured ΔT_{ad} larger than 35 K under tension were achieved. The large ΔT_{ad} and ΔW_u can be ascribed to the grain refinement and the heterogeneous internal stress fields after the thermo-mechanical treatment, which have enhanced the critical stress of superelasticity and recoverability of martensitic transformation during unloading.

Smart Topological Elastic Metamaterials with Tunable Spin Hall Effect

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Abstract: Recently, valley Hall effect have been observed in mechanical systems. It has attracted enormous attention from researchers due to its exceptional capacity in inducing topologically protected interface modes, which have shown high robustness against structural defects. However, most of current topological metamaterials suffer from narrow working frequency ranges. A feasible approach to broaden the frequency range is using modern control techniques to tune the behaviors of metamaterials to match the needs, so that the narrow working frequency range can be changed in a wide range. Furthermore, control techniques can make topological metamaterials intelligent. Their functions can be changed or even switched at will. In this work, we start from the analysis of a theoretical model and find a suitable way to design tunable topological plate-type metamaterial by using piezo-patching techniques. Finite element simulations show the existence of topologically protected interface mode, whose working frequency can be tuned by changing the capacitances in the electric circuits. The tunable topological metamaterial proposed in this work may guide the design of intelligent acoustic devices with robust wave guiding performances.

Static Deformation and Dynamic Response of Multilayered Magnetoelectroelastic Nano-Plates

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Abstract: Due to their powerful functions for transforming energy among mechanical, electric and magnetic fields, the magnetoelectroelastic (MEE) materials have been paid much attention. Developments of new advanced materials/composites involve nanostructures, both the size-dependent effect and the MEE multi-field coupling should be taken into account. In fact, size-dependent effect in magnetoelectric materials was observed experimentally and could be useful in designing various miniaturized multifunctional devices. It is well-known that the classical elasticity theory is not capable of describing the size-dependency because it assumes that the matter is continuously distributed throughout the body by neglecting its microstructure. Therefore, several size-dependent elasticity theories, such as nonlocal elasticity theory, strain gradient elasticity theory, surface/interface theory and modified couple-stress theory have been developed to characterize the size-dependent effect in nanostructures. Layered structures such as sandwich ones are widely used in different engineering branches due to their high stiffness, good insulation, and weight efficiency as compared to the conventional structural members. Therefore, size-dependent elasticity theories are developed for static deformation and dynamic response of three-dimensional layered structures composed of smart materials such as piezoelectric and magnetic materials in this work. Three-dimensional exact solutions of the extended displacements, extended stresses, natural frequencies, critical buckling loads and dispersion relation for bending, vibration, buckling and wave propagation of layered MEE nanoplates are derived, respectively, by solving the linear eigensystem and using the propagator matrix method. Numerical examples are presented the effects of thickness of nanoplates, nonlocal parameter, material length scale parameter, stacking sequence, shear modulus of the elastic medium and the orientation of incident wave on static deformation and dynamic response. The obtained results will provide theoretical basis for the optimal design of nano-devices and structures of advanced materials/composites.

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Session 3: Energy Materials

Achieving Strong Coherency for a Composite Electrode via One-Pot Method with Enhanced Electrochemical Performance in Reversible Solid Oxide Cells

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Abstract: The oxygen electrode with a fast oxygen reduction reaction (ORR), oxygen evolution reaction (OER), and sufficient durability plays a pivotal role in reversible solid oxide cells (RSOCs). Here, we demonstrate a NdBa0.5Ca0.5Co1.5Fe0.5O5+δ@ Gd0.1Ce0.9O2-δ (NBCCF@GDC) composite oxygen electrode via a one-pot method for exhibiting strong coherency, which result in boosting the electrochemical performance of RSOCs. The NBCCF@GDC electrode yields a very low polarization resistance (0.106 Ω-cm^2 at 800 °C), high electrolysis current density (1.45 A cm^{-2} with 70 vol % absolute humidity at 1.3 V), and high power density (~1.3 W cm^{-2} at 800 °C) and shows excellent reversibility and stability. Notably, strong coherency in these NBCCF@GDC composite materials was successfully revealed by HT-XRD, XPS, STEM, and EELS. The phase contiguity and interfacial coherence between NBCCF and GDC increase the Co oxidation state and the number of active sites, which enhanced the electrocatalytic activity for perovskites. Overall, this work demonstrates a highly desirable strategy for the production of functionalized electrodes for next-generation reversible solid oxide cells

Insight into the Stabilized Water Oxidation Performance on Highly Active Manganese Nickel Oxides

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Abstract: Manganese oxides (MnO_x), though show highly catalytic activity for water oxidation, have suffered from poor performance stability during prolonged electrolysis. This work introduces a novel method to produce manganese nickel oxides ($MnNi_yO_x$) on FTO glass by co-electrodeposition from an ionic liquid medium, which shows significantly improved water oxidation catalytic activity and stability. The electrodeposited films shows low crystallinity and the morphology change from nanoparticles in the MnO_x to a network-porous structure in the $MnNi_yO_x$. The Ni content in the $MnNi_yO_x$ can be controlled from y = 0.33 to y = 1 by altering the concentration of Ni^{2+} and acidity of the deposition electrolytes. The catalytic activity for water oxidation on the obtained $MnNi_yO_x$ increases compared with MnO_x and NiO_x, and it is further improved after prolonged water electrolysis. The $MnNi_yO_x$ shows high water oxidation activity (as low as 280 mV for 1 mA cm^{-2} in 1.0 M NaOH) and improved long-term stability in the examined electrolytes (stable current of 8 mA cm^{-2} at 1.64 V for 20 hr prolonged electrolysis in 1.0 M NaOH). It is proposed that the stabilized Mn at high oxidation states by Ni, and the homogeneous distribution of Ni-O and Mn-O structure in the binary metal oxides, contribute to the high catalytic activity and improved stability.

An Efficient and Non-Precious Anode Electrocatalyst of NiO-Modified Carbon Nanofibers towards Electrochemical Urea Oxidation in Alkaline Media

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Abstract: Non-precious NiO nanoparticles were combined with carbon fibers (CFs) to design the novel electrode material; NiO-CFs. The as-synthesized NiO-CFs material was investigated in terms of Field emission scanning electron microscope (FE-SEM), Fourier-transform infrared spectroscopy (FT-IR), Brunauer-Emmett-Teller (BET) surface area, Energy-dispersive X-ray spectroscopy (EDX), UV–vis spectra, Transmission electron microscope (TEM), selected area diffraction (SAED) pattern and X-ray diffraction (XRD) techniques. These analyses indicate the successful synthesis of a nanocomposite of NiO-CFs. Cyclic voltammetry (CV) in addition to chronoamperometric (CA) and electrochemical impedance spectroscopy (EIS) methods were studied in the 3-electrodes system to examine the electrochemical performance of NiO-CFs material for urea oxidation in KOH medium. The synthesized nanocomposite showed improved electrochemical oxidation of urea at various urea concentrations up to 1.5 M. The decreasing of both charge transfer impedance and series resistance indicates the enhanced transfer of electrons in the occurrence of urea which could be related to the high electrochemical performance of NiO-CFs material as an electrocatalyst. The superior electrochemical activity can be due to the assembly of C-structure with NiO nanoparticles during the synthesis steps which enhance electrocatalysis, charge transfer, and structural defects.

A facial and effective way to prepare high-performance hetero-structured composite cathode for Intermediate temperature solid oxide fuel cells

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Abstract: A hetero-structured composite porous cathode has been simply prepared by mixing 90 wt% single-phase perovskite (SP) $La_{0.6}Sr_{0.4}Co_{0.2}Fe_{0.8}O_{3-\delta}$ (LSCF113) and 10 wt% Ruddlesden-Popper layered perovskite (RP) $LaSrCo_{0.2}Fe_{0.8}O_{4-\delta}$ (LSCF214) nano-powders. The nano-powders of LSCF113 and LSCF214 were separately synthesized by wet chemical coprecipitation (CP) method, and subsequently mixed by ball-milling to obtain the composite CP-LSCF214-113 cathode with RP/SP hetero-interface. The hetero-interface of the cathode has been confirmed by XRD and TEM. The polarization impedance (R_P) of a symmetric cell with the composite cathode achieved 0.06 and 0.24 $\Omega \cdot cm^2$ at 800 and 700 °C, respectively, due to the presence of the RP/SP hetero-interface, respectively 72.3% and 56.1% of the cathode impedance of CP-LSCF113 counterparts. The cell also showed excellent stability over 100 h at 750°C. An anode supported SOFC with the CP-LSCF214-113 composite cathode achieved maximum power density of 1.02 $W \cdot cm^{-2}$ at 800°C. Moreover, the CP-LSCF214-113 effectively inhibits the coarsening of grains and the growth of RP phase. As comparison, LSCF113 and LSCF214-113 cathodes were prepared by solid state reaction (SSR) method. The R_P of the SSR-LSCF214-113 is even higher than that of SSR-LSCF113, indicating that the RP/SP hetero-interface was not effectively formed for the composite prepared by SSR. Our results reviewed that the CP method combined with ball-milling and subsequent calcining is an effective way to construct RP/SP hetero-interface in porous cathodes for intermediate temperature solid oxide fuel cells (IT-SOFCs).

Chemical Vapour Deposited Si@Carbon Nanotubes as Anode Materials for Low-Cost Multivalent Battery Systems

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Abstract: Although, Si is an attractive anode material due to its high specific capacity (i.e. about ten times higher than graphitic carbon), it exhibits volume expansion during the intercalation/deintercalation processes, leading to poor stability performance. In order to overcome this shortcoming, one possible strategy is the development of nanocomposites of Si with carbon-based structures such as carbon nanotubes. The carbon nanotubes act as both mechanical support and electrical conductor, while Si as a high-capacity anode material. Furthermore, research efforts have been focused on developing Zn^{2+} and Al^{3+} batteries, since two or three times more charge per ion can be transferred compared with Li^{+}-based ones. Nevertheless, there are limitations to find suitable electrode materials with fast mobility and kinetics during the intercalation/deintercalation processes. In this work, the chemical vapour deposition process was implemented in two steps to grow porous CNT-Si nanocomposite coatings at 480 °C. The growth of randomly oriented CNT films was attained starting from ethanol as the carbon source, while that of amorphous Si around the individual CNTs was obtained by the thermolysis of silane. The structure, morphology and electrochemical performance of the samples are examined to investigate the effect of Si amount on the efficiency and stability of the electrode. A proposed mechanism during the Zn^{2+} and Al^{3+} intercalation/deintercalation processes is discussed.

Defect Modulation in Piezoelectric ZnO Nanorods and Impact on Nanogenerator

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Abstract: The piezoelectric nature of the wurtzite structure of ZnO nanorods with a high aspect ratio at nanoscale dimensions is of high interest for energy harvesting devices. Thanks to the advances in nanomaterials production techniques that enable several limited real-life applications. But a number of issues related to enhancing the piezoelectric effect and hence energy harvesting are still open and deserve particular attention. The main aim of several studies has been to produce high-quality crystalline piezoelectric nanostructures. Therefore, herein investigated the role of point defects that arise due to different production techniques and their eventual impact on the functional piezoelectric effect is demonstrated. In this context, two different production methods feasible for a scale-up process are adopted and the produced ZnO nanorods are duly assessed by Scanning Electron Microscopy (FE-SEM), X-ray diffraction (XRD), and Photoluminescence (PL). The modulation of point defects by thermal annealing is also investigated. Further, flexible piezoelectric nanogenerators are fabricated using nanocomposite films comprised of the resultant nanomaterials. The flexible devices with the respective compositions demonstrate that the potentiality of the point defects on achieving higher piezoelectric voltages is reported. This novel insight on improving the device performance by modulating the point defects would be highly beneficial for researchers in the field.

Design and Preparation of Polymeric Carbon Nitride-Based Photocatalysts for CO_2 Reduction

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Abstract: Conversion of CO_2 to chemicals and fuels via photocatalysis technology is a sustainable route to solve both energy crisis and environmental impacts. Polymeric carbon nitride (CN) is a promising photocatalytic material for CO_2 reduction due to its visible light response, high chemical stability, low-cost and easy preparation [1]. However, the CO_2 photoreduction performance for bulk CN obtained from direct pyrolysis is still far from satisfactory due to the limited visible light absorption, serious recombination of photogenerated charges and low surface area. We designed and prepared a series of CN based photocatalytic materials including N-defective CN nanosheets, N-rich porous CN, TiO_2 quantum dots/CN nanosheets, hollow In_2S_3/CN, Fe_2O_3 nanoparticles/CN nanosheets, etc [2–5]. Our work indicates that the introduction of defects, controlling the morphology (nanosheets or porous structure) and the construction of heterojunction can efficiently promote visible light absorption, CO_2 adsorption as well as charge separation and transfer of CN, leading to enhanced activity of CO_2 photoreduction. This work provides insights into the design and preparation of high-efficiency CN-based photocatalysts for energy and environmental applications.

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Effect of Si Doping on the Stability and Efficiency of Graphene Oxide as an Anode Material for Aqueous Zn-ion Batteries

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Abstract: Towards the great demand for energy storage applications, Si has attracted increasing attention due to its high theoretical capacity and extensive sources. Nevertheless, it presents large volume expansion and structural changes during the charging and discharging processes causing irreversible capacity loss of the electrode. To overcome the aforementioned limitations, a conjugation with graphene oxide is proposed. It is expected that the synergetic functionality will improve the electrochemical performance of the electrode through the release of Si volume change stress and the increase of its conductivity. In particular, a dispersed solution of Si nanoparticles and graphene oxide has been prepared and then the solution is immobilized through a spray procedure on a solid substrate. The graphene oxide was prepared through the modified Hummer's method using 1 g graphite in 46 ml H_2SO_4. Then 5, 8, and 12 at. % of Si nanoparticles were added in the GO solution to form an aqueous mixture of the two entities under low temperature (60 °C). The structural and morphological features of the electrodes have been investigated after the cycling to investigate the effect of Si doping on the efficiency and stability of the electrodes. A proposed mechanism during the Zn^{2+} charging and discharging processes is discussed.

Mitigating Electrical Loss of $CsPbI_2Br$ Solar Cells by Molecularly Manipulating Orientation of Hole Transport Material

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Abstract: Inorganic cesium lead halide perovskites ($CsPbI_{3-x}Br_x$) offer a pathway towards excellent photovoltaics due to their superb thermal stability. However, moisture-induced phase degradation restricts the application of the widely employed hole transport layers (HTLs) with hygroscopic dopants. State-of-the-art dopant-free HTLs fail to realize efficient inorganic perovskite solar cells (PSCs) due to severe electrical losses. In this work, a conjugated donor-type small molecule (i.e., SMe-TATPyr) was synthesized to mitigate the electrical loss pathways by simultaneously manipulating the hole transport material (i.e., P3HT) stacking characteristics, passivating the $CsPbI_{3-x}Br_x$ perovskite surface defect, and creating favorable energy level alignment between perovskite and hole transport layer. This leads to a reduced Voc deficit and a PCE of 16.93% for $CsPbI_2Br$ PSCs with dopant-free HTMs. In addition, the unencapsulated devices maintain 96% of their initial PCE after aging at low humidity condition (R. H. 25%) for 1500 hours and over 95% PCE after annealing at 85 °C for 1000 hours.

The Atomic Arrangement of Electrocatalyst

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Abstract: It is of great importance to explore the highly efficient, stable electrocatalysts with low costs to realize the development of the energy storage and conversion. So far, much more attention has been paid to the modulations of the compositions, sizes, and morphology structures of electrocatalysts to enhance their electrocatalytic performances, however, the atomic arrangement, which is a key factor influencing the properties of electrocatalysts, is less studied, and the effect of atomic arrangement on the performance as well as corresponding regulatory mechanisms are significant, but still remain unknown. Here, we report novel strategies for the synthesis of noble metal based nanostructures with the unconventional crystal phase (i.e. metastable phase, amorphous phase and intermetallics), which exhibit excellent electrocatalytic performances toward hydrogen evolution reaction, oxygen evolution reaction, and methanol (ethanol) oxidation reaction. Our research will provide theoretical foundation and technical support for the exploitation of the high-performance electrocatalysts with low cost.

Pt-Based Electrocatalysts with High Atom Utilization Efficiency: From Nanostructures to Single Atoms

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Abstract: Platinum is a key component of the catalysts in a proton-exchange membrane fuel cell (PEMFC), which exhibited good oxygen reduction reaction (ORR) activity. Notwithstanding the superior properties of Pt catalysts, the low abundance of Pt, and subsequent high cost have created a major barrier for the large-scale commercialization of Pt catalysts in PEMFCs. One effective route for reducing the cost of Pt is to increase the atom utilization efficiency by reducing the particle size to clusters or even single atoms catalysts.[1] Herein, we will demonstrate our recent approaches about the preparation of Pt single atom catalysts by atomic layer deposition method (ALD). Nearly 100% Pt single atom catalysts were successfully deposited on N-doped carbon nanotubes. Pt-Pd single atom alloys were prepared through ALD method and applied in electrochemical oxygen reduction for the first time. We also successfully prepared successfully prepared Pt-Ru dimers on NCNTs through ALD process. All these different types of single atom catalysts exhibited superior activity in ORR and HER reactions. In conclusion, we demonstrate a series types of Pt single atoms, including high-quality Pt single atom, Pt-Pd single atom alloy and Pt-Ru dimer structures. The results show that the formation of single atom structure can effectively improve the electrochemical performance. It is also worth to mention that we have first introduced ALD technique in the single atoms. It is believed that our study opens up a new avenue of developing new types of Pt-based catalysts for fuel cells and brings new understanding about catalytic performances of single atoms.

The Photocatalytic Performance of Hydrogen Production and Mechanism of $Co_3S_4/Zn_{0.5}Cd_{0.5}S$

Yidong Sun, Chunxu Pan

Wuhan University

Abstract: As a kind of CdS-based semiconductor photocatalyst, the band gap of the $Zn_xCd_{1-x}S$ solid solution can be adjusted by adding Zn^{2+} to change the internal proportional structure, and the $Zn_xCd_{1-x}S$ has been considered the best catalysts for photocatalytic hydrogen production. However, its application is still limited, because of rapid recombination of photo-generated electrons and holes and photo-corrosion during photocatalytic reaction, which make its hydrogen production rate cannot meet the requirements of industrial usages. In this study, layered Co_3S_4 has excellent conductivity, and the $Co_3S_4/Zn_{0.5}Cd_{0.5}S$ heterojunction can effectively enhance the separation efficiency of photogenerated carriers and the layered structure also increases the refraction of light. Comparing with pure $Zn_{0.5}Cd_{0.5}S$, the 10%$Co_3S_4/Zn_{0.5}Cd_{0.5}S$ heterojunction exhibits the highest visible light response, and the transient photocurrent and hydrogen production rate reach to 14 μA and 1511 μmol/h/g, respectively, which are 70 and 14.6 times higher than pure $Zn_{0.5}Cd_{0.5}S$. While a theoretical calculation is carried out for exploring Co_3S_4 as a qualified cocatalyst and the high property of the $Co_3S_4/Zn_{0.5}Cd_{0.5}S$ heterojunction. The mechanism is that during the reaction, the photogenerated electron-hole pairs are separated in regard to the following processes, i.e., the photogenerated electrons on the Co_3S_4 conduction band transfer to the $Zn_{0.5}Cd_{0.5}S$ conduction band, while the photogenerated holes transfer from the $Zn_{0.5}Cd_{0.5}S$ to the Co_3S_4 valence band combine with lactic acid to form pyruvate. This work provides a new idea for experimental design, and the process exhibits advantages, such as simple, environmentally friendly, and possible large-scale production, etc. It expects a broad application prospects.

Session 4: Functional Ceramics, Thin Films and Crystalline Materials

A New Acentric Borate-nitrate Cs3B8O13(NO3) with Interpenetrating Porous 3D Covalent and Ionic Lattices

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Abstract: A new acentric borate-nitrate Cs3B8O13(NO3) was synthesized by molten salt method which consists of two novel interpenetrating porous three-dimensional (3D) lattices: covalent lattice [B8O13]– and ionic lattice [(NO3)Cs3]–. It shows a low ultraviolet cut-off edge (202 nm) and a phase-matching second harmonic generation (SHG) intensity (0.7 KDP @1064 nm).

Figure 1. (a) [B8O16]8− FBB and [(NO3)Cs6]5+ SBU. (b) 3D open porous covalent lattice [B8O13]∞. (c) 3D open porous ionic lattice [(NO3)Cs3]∞. (d) The interpenetrating 3D framework of CBN.

Figure 2. (a) Powder SHG measurements at 1064 nm for CBN and KDP. (b) UV-vis-IR diffuse reflectance spectroscopy. (c) Calculated birefringence and the band structure of CBN (d).

Figure 3. (a) The density of states. (b) SHG density in the occupied and (c) unoccupied states in the VE process for CBN. (d) The arrangement of the NLO-active units of CBN.

The novel structure of the title compound enriches the structural chemistry of borates and the current work shed some light on the exploration of new NLO materials in the rarely studied borate-nitrate system.

Active Manipulation of Metamaterials and Plasmonics with Thin-film IGZO Schottky Diodes

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Abstract: Metamaterials and surface plasmonics have gained great interest in the applications of light manipulation, biosensing, cloaking, flat lenses, communication etc. As passive devices, the optical properties of metamaterials and surface plasmonics are set in stone after design, which stimulates the researches on how to actively control these passive devices. Recently, we have developed using In-Ga-Zn-O (IGZO) thin-film Schottky diode to actively modulate metamaterials and surface plasmonics at millimeter wave and terahertz frequencies. IGZO is an optical transparent metal-oxide semiconductor widely used for large-area displays and flexible electronics due to its low cost, high yield, high uniformity, flexibility, and room-temperature process. Typically, the operating frequency of IGZO devices, such as transistors and diodes, is less than 6 GHz due to the low electron mobility of IGZO film. In this talk, we will show using IGZO Schottky diodes to actively control matemetrials at several hundred GHz, i.e., terahertz frequencies, and multi-frequency, multi-bit manipulate surface plasmon polaritons at millimeter wave frequencies.

Effect of hexamethylenetetramine on enhanced corrosion resistance of AZ31B magnesium alloys by micro-arc oxidation

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Abstract: In order to fabricate calcium-phosphate (Ca-P) coatings on AZ31B magnesium alloys by micro-arc oxidation (MAO), hexamethylenetetramine was selected as a novel inhibitor for magnesium alloys in neutral solutions. The influences of hexamethylenetetramine concentrations on coatings property were systematically studied. The surface morphologies, chemical compositions and corrosion resistances of magnesium samples were investigated using SEM, EDS, XRD and potentiodynamic polarization tests and electrochemical impedance spectroscopy (EIS). The results showed that the coatings with different concentrations had unequal microstructures. The coatings were composed of Mg and MgO. Hexamethylenetetramine was a corrosion inhibitor for Mg alloys and increased the solubility of calcium salts. When the concentration was 360 g/L, the coating achieved the lowest corrosion current density (8.75×10^{-9}A/cm^2) in Hank's solution, and higher inhibition efficiency (94.57%) in 3.5wt % NaCl solution. However, once the concentration was lower than 240 g/L, the magnesium alloy hardly was passivated and anodic coatings could not be developed. With the concentration increasing, the solution got clearer, besides, final oxidation voltage and the pH values got higher except the conductivity. The anti-corrosion ability gradually alleviated when the concentration was more than 360 g/L. And the reasons why hexamethylenetetramine enhances the corrosion resistance of AZ31B magnesium alloys may be due to its interaction with Mg^{2+} ions, which can be adsorbed on the surface of magnesium alloys.

High-performanced Piezoelectric Energy Harvester Based on PIN-PMN-PT Crystals

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Abstract: Wireless sensing is widely adopted in internet of things (IoT) systems, but battery replacement is a critical issue for these devices. Triboelectricity, solar, heat, and vibration can be potential energy sources. Piezoelectric energy harvesters that can obtain energy from ambient vibrations are thought to be a promising approach to this problem. However, state-of-the-art energy harvesters made from cantilever-structured piezoelectric ceramics exhibit low output power densities and degradation in long time service.

Herein, we propose two piezoelectric energy harvesters based on $Pb(In_{1/2}Nb_{1/2})O_3$-$Pb(Mg_{1/3}Nb_{2/3})O_3$-$PbTiO_3$ (PIN-PMN-PT) single crystals to solve the above issues. The first one is a bridge-type shear-mode piezoelectric energy harvester. Owing to the large figure-of-merit $d_{15}\times g_{15}$ (1.296×10^{-10} C V m N^{-2}) of the crystal and the higher electromechanical transfer efficiency of the flex-tensional structure when compared to a ceramic cantilever structure, the newly designed shear-mode energy harvester exhibits a power density of up to 1.378×10^4 W m^{-3}. This is much higher than the power densities provided by conventional cantilever energy harvesters based on piezoelectric ceramics (~10^2 W m^{-3}). The output voltage and maximum output current are 21.6 V_{pp} and 6×10^{-4} A_{pp}, respectively under an inertial force of 0.25 N. This output current and power density are 5.5 times and 3.0 times, respectively, higher than those of the same structured energy harvester made from soft piezoelectric ceramics. The second one is a modified barbell-shaped piezoelectric energy harvester (BSPEH) based on two d_{33}-mode cuboid PIN-PMN-PT multilayer single crystal stacks (ten wafers with a thickness of 0.5 mm and d_{33} ~ 1300 pC/N). Due to the electrically parallel and series connections of multilayer piezoelectric elements and the high figure-of-merit $d_{33} \times g_{33}$ of the single crystal, the maximum power density of BSPEH could reach 39.7 mW cm^{-3} (under an acceleration of 5 g), which is much higher than that of traditional cantilever piezoelectric energy harvesters (CPEHs), ~0.1 mW cm^{-3}. A maximum output voltage of 50.4 V_{pp} was obtained when two crystal stacks are connected in series, and a maximum output current of 880 μA can be obtained when two crystal stacks are connected in parallel. Furthermore, the energy harvesting properties of BSPEH stay almost the same after 10^6 vibration cycles, while the properties of CPEH decrease 20% after 10^5 vibration cycles.

A sample wireless sensing and data transmission system is successfully powered by the newly designed energy harvester. This work may help to address the issue of sustainable energy supplies for IoT systems.

Artificial Chameleon Skin with Super-Sensitive Thermal and Mechanochromic Response

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Abstract: Both the nonclose-packed structure and the large refractive index contrast of guanine nanocrystals and cytosols in iridophores play a vital role in the dynamic camouflage of chameleons, including the bright skin color and color tuning sensitivity to external stimulus. Here, the nonclose-packed photonic crystals consisting of ZnS nanospheres and polymers, which have similar refractive indices with guanine nanocrystals and cytosols, respectively, are constructed by a twostep filling strategy. ZnS@SiO2 nanospheres are self-assembled to build intermediate close-packed photonic crystals followed by filling polymers in their interstices. The nonclose-packed photonic crystal is successfully achieved when the silica portion is etched by HF solution and refilled by polymers. Excitingly, the stimulus response of the designed photonic crystal is as sensitive as the skin of chameleons due to the similar contrast of refractive indices and nonclose-packed structure. The reflection peak of the structure can blue-shift more than 200 nm as the temperature increases from 30 to 55 °C or under 20% compressional strain. This work not only builds the nonclose-packed photonic crystals by introducing a two-step filling strategy but also proves that high refractive contrast in photonic crystals is an effective strategy to achieve ultrasensitivity, which is highly desirable for various applications.

Biphasic Liquid–Liquid Interface Limit Architecture of High-Quality Perovskite Single-Crystal Sheets

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Abstract: Surface defects have a greater impact on UV detection because of high UV absorption on the shallow surface. $MAPbCl_3$ is considered one of the most promising materials for visible-blind UV detectors because of its large optical band gap. The high growth temperature for $MAPbCl_3$ single crystals is about 60–100 °C by the antisolvent evaporation method. Therefore, the low temperature gradient can restrain the growth condition and obtain higher crystal quality. The growth temperature and precursor concentration play key roles in obtaining high-quality bulk single crystals of $MAPbX_3$ by the reported methods. However, the above methods are also unsuitable for preparing high-quality single-crystal thin films or sheets.

We herein propose a novel liquid–liquid (dimethicone/dimethyl sulfoxide (DMSO)) interface limit method to synthesize thin high-quality single-crystal perovskite sheets for the first time. The thickness of the sheets could be controlled in the range from 1 to 50 μm by adjusting the liquid–liquid interface, precursor concentration, and solution volume. DMSO molecules can slowly diffuse into the dimethicone through the biphasic liquid interface rather than ions, resulting in single-crystal sheet increases when the solution becomes saturated without antisolvents. The thin single-crystal sheet was utilized to prepare a photodetector because of its high crystal quality and fewer surface defects, which are beneficial to improve the photoelectric properties. The results demonstrate that our photodetector has superior properties with a high responsivity of 0.88 A W- and external quantum efficiency (EQE) of 276.8% for $MAPbCl_3$ at a bias of 3 V under illumination with 395 nm light at 0.43 mW cm^{-2}. Moreover, the single-crystal $MAPbCl_3$ sheet-based photodetector also has excellent stability with 4200 continuous on–off cycles.

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Design and Synthesis of Deep-Ultraviolet Optoelectronic Crystals Based on Borates

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Abstract: Borate is one of the most important systems for exploring novel optoelectronic materials, especially deep-ultraviolet (DUV) nonlinear optical (NLO) and birefringent crystals, due to its wide optical transparency window, excellent chemical stability, and large optical polarizability and anisotropy that are benefit to NLO coefficient and birefringence, respectively [1,2]. In this report, the current progress on the exploration of new DUV NLO and birefringent crystals based on borates has been summarized. Specifically, the effects of fluorine atoms on the structural chemistry and NLO properties of borates have been analyzed [2,3]. A strategy for the design of DUV birefringent crystal by using of $[BO_2]_\infty$ infinite chains was proposed based on the systematic investigation of the B-O anionic groups using the classical dipole-dipole interaction model [4,5].

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Fabrication and Magneto-Optical Property of $(Tb_{0.8}Lu_{0.16}La_{0.04})_2O_3$ Transparent Ceramics by PLSH Technology

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Abstract: Novel $(Tb_{0.8}Lu_{0.16}La_{0.04})_2O_3$ magneto-optical transparent ceramics have been fabricated through a modified wet chemical co-precipitation route combined with pressureless sintering in reductive H_2 atmosphere (PLSH). The primary particle sizes of $(Tb_{0.8}Lu_{0.16}La_{0.04})_2O_3$ nanocrystalline powders pre-calcined in air at 900 °C–1100 °C for 2h followed by annealing treatment in hydrogen atmosphere were 25.5 nm, 26.32 nm and 38.13 nm, respectively. The $(Tb_{0.8}Lu_{0.16}La_{0.04})_2O_3$ ceramics could be obtained by one-step sintering at 1600°C for 8–18h in H_2 atmosphere. Mechanical polished $(Tb_{0.8}Lu_{0.16}La_{0.04})_2O_3$ ceramic with a thickness of 1mm showed good transmittance from visible to near infrared wavelength, corresponding to a 75.2% transmittance at 1400nm wavelength. The measured Verdet constant at 632.8 nm wavelength was -353 rad/(T·m), 263.4% higher than that of commercial TGG crystal. Using magneto-optical materials with high Verdet constant helps shorten the required length of the magneto-optical devices. $(Tb_{0.8}Lu_{0.16}La_{0.04})_2O_3$ magneto-optical ceramics, with the Φ over 30 mm and the thickness over 2 mm, have been proved to be obtained by PLSH technology. It's promising to fabricate compact and large-size Faraday rotators by using $(Tb_{0.8}Lu_{0.16}La_{0.04})_2O_3$ transparent ceramics.

Fabrication of Monodispersed core-shell Co3O4@C and Co@C nanocomposites with enhanced electromagnetic performance

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Northeastern University

Abstract: In order to deal with the increasingly serious electromagnetic wave pollution, the development of high-performance absorbing materials has become the focus of current research. Based on transition metals, combining dielectric loss materials to prepare composite lossy core-shell structure absorbing materials, which can effectively improve the absorbing performance of the material. Among them, carbon is often used as a component of the core-shell structure because of its simple preparation process and strong dielectric loss ability.

This work uses solvothermal method and in-situ polymerization to prepare Co3O4@phenolic resin. By increasing the carbonization temperature and time, Co@C nanoparticles are prepared. Co3O4 is reduced to Co particles under the action of the carbon layer, providing strong dielectric loss, The carbon layer deepens the degree of graphitization under the catalysis of metal cobalt, providing excellent dielectric loss and conduction loss. The composite loss characteristics make the Rlmin value of the material reach -21.1 dB when the thickness is 2.3 mm, which is effective The absorption bandwidth has reached 4.3 GHz.

Fabrication of MXene@Co_3O_4 nanosheet for a high-performance supercapacitor

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Abstract: The excessive consumption of traditional fossil energy has caused serious energy crises and environmental pollution phenomenon. The rapid development of new energy storage devices improves the utilization rate of electric energy with the merits of low cost, eco-friendliness, and abundance.The new energy storage devices with batteries and supercapacitors have attracted worldwide attention. When the battery is charged at a high speed, the various polarizations (ohmic, concentration and electrochemistry) inside the battery can reduce the utilization of the active material, increased tendency of lithium plating, excessive heat generation. Supercapacitors have attracted increasing attentions due to their advantages such as fast charging and discharging speed, long cycle life and high power density. This paper develops a novel nanosheet structure MXene@Co_3O_4 enriched with oxygen vacancies for supercapacitor applications. The introduction of oxygen vacancies can provide more active sites, which improve the electrochemical performance of the material. The Co_3O_4-MXene electrode materials are developed and demonstrated outstanding electrochemical performance, which indicates that the Co_3O_4-MXene are promising alternatives to the supercapacitor applications.

Growth and Characterization of Novel Mid-IR Laser Crystals

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Abstract: Mid-IR (MIR) lasers operating around 2.0–5.0 μm have received extensive attention for numerous applications in medicine, remote sensing, military countermeasures, and atmosphere pollution monitoring due to the strong water absorption and short penetration depths of a few micrometers into biological tissue around this spectral region. The growth and characterization of novel Mid-IR laser crystals will be introduced in this report. A series of novel rare earth (Ho^{3+}, Er^{3+}, Dy^{3+}) doped fluoride (PbF_2, $LuLiF_4$) mid-infrared laser crystals were firstly grown. The use of codoping sensitized (Yb^{3+}, Tm^{3+}) and deactivated (Pr^{3+}, Eu^{3+}, Tb^{3+}) ions for enhancement of mid-infrared emissions were investigated in details. Moreover, the energy transfers between the Rare Ions were also investigated. The results show that the fluoride (PbF_2, $LuLiF_4$) crystals are the suitable mid-infrared laser crystal matrix materials due to their lower maximum phonon energy. The co-doping of sensitized (Yb^{3+}, Tm^{3+}) and deactivated (Pr^{3+}, Eu^{3+}, Tb^{3+}) ions are an effective way to improve the luminescence properties of mid-infrared laser crystals.

Novel Structural Topotactic Transformation Synthetic Strategy for Lanthnide-based Micro/Nanocrystals with Multicolor Emissions

Baiqi Shao

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Abstract: Design and synthesis of inorganic micro/nanocrystals with target phase/morphology is a focal theme in nanoscience and nanotechnology. Although nanogrowth kinetics has been conceptually established accompanying great progress during the past few decades, the intrinsic nature of a crystal structure and the elusive kinetic and thermodynamic factors in an aqueous system make it still a challenge to target a specific crystal phase, particularly under routine conditions. In view of this, we have developed a novel green synthetic strategy that use an ideal structural template on the basis of the topotactic structural matching between the template and the target phase to induce specific phase formation under conventional reaction conditions. Under this way, we have realized the systematic engineering of series of lanthnide fluorides, orthophosphate, and oxysulfides micro/nanocrystals with target crystal phases and tunable size/morphology. Our work may bring a new direction of thought for the targeted synthesis of inorganic micro/nanocrystals that are difficult to get via conventional synthetic routes.

Magneto-optical Dy_2O_3 Transparent Ceramics

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Abstract: Dy_2O_3 transparent ceramics with 4at.% La_2O_3 as sintering aid have been successfully fabricated by a modified wet chemical co-precipitation combined with pressureless sintering in reductive H_2 atmosphere (PLSH). The average particle size of the powders after calcining in air of as synthesized Dy_2O_3 precursors at 900 °C, 1000 °C and 1100 °C is about 55 nm, 65 nm and 78 nm by SEM observation, showing good dispersibility and homogeneity. The Dy_2O_3 ceramic can be sintered to be transparency at 1600 °C for 8–12h in pressureless reductive H_2 atmosphere. The transmittance of mechanical polished Dy_2O_3 ceramic with 1mm thick at 633 nm is 73.71%. The scattering loss of as sintered Dy_2O_3 transparent ceramic is about 0.137%/cm at 2000nm wavelength. The Verdet constant of the Dy_2O_3 transparent ceramics at 632.8 nm is −310rad/(T·m), which is 2.31 times that of the commercial TGG single crystal, showing great application potential on magneto-optical devices.

Piezoelectric Single Crystals for High Temperature Sensing: Recent Development

Fapeng Yu, Xueliang Liu, Chao Jiang, Yanlu Li, Xian Zhao

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Abstract: Monitoring of structural health at high temperatures is required in many industrial applications, including turbine engines, automotive combustion systems, and aerospace propulsion systems. With recent scientific and technological developments, there is a pressing need for high-performance piezoelectric sensors for in-situ monitoring of the dynamic mechanics of such industrial systems for feedback control and system optimization, as well as for the monitoring of the health of structural components for safety improvements. Extensive studies have been carried out to design different kinds of vibration sensors for high-temperature applications, including piezoresistive, capacitive, fiber optic and piezoelectric sensors. Piezoresistive sensors are less susceptible to electromagnetic interference than other types of sensors, but they are not suitable for high-temperature applications due to the inherent temperature dependence of material resistivity. Capacitive sensors can offer the advantages of low thermal drift, high resolution, and good noise performance, however, their use in high-temperature applications is often limited by the low working temperature (400 °C) and the parasitic capacitance of the sensor itself. Fiber optic sensors have the advantages of high operating temperature and high tolerance of electromagnetic interference, but they are complex to fabricate and require expensive signal processing systems. Piezoelectric sensors have many advantages over the sensors mentioned above. Firstly, they usually have simple structures and fast response times. Secondly, they are robust and long-lasting, even in harsh environments. Last but not least, external power sources are not an essential requirement for piezoelectric sensors, which greatly facilitates their application in high-temperature environments. In this report, several kinds of high-temperature piezoelectric crystals (LGS type, BTS type, and ReCOB type crystals etc.) are introduced and their potential applications for high-temperature (≥482 °C) sensing are reported.

Polymer Based Conductometric Gas Sensor for Hydrogen Detection.

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Abstract: Hydrogen measurement is crucial in emerging industries that employ liquid H_2 as an energy source. Hydrogen gas leak detectors, such as the one described in the present work, are used to prevent any accident because of the high explosion risks it has in the presence of air, as these can lead to serious injuries and damage. Polyaniline (PANi) has been proven to be an advantageous material for producing gas sensing devices, having very good sensitivity and short response times.

In this work, conductive PANi thin films were obtained via chemical polymerization of aniline directly on gold thin film and have been characterized by scanning electron microscopy (SEM) and X-ray photoelectron spectroscopy (XPS), and then electrically characterized in a gas chamber. Aniline was polymerized on the substrate in an acidic solution bath with ammonium persulfate and hydrochloric acid according to a method described in the literature. The electrical properties of the sensor inside the gas chamber have been investigated using a source-meter while under direct expose to hydrogen gas at varying concentrations.

The developed PANi based sensor proved to be a very good hydrogen gas detector with reasonable sensitivity at very low concentrations of just 1 ppm H_2.

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Pulsed Laser Deposited Bi-phasic Calcium Phosphate Implant Coatings Fabricated from Fish Bones

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Abstract: We report herewith on the fabrication of biological BCP implant-type coatings, by Pulsed Laser Deposition (PLD), from bioceramic targets prepared from Salmo salar (salmon) and Sparus aurata (sea-bream) fish bones using a KrF* excimer laser source (λ = 248 nm, $\tau_{FWHM} \leq$ 25 ns). Physical–chemical characteristics of targets and deposited nanostructures were assessed by SEM and XRD, and also by Energy Dispersive X-ray (EDX) and FTIR spectroscopy. Films were Ca-deficient and contained a significant fraction of β-tricalcium phosphate apart from hydroxyapatite, which could contribute to an increased solubility and an improved biocompatibility for bone regeneration applications. The synthetized coatings proved efficient against Escherichia coli colonization, while presenting unchanged cytocompatibility with human gingival fibroblast cells in respect to the biological control, making them promising for fast osseointegration implants.

Progress is therefore expected in the realm of multifunctional thin film biomaterials, combining antimicrobial, anti-inflammatory and regenerative properties for advanced implant coatings.

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Research on the Component Design, Fabrication and Performance Control of Terbium Oxide Magneto-optical Transparent Ceramics

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Abstract: Novel Terbium oxide is a magneto-optical material with the highest Verdet constant in visible light band, which has important application in high-energy laser system. In this paper, three kinds of doping ions such as Lu^{3+}, $La^{3+}$and Ce^{3+} were introduced by wet chemical co-precipitation to control the phase transitions, sintering activity and magneto-optical properties of terbium oxide ceramics. Optical grade Re:Tb_2O_3 was obtained by one-step sintering at 1600 °C for 8–18h in folwing H_2 atmosphere. Mechanical polished Re:Tb_2O_3 ceramic with a thickness of 1 mm showed good transmittance from visible to near infrared wavelength, corresponding to a 73.1% transmittance at 1400 nm wavelength. The measured Verdet constant at 632.8 nm wavelength was −353 rad/(T·m), 2–3 times higher than that of commercial TGG crystal. In this study, the preparation of Re:Tb_2O_3 magneto-optical ceramics with size over Φ 30mm by NC-PLSH technology was proved feasible, which shed light on the fabrication of high performance magneto-optical isolators and rotators. The relationships among component design, process parameters, and microstructure were discussed as well.

Single-crystal Lithium Niobate Thin Films

Hui Hu

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Abstract: Lithium niobate crystal has excellent electro-optical, nonlinear optical, piezo-electrical, and ferroelectric properties. Optical waveguides on lithium niobate crystals are generally fabricated using methods such as Ti diffusion and proton exchange. However, due to the low refractive index contrast of the waveguide, the bending radius of the waveguide is large, which greatly limits the miniaturization of the waveguide devices. Single-crystal LN thin films (lithium niobate on insulator, LNOI) was fabricated by ion implantation and direct wafer bonding technology, which retained the physical properties of lithium niobate bulk material and had high refractive index contrast. LNOI with 6-inch diameter was developed. LN thin films with various substrates such as Si, sapphire, and quartz were demonstrated. Many high-performance photonic devices based on LNOI have been reported, including electro-optic modulators, optical resonators and optical wavelength conversion devices. LNOI could also be used for surface acoustic wave devices. Recently, hybrid thin films such as single-crystal Si thin film on LNOI were developed, which could provide more flexibilities to the device design.

Synthesis of $Gd_xIn_{2-x}(MoO_4)_3:Eu^{3+}$ Red Phosphor and Its Luminescent Properties

Chengling Mao, Zefen Li, Wei Liu, Zhen Gong, Tian Tian, Jiayue Xu

Shanghai Institute of Technology

Abstract: Rare-earth-activated molybdate phosphor has attracted extensive attention in the field of LED lighting and display because of its good thermal and chemical stability, high color purity, narrow emission spectrum band and low synthesis temperature. For example, Tang et al. sintered $In_2(MoO_4)_3:Eu^{3+},Bi^{3+}$ phosphors by solid-state reaction method, and enhanced the luminous intensity of Eu^{3+} by sensitization of Bi^{3+}[1-3]. In this paper, Gd^{3+} is designed to replace In^{3+} in the matrix to enhance the luminous intensity of $In_2(MoO_4)_3:Eu^{3+}$. $Gd_xIn_{2-x}(MoO_4)_3:Eu^{3+}$ (x = 0.1, 0.3, 0.5, 0.7, 0.9) was synthesized by high-temperature solid-state method, and the molar fraction of $Eu^{3+}$was 0.4. XRD results showed that the pure phase with the same structure as $In_2(MoO_4)_3$ is obtained. The luminescent properties of the phosphor were systematically studied. The diffuse reflection test results showed that the phosphor had a broad absorption in the range of 200–350nm, which belonged to the charge transfer state (CTS) of molybdate group, and also had the characteristic absorption peak of Eu^{3+}. The phosphor can be effectively excited by ultraviolet light (395 nm), and its emission center is red light at 614 nm ($^5D_0 \rightarrow {}^7F_2$ of Eu^{3+}). Its color coordinate is (0.6624,0.3372), which is close to the ideal red light (0.67,0.33), and its color purity is as high as 99.96%. $Gd_xIn_{2-x}(MoO_4)_3:Eu^{3+}$ phosphor and ultraviolet chip are packaged to obtain LED devices, which can emit bright red light. Therefore, $Gd_xIn_{2-x}(MoO_4)_3:Eu^{3+}$ is a potential new red phosphor which can be applied to ultraviolet white LEDs.

Luminescence Dynamics of Inorganic Perovskite CsPbX3 Nanoparticles and Thin Films

Bingqiang Cao

University of Jinan

Abstract: Nano scale all inorganic cesium lead halide perovskite (cspbx3, x = Cl, Br, I) quantum dots and films have the advantages of high purity, adjustable emission wave growth range, narrow half peak width, high fluorescence quantum yield (up to more than 95%) and full solution treatment. They have attracted great attention of researchers and have broad application prospects in display lighting, solar cells and other fields. However, the detailed photophysical mechanism of perovskite nanoparticles and films needs to be further studied. We synthesized a series of different nanoscale cspbbr3 nanoparticles by thermal injection method, and studied the effects of synthesis temperature and different ligands on their size and photophysical properties. It is found that the size of cspbbr3 nanoparticles increases significantly with the increase of synthesis temperature or ligand electronegativity, showing quantum confinement effect. The ligand molecules adsorbed on the surface of nanoparticles effectively passivated the surface. The luminescence kinetics was studied by time-resolved fluorescence spectroscopy and transient absorption spectroscopy, and the physical mechanism of fluorescence peak shift of cspbbr3 nanoparticles was studied. Using special ligands as growth templates, ultra-small quantum dots can be synthesized, and significant ste luminescence is observed. The recent research progress in photophysics of cspbbr3 perovskite films will also be discussed. Our work provides new insights into the size dependent photophysical properties of cspbbr3 nanoparticles.

Session 5: Rare Earth Materials and Optics and Photonics

Cadmium Ions Detection Using an Optical Fiber Based Sensor

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Abstract: Heavy metals (eg cadmium, arsenic, mercury, lead, etc.) are classified as environmental pollutants due to their toxic effect on humans, animals and plants. They are not biodegradable, therefore they remain in the permanent ecological system. Contamination of the environment with heavy metals, including cadmium (Cd), is a serious problem in the modern world. Cd is therefore one of the most toxic heavy metals, acute poisoning include symptoms such as kidney damage, hypertension, anemia, hypertension or cancer, among others.

Herein, a palladium (Pd) / polyaniline (PANI) FO-SPR sensor will be manufactured, and coated further with chitosan for the specific detection of Cd^{2+} in drinking water. The thin Pd film will be deposited by magnetron sputtering, replacing the conventional gold layer, commonly preferred in the construction of classic FO-SPR sensors. PANI will be synthesized using an electroless polymerization approach, in order to be deposited as uniformly as possible on the optical fiber coated with Pd. The Pd/PANI/Chitosan FO-SPR sensor exhibited Cd^{2+} detection limit at pM level.

The authors acknowledge support from “Academy of Romanian Scientists, 3 Ilfov str, Bucharest, Romania”.

Ceria-based Catalyst for Low Temperature Denitration via SCR Technology

Changjin Tang

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Abstract: NOx is one of the most notable air pollutants in world that induces a series of environment issue like acid rain, chemical smog and O3 generation. As a powerful control strategy, the employment of NH3 as a reductant to convert NOx to N2 in the presence of catalysts has been widely investigated. In this presentation, I will give our recent studies on the using of ceria-based catalysts for NOx control at low temperatures. In addition to talk about activity enhancement, the strategies to improve the resistance to H2O, SO2 and alkaline K are also reported. Particularly, how to modify the acid property of ceria is address, and their effect on the redox property and catalystic performance of ceria will be discussed in this talk. It is hoped this report can help us to know more about the designation of ceria-based catalysts for control of NOx from stationary sources, especially for non-electricity areas like sintering, coking and cement kiln.

External Current-controlled Dynamic Display by Integrating Upconversion Micro-disks with Power Density-dependent Color into NIR Luminescent Diodes

Zhipeng Meng, Suli Wu

Dalian University of Technology

Abstract: Developing materials, which can emit tunable colors on changing external stimuli in a fixed composition, will avoid the energy loss by mixing different materials emitting a single color. We designed a core–shell upconversion micro-disk structure with high concentration of Yb^{3+} doped in the core. Fine-tuning color output is achieved by varying the power density of the excitation light within a range of 0.8–12.9W/cm^2, which is lower than most of the reported ones and can be realized by commercial NIR-LED (near infrared luminescent diodes). Importantly, we designed a dynamic display device by integrating the micro-disks in a series of NIR-LEDs. For the first time, the dynamic red, orange, yellow and green colors can be demonstrated by simply changing the external current. A red shape of a standing human and a green shape of human with walking step can be dynamically realized in a LED array by varying the external current.

Luminescence Behavior of Mn^{2+} Co-activated $SrZn_2(PO_4)_2$ Persistent Phosphor

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Abstract: The light yellow $SrZn_2(PO_4)_2:Mn^{2+}$ samples were prepared using solid state reaction in air and the photoluminescence properties of the phosphors were investigated. The as-prepared phosphors were studied systematically by X-ray diffraction, scanning electron microscope (SEM) and energy dispersive X-ray spectroscopy (EDS), photoluminescence (PL) spectra, afterglow decay curves, thermoluminescence (TL) glow spectra, X-ray photoelectron spectroscopy (XPS) and electron paramagnetic resonance (EPR). The luminescence of Mn^{2+}activated $SrZn_2(PO_4)_2$ exhibited a strong emission peak at 550 nm under 417 nm excitation. The ions of Mn^{2+} acted as not only the activators but also the providers of traps. The doping concentration of Mn^{2+} has a significant effect on the photoluminescence and long afterglow luminescence. The TL process and possible luminescence working mechanism of the $SrZn_2(PO_4)_2:Mn^{2+}$ were discussed in detail. The suitable and effective trap depths as well as the high concentration of defects for $SrZn_2(PO_4)_2$ phosphors were obtained though the introduction of Mn^{2+} ions, greatly extending the lifespan of the electron-hole pair in the lattices for the improvement of the luminescent properties of $SrZn_2(PO_4)_2$ long afterglow phosphors.

Near-infrared Spectroscopic Properties of Rare-earth/Ag Nanoparticles Single and co-doped Bismuth Glass

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Abstract: Erbium-doped fiber amplifier (EDFA) has promoted the development of the global fiber-optic communications network. With the development of the Internet and multimedia information, the conventional erbium-doped silicate fiber has difficulty in meeting information transportation requirements, because its average gain bandwidth is limited to be 35 nm (from 1530 to 1565 nm). In order to achieve the more multi-channel number and the wider bandwidth, developing materials which can realize broadband light emitting in near infrared range has become an interesting work. In this study, many single, co-doping types of rare earth and silver nanoparticles have been adopted in bismuth glass to enhance near-infrared emission intensity. The choice of glass proportions is based on high refractive index, high nonlinearity refractive index, excellent infrared transmission, low melting temperature and glass transition temperature of bismuth glass. The wider and stronger near infrared emission of rare-earth ions were obtained. The detail characteristics parameters were exhibited. The energy transfer mechanism among rare earth ions or silver nanoparticles has been analyzed.

Preparation of High-performance Rare Earth-based Perovskite Catalysts for Heterogeneous Catalysis

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Wuhan Textile University

Abstract: Rare earth-based perovskite oxides with ABO3 structure are a type of promising materials for heterogeneous catalysis due to their unique properties, such as stable and definite structure, controllable physical and chemical properties. For example, the oxygen vacancies, the metal oxidation states, and the redox behaviors can be tuned by simply replacing the cations at either A- or B-site with a foreign one, thus offering the possibility to correlate physicochemical properties and catalytic performances. However, the inherent electronic properties of perovskite and the low specific surface area caused by high temperature calcination limit its application. In order to enhance the catalytic performance of perovskite oxides, many efforts have been attempted to improve intrinsic properties (e.g., redox capacity, oxygen vacancy activation capacity, etc.) and specific surface area (e.g., generation of pores, coating with porous materials, etc.). This work reported the recent research achievements of our group on the regulation of inherent properties and specific surface area of perovskite oxides, and their varied applications in heterogeneous catalysis.

Rare Earth Doped Solid Materials for Optical Quantum Technologies

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Abstract: Rare earth (RE) ions possess abundant energy levels, and the optical and electron/nuclear spin transitions between two levels in the 4*f* electron shell exhibit very good coherence properties, among which the best coherence time can reach a few hours. Solid state materials are characterized by high structural and physicochemical stability, strong operability and easy synthesis and processing. Therefore these unique properties have enabled RE doped solid state materials as one of the most promising light-matter interfaces and quantum information storage platforms for optical quantum applications. Great improvements can be further achieved, e.g. on the quantum storage performance, the control ability and the operation precision of the quantum systems, by tuning the morphology, size of the materials and the doping concentration, dephasing dynamics of RE ions in solids. Incorporated with superconducting or trapped ion quantum systems, the RE solid systems could enable the construction of a powerful quantum hybrid system where more practical applications can be harvested in quantum communications, quantum computing, quantum network and quantum sensing areas. The aim of this work is to introduce related developments on RE solid state materials that the author and their groups studied for optical quantum applications, including Eu^{3+} doped bulk single crystals, polycrystalline transparent ceramics and nano-structural powders. Since the processes involved in dephasing and the coupling to other quantum systems are studied, main characterizations are performed using high-resolution coherent spectroscopy under ultralow temperatures, and a fine control of temperature, magnetic field, optical laser and radio frequency pulses is needed.

Rare Earth Doped Upconversion Luminescent Oxyfluoride Glass Ceramics: Microstructure Study Using Advanced Solid-state NMR Spectroscopy

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Abstract: Rare earth doped oxyfluoride glass ceramics have wide promising application in three-dimensional display, solar energy conversion, white light-emitting and so on due to their high efficiency upconversion luminescence properties. The luminescent properties of rare earth doped glass ceramics are closely related to the microstructure of glass, the distribution of rare earth ions, and the crystallization of fluoride. We will report the glass structure at atomistic scale characterized using advanced solid-state NMR technology, including the changes of glass structure with composition and the evolution of glass microstructure during the precipitation of various fluoride crystals. On the atomistic scale, the micro crystallization mechanism, the role of various elements in the fluoride crystallization, and the distribution of rare earth ions in glass ceramics are reported. Finally, we reveal the internal relationship between compositions, microstructure, crystallization and luminescent properties, and propose the composition design strategy of rare earth doped glass ceramics for upconversion luminescence.

Synthesis and Properties of Ultrathin Rare Earth Nanostructures

Yaping Du

Nankai University

Abstract: Rare earth elements have abundant optical, electric, magnetic and catalytic properties arising from the special 4*f* electron configuration, large atomic magnetic moment, strong spin and orbit interaction, diverse coordination number and specific crystals structures. In recent years, the rationally controlled synthesis and structure-property relation studies on the rare earth compounds have drawn a lot of attentions, in particular, ultrathin rare earth compound nanocrystals which have at least one dimension approaching the size of corresponding crystal unit cells, possess the unique properties and resulting applications owing to the obvious small size and strong surface effect arising from their exceptionally small dimensions. In this talk, we demonstrated some typical ultrathin rare earth compound nanostructures such as oxides, chalcogenides, oxyhalides, gadolinium porphyrin metal-organic framework as well as hydroxyl carbonates synthesized based on the solution chemistry method, and investigated the as-obtained material's properties and applications in terms of biomedicine and energy storage and conversion.

The Radiation-induced Darkening and its Suppression Methods in Yb^{3+}-doped Silica Fibers

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Abstract: Yb^{3+}-doped silica fiber (YDF) amplifiers have been demonstrated to meet future long-haul inter-satellite optical communications needs by NASA in 2005, because of their low weight, size, and high average power combined with good beam quality. However, the YDFs will face a harsh ion radiation of various types (such as proton, electron, X- and γ-ray) during their space mission. The radiation-induced darkening (RD), mainly due to the generation of color centers at the microscopic scale, can seriously deteriorate the laser performance of YDF. In this report, three aspects will be covered [1]. First, the space radiation environment, and the challenges that optical fiber will face in space will be briefly introduced. Second, the nature, generation mechanism of color centers responsible for RD in YDFs will be reviewed. Finally, five methods to inhibit RD and their inhibition mechanism will be introduced systematically.

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Theory-guided Design and Synthesis of Emerging Luminescent Materials

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Abstract: Luminescent materials play an important role in our daily life and are intimately linked with a wide range of forefront research fields. Design and synthesis of novel luminescent materials are thus far largely the results of trial and error, which signifcantly slows down the discovery of emerging systems with desired properties. Theoretical calculations can provide deep insights into the underlying mechanisms in various functional materials, and have gradually been recognized as a powerful approach to accelerating the discovery of emerging systems. In this talk, I will introduce our works in the field of theory-guided design and synthesis of emerging luminescent materials. Specifically, I will show how theoretical calculations enable us to obtain highly luminescent halide perovskite nanocrystals that cannot be achieved through trial-and-error experiments [1], followed by talking about theory-guided defect tuning for accelerated discovery of UVC persistent phosphors [2].

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Thermal-induced Ion Migration in Solids: An Optical Perspective with Rare-earth Luminescence

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Abstract: Thermal-induced ion migration/diffusion in solids not only affects the preparation, processing and performance of materials, but also is one of the essential factors to dominate the device lifetime, particularly for the materials used in the high power lasers and high power laser-driven displays. The ion migration in solids induced by thermal effects in device or upon laser irradiation is random and short-ranged, the process of which is strongly correlated with the point defects. All the available equipments or methods are not able to characterize the thermal-induced ion migration behavior in the optofunctional materials in a facile and *in situ* way. This report reviews the method of using the rare-earth luminescence to investigate the ion migration behavior and the microstructure change in the rare-earth doped optofunctional materials. Generally, the intensity pairwise ratios of the emission peaks of Er^{3+} versus temperature show a continuous but not derivable behavior with a break point (the ignition point of ion motion), which is analogous with the behaviours of thermal properties and the deduced configurational entropy.

Ultrathin Metallic Gap-enabled Extreme Nanophotonics

Pan Wang

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Abstract: Ultrathin metallic gap-based plasmonic nanocavities can provide extreme confinement and enhancement of optical fields, and have attracted great research interests recently. In this talk, I will first introduce high-quality nanoparticle-on-mirror plasmonic nanocavities based on ultrasmooth single-crystalline gold microflakes and their integration with optical fibers [1]. Then, by constructing tunnel junctions on the top of high-density Au nanorod array, we demonstrated large-scale and efficient electrical launching of surface plasmons in the metamaterial based on inelastic electron tunneling, which as well results in an eye-visible light emission due to the radiative decay of the plasmonic modes [2]. By engineering the geometrical parameters of the metamaterials, we can tune the tunneling-induced emission throughout the visible and near-infrared spectral range [3]. Moreover, by harvesting the simultaneously generated hot electrons from the elastic tunneling process, we show that the light emission can be dynamically modulated due to the hot-electron-activated chemical reactions in the highly confined junctions [2,4]. Therefore, ultrathin metallic gaps with the capability of extreme electric and optical confinement can significantly enhance light-matter interactions, and will find promising applications in fundamental researches as well as in developing optoelectronic devices with small size and high performance.

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Upconversion Emission Properties and Applications of RE^{3+}: $Y_nO_{n-1}F_{n+2}$ Nanocrystals Embedded Glass-ceramics

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Abstract: Rare-earth doped nanocrystals embedded oxyfluoride glass-ceramics combines the advantages of nanocrystals and glass, providing multiple environments for rare-earth dopants and leading to many interesting optoelectronic properties. In most oxyfluoride glass-ceramics, fluoride nanocrystals frequently precipitated, since they can provide low-phonon energy environment for rare-earth ions. In this work, rare-earth doped oxyfluoride nanocrystals, i.e., $Y_nO_{n-1}F_{n+2}$ nanocrystals are successfully precipitated in oxyfluoride glass-ceramics. It is found that both structures and shapes of these oxyfluoride nanocrystals can be controlled by the doping concentration of rare-earth ions, resulting in the controllable formation of spherical and rod-like nanocrystals. The particular structure of these oxyfluoride nanocrystals provide multiple doping sites for rare-earth ions and particular Stark splitting of rare-earth ions, leading to every efficient upconversion emission in the visible and ultraviolet spectral range. Based on these efficient upconversion emission properties of RE^{3+}: $Y_nO_{n-1}F_{n+2}$ nanocrystals embedded glass-ceramics, their potentials towards optical thermometry and infrared-driven sterilization will be discussed in this talk.

Rare earth Doped Upconversion Luminescent Oxyfluoride Glass Ceramics: Microstructure Study Using Advanced Solid-state NMR Spectroscopy

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Abstract: Rare earth doped oxyfluoride glass ceramics have wide promising application in three-dimensional display, solar energy conversion, white light-emitting and so on due to their high efficiency upconversion luminescence properties. The luminescent properties of rare earth doped glass ceramics are closely related to the microstructure of glass, the distribution of rare earth ions, and the crystallization of fluoride. We will report the glass structure at atomistic scale characterized using advanced solid-state NMR technology, including the changes of glass structure with composition and the evolution of glass microstructure during the precipitation of various fluoride crystals. On the atomistic scale, the micro crystallization mechanism, the role of various elements in the fluoride crystallization, and the distribution of rare earth ions in glass ceramics are reported. Finally, we reveal the internal relationship between compositions, microstructure, crystallization and luminescent properties, and propose the composition design strategy of rare earth doped glass ceramics for upconversion luminescence.

Keywords: rare earth doped glasses, solid state nuclear magnetic resonance, and luminescence

Luminescent Nanocrystal-doped Glass and Fiber

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Abstract: Near/mid-infrared fiber lasers have attracted significant attention due to their widespread applications in remote sensing, environmental monitoring, laser processing, and so forth. Combining the merits of the low phonon nature of fluoride nanocrystals and the excellent fiber-drawing ability of the oxide glass matrix, nanocrystal-doped glasses have been considered as potential candidates for rare-earth-doped fiber lasers. Herein, the nanocrystal-doped glass fibers are fabricated by the modified melt-in-tube fiber-drawing method, which provides an ingenious way to break through the bottleneck problem of uncontrollable rapid growth of nanocrystal existing in traditional fiber-drawing method. Thermal and optical properties between fiber core and cladding glasses are well matched, which ensure that the structure of the precursor fiber is well preserved during the fiber-drawing process. The obtained nanocrystal-doped glass fibers with excellent optical properties and well-preserved structure are expected as potential gain materials for near/mid-infrared fiber lasers. Importantly, we have obtained enhanced near/mid-infrared laser output in nanocrystal-doped glass fibers, strongly manifesting that the obtained nanocrystal-doped glass fiber is a promising gain fiber material.

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Development and Fabrication of Multispectral Chalcogenide Glasses

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Abstract: Due to advances in detection/acquisition systems, spectral measurement, and data processing, multispectral imaging technology has experienced rapid development over the past decade. It brings many new applications to the commercial and defense sectors.The so-called multispectral imaging system currently requires optical materials transparent from visible light to critical thermal windows. These multispectral materials would simplify the design of cameras that currently rely on several discrete optical elements to perform thermal and visible imaging at these wavelengths. The traditional lens materials used for multispectral imaging are the crystalline materials of ZnSe and ZnS, which are difficult to produce large-size samples through vapor deposition. Finding a multispectral lens material with the capability of large-size fabrication, high cost performance and easy to process has become an inevitable choice for the popularization of multispectral imaging technology. This work is to develop large-size (Φ>100 mm) multispectral chalcogenide glass transparent from 0.6 to 12 μm. A new method of three-stage thermal analysis is developed for evaluating and screening the glass composition suitable for large-size fabrication (Figure 1). And partial substitution of S by Se results in a novel chalcogenide glass sample transmitting from 0.6 to 12 μm and retaining the ability for large-size fabrication.

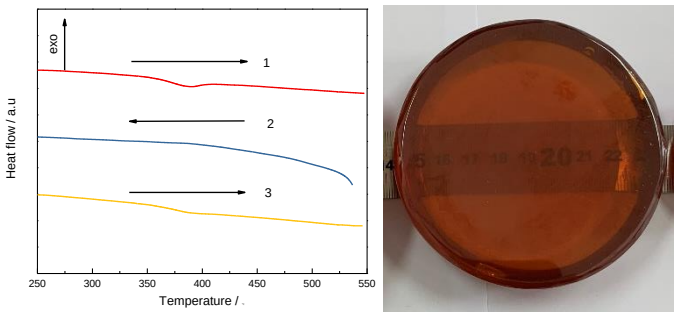

Figure 1. Three-stage DSC analysis and large-size (Φ100 mm) multi-spectral chalcogenide glasses.

Session 6: Advanced Nanomaterials and Nanotechnology

Characteristics of Composite Materials Based on a Modified SPEEK Matrix and Fe@MWCNT-OH Carbon Nanotubes and Their Potential Application in CO2 Separation

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Abstract: The development of industry and civilization causes an increased demand for energy, which in turn results in an increase in fuel combustion and CO_2 emissions. Unfortunately, CO_2 accumulation is responsible for global warming and major climatic changes. Therefore, further action should be related to the reduction of greenhouse gas emissions, which can be achieved by using various strategies such as reducing energy demand, implementing cleaner energy sources, capturing, storing, or sequestering CO_2 and using CO_2 as a raw material. CO_2 separation can be carried out by various conventional methods, however most of them are very energy-consuming and expensive. A real alternative to them can be membrane techniques, based on the latest type of hybrid membranes, combining the advantages of both organic and inorganic membranes. The authors in the above work propose a new type of inorganic-organic hybrid materials Fe@MWCNT-OH/SPEEK (with a new type of CNTs characterized by increased iron content 5.80wt.%). It was found that the introduction of nanofillers into polymer matrix has significantly improved hybrid membrane's gas transport (D, P, S, and $\alpha_{CO2/N2}$), magnetic, thermal, and mechanical parameters. It was stated that magnetic casting has improved the alignment and dispersion of Fe@MWCNT-OH carbon nanotubes. At the same time, CNT's and polymer chemical modification enhanced interphase compatibility and membrane's CO_2 separation efficiency. The thermooxidative stability, mechanical and magnetic parameters of composites were improved by increasing new CNTs loading. Cherazi's model turned out to be suitable for describing the CO_2 transport through analyzed hybrid membranes.

Design of Polymeric Nanoparticles Based on Hydrophobized Pullulan with Application in Cancer Therapy

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Abstract: Pullulan is a microbial exopolysaccharide with biocompatible, biodegradable, nonmutagenic, nontoxic, noncarcinogenic, and nonimmunogenic properties. Even though pullulan presents remarkable features it cannot self-associate in aqueous solutions due to its high solubility in water; functionalization can be applied to widen its applicability. The main aim of this paper was to design polymeric nanoparticles with application in cancer therapy using pullulan acetate as a hydrophobized form of pullulan and curcumin as an anticancer drug. Pullulan acetate was obtained by chemical functionalization of pullulan produced through a fermentation process by Aureobasidium pullulans strain. Polymeric nanoparticles loaded with curcumin were prepared by using the nanoprecipitation method. The pullulan nanoparticles loaded with curcumin were characterized in terms of entrapment efficiency, size, polydispersity, and stability. The curcumin-loaded nanoparticles showed good entrapment efficiency of curcumin, nanometric sizes, and narrow polydispersity index. The pullulan nanoparticles loaded with curcumin were stable for at least three months, with approximately the same amount of drug entrapped after three months of storage. This work was supported by the Ministry of Research, Innovation and Digitalization project PN 1941-04 01.

Hybrid Organic/Inorganic Chalcogenides Based Conductive Materials: Synthesis, Characterizations and Performances

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Abstract: Hybrid organic/inorganic chalcogenides refer to materials constructed with organic ligands bearing thiol (or selenol) units and metal ions, in which continuous 1D, 2D or 3D M-X (M: metal ions, X: S or Se) chains or networks are formed. M-X chains and networks provide the path for efficient charge transport, organic subunits provide the potential for tuning the electronic structure and corresponding electrical performance, and all these factors make hybrid organic/inorganic chalcogenides find applications in energy conversion and storage, electrocatalysts, chemiresistive sensors and so on. Besides these practical applications, conductive CPs display fascinating features in more fundamental areas, such as spintronics, superconductors, quantum materials, and topological insulators.Recently, we have constructed a series of hybrid organic/inorganic chalcogenides based on benzenehexathiol (BHT) and its analogues. Besides the developing of synthesis method, structure characterization, their potentials as thermoelectric materials and electrocatalysts have been explored. Superconductivity was also found in one of the most conductive materials Cu_3BHT.

Intrinsic Nanostructure Induced Ultralow Thermal Conductivity in Eu_2ZnSb_2 Zintl Phase Thermoelectric Materials

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Abstract: The Zintl phase Eu_2ZnSb_2 has a remarkable combination of high mobility and low thermal conductivity that leads to excellent thermoelectric performance. The key feature of this compound is a crystal structure that has a Zn-site with a 50% occupancy. The intrinsic phonon–phonon interactions with rattling behavior, low bulk modulus, and scattering from disorder on the Zn sublattice lead to the ultralow lattice thermal conductivity of Eu_2ZnSb_2. Here we use comparison of experimental thermal conductivity measurements and first principles thermal conductivity calculations to characterize the thermal conductivity reduction. We find that partial ordering, characterized by local order, but Zn-site disorder on longer scales, leads to an intrinsic nanostructuring induced reduction in thermal conductivity, while retaining electron mobility. This points the way to a new mechanism that can be applied to Zintl phase materials, particularly the design of systems with disorder on one sublattice, but a local ordering tendency that produces different behavior on different length scales, effectively an intrinsic bulk nanostructured material.

Investigation on the Stability of Liquid-like Thermoelectric Materials and Modules

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Abstract: Recently, the application of superionic conductors with liquid-like sublattice has been extended to the field of thermoelectrics. Extremely high thermoelectric figure of merit with the maximum $zT > 2.0$ have been observed and reported in a large family of novel Cu- and Ag-based liquid-like materials. However, despite the high performance, the stability and reliability of these liquid-like materials are key concerns for long-term service in the real applications. In this study, through systematically investigating the behavior of various liquid-like materials in an electric field or thermal gradient, we reveal the relations of atom migration, deposition, and material's degradation. A general model is proposed to reveal the threshold for decomposition of liquid-like materials to prevent metal deposition upon atom migration. It is found that each liquid-like material has a threshold for metal deposition, named as the critical voltage. When the voltage stressed on the material is lower than the V_c, the mobile ions just form a steady concentration of gradient inside the material without any deposition. In this case, the liquid-like materials will demonstrate similar good stability with the traditional stable materials. With these understanding, a new strategy is proposed to design the stable and efficient TE modules based on liquid-like materials via geometry and interface optimization. By using this strategy, a TE module based on Cu_2Se with both good stability and high energy conversion efficiency up to 9.1% was successfully achieved.

Molecular Engineering and Application Exploration of Antiadhesion Coating Surfaces and Interfaces

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Abstract: Antiadhesion coating materials have promising applications in various fields such as crude oil pipelines and artificial blood vessels. However, the widely concerned Teflon as well as the lotus- and nepenthes-inspired antiadhesion coatings are plagued with insufficient performance or durability, or unscalable process that restrict their industrialization. We have proposed the conceptional different idea of molecular engineering at soft and flat coating surfaces and interfaces through which to tackle issues associated with crude oil and blood adhesion, creatively introduced liquid silicon and fluorine antiadhesion functional molecules into industrial polymer systems, achieved the coexistence of key parameters for flat coating materials (such as antiadhesion performance against crude oil and blood, high stretchability, transparency, and recyclability), and has industrialized several antiadhesion resins. Currently, the author has presided over 12 scientific research projects such as the National Natural Science Foundation of China and several enterprise cooperation projects, published 48 SCI papers in journals such as AIChE Journal, held 16 granted patents, given 12 invited and oral presentations at international and national academic conferences, and has been awarded as a Pearl River Scholar of Guangdong province. We wish that our research will provide important theoretical, material and technological bases for the development of molecular engineering of antiadhesion coating surfaces and interfaces.

A Keggin-type Polyniobate Bonds on Ti-containing Metal-organic Framework MIL-125(Ti) for the Separation and Purification of Cytochrome C in Porcine Heart

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Abstract: A novel composite Nb_6O_{19}@MIL-125(Ti) was obtained which a Keggin-type polyniobate ($K_7H[Nb_6O_{19}]\cdot 13H_2O$]) bonded on ti-containing metal-organic framework MIL-125(Ti) by intermolecular hydrogen bonding. It was successfully confirmed by characterizations with FT-IR, EDS, SEM, TEM and TGA. The experimental of protein adsorption showed that Nb_6O_{19}@MIL-125(Ti) composite had selective adsorption for cytochrome c by electrostatic interaction and hydrogen bonding. At pH10.0 (BR buffer), the maximum adsorption efficiency of 300 μL 100 $\mu g\cdot mL^{-1}$ cytochrome c on 1.0 mg Nb_6O_{19}@MIL-125(Ti) composite was 99.5%. The adsorption behavior of cytochrome c onto Nb_6O_{19}@MIL-125(Ti) composite corresponds to Langmuir adsorption model and the maximum theoretical adsorption capacity is 168.35 $mg\cdot g^{-1}$. By using 3 $mol\cdot L^{-1}$ NaCl to strip the adsorbed cytochrome c on Nb_6O_{19}@MIL-125(Ti) composite, an elution efficiency of 92.19% is achieved. In addition, the application of Nb_6O_{19}@MIL-125(Ti) as sorbent in porcine heart samples has been investigated by sodium dodecyl sulfate-polyacrylamide gel electrophoresis (SDS-PAGE) analysis, and the result showed that cytochrome c was successfully isolated and purified.

Bioinspired Nanofluidic Materials: Ions Transport Based Energy and Sensory Systems

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Abstract: All biological systems including animals and plants communicate in a language of ions and small molecules, while our modern information infrastructures and technologies rely on a language of electrons. Although electronics and bioelectronics have made great progress in the last several decades, they still face the disadvantage of "signal transformation" when communicating with biology because both sides speak "different languages". To narrow the gap between biological systems and artificial intelligence systems, bioinspired ion transport-based sensory and energy systems should be developed as the successor of electronics because they can emulate biological functionality more directly and communicate with biology seamlessly. Our work interests mainly focus on the fabrication of novel nanofluidics and the realization of biological-inspired ion transport properties. The work interests are to learn from biological nanoionics, construct artificial nanoionics, and build a bio-artificial hybrid nanoionics system, able to realize seamless signal transduction between external stimuli, responsive artificial machines, and biological systems.

Antimicrobial Biodegradable Polymeric Implants

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Abstract: Our study focused on the long-term degradation under simulated conditions of coatings based on different compositions of polycaprolactone-polyethylene glycol blends (PCL-blend-PEG), fabricated for titanium implants by a dip-coating technique. The degradation behavior of polymeric coatings was evaluated by polymer mass loss measurements of the PCL-blend-PEG during immersion in SBF up to 16 weeks and correlated with those yielded from electrochemical experiments. The results are thoroughly supported by extensive compositional and surface analyses (FTIR, GIXRD, SEM, and wettability investigations). We found that the degradation behavior of PCL-blend-PEG coatings is governed by the properties of the main polymer constituents: the PEG solubilizes fast, immediately after the immersion, while the PCL degrades slowly over the whole period of time. Furthermore, the results evidence that the alteration of blend coatings is strongly enhanced by the increase in PEG content. The biological assessment unveiled the beneficial influence of PCL-blend-PEG coatings for the adhesion and spreading of both human-derived mesenchymal stem cells and endothelial cells.

Combined Defect, Interface and Structure Engineering in Nanofibrous Catalysts for High-Efficiency Electroreduction of N_2

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Abstract: NH_3 plays an important role in enriching our lives since it vitally participates in modern agricultural, pharmaceutical, and plastic industries. The fixation of N_2 in the atmosphere is essential to the NH_3 synthesis, which is a challenging task since it requires an extremely high energy to break the inert N≡N bond (940.95 kJ mol^{-1}). As such, the century-old Haber–Bosch process for the artificial N_2 fixation depends on harsh reaction conditions (300–550 °C, 200–350 atm), which lead to huge energy consumption. Besides, the excessive consumption of fossil fuels associated with this process leads to serious CO_2 emissions. In this circumstance, the electroreduction of N_2 stands out as one of the most promising candidates, since it can realize N_2 fixation under ambient conditions.

The key to the electroreduction of N_2 lies in the development of highly active and selective catalysts. Inherently, transition metals suffer from inferior selectivity due to fierce competition from H_2 evolution, while *p*-block metals exhibit poor activity due to insufficient "π back-donation" behavior. Considering their distinct yet complementary electronic structures, herein we propose an efficient strategy to tackle the activity and selectivity challenge through the atomic dispersion of *p*-block metal on a novel, all-amorphous transition metal matrix. Specifically, lotus-root-like, amorphous TiO_2 (a-TiO_2) nanofibers are synthesized for the first time, which are featured by large surface area and easy electrolyte infiltration. Besides, it is found that amorphization produces abundant O vacancies (V_O) in the whole bulk, endowing a-TiO_2 with enhanced N_2 activation and electron transport capacity. Moreover, well-isolated single atoms of Ga are confined within V_O, enabling selective N_2 adsorption at the catalyst surface due to suppressed H_2 evolution.

Stability and safety also play important roles in the design of catalysts. The traditional particulate nanomaterials exclusively exist in the powder form, which may cause health risks and environmental hazards. To overcome these shortcomings, we report a novel, highly elastic bulk form of TiO_2 for safe use and easy recycling. Specifically, TiO_2 nanofibrous aerogels (NAs) consisting of resiliently bonded TiO_2 nanofibers are constructed, which are featured by ultralow bulk density, ultrahigh porosity, and excellent elasticity. Profited by combined defect, interface and structure engineering, the TiO_2 NAs serve as high-efficiency catalysts towards the electroreduction of N_2, delivering high NH_3 yield and Faradaic efficiency comparable to, or even better than those of noble-metal-based catalysts.

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Conducting Polymer/Carbon Nanotube Thermoelectric Composites

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Abstract: Thermoelectric (TE) materials are vital for inter-converting heat and electricity in a green way. The formation of composites consisting of single-walled carbon nanotubes (SWCNTs) and conducting polymers (CPs) overcomes numerous disadvantages inherent in inorganic TE materials and organic TE materials, hence benefiting the manufacture of wearable electronics, vehicle-mounted refrigerator, *etc*.

Herein, polypyrrole (PPy), polyaniline (PANI), and poly(3,4-ethylenedioxythiophene) (PEDOT) were composited with SWCNTs to form TE nanocomposites which possessed greatly enhanced power factors due to the tuning of polymerization parameters and the modification of SWCNTs. The PPy/SWCNT nanocomposites are super flexible, stretchable and mechanically stable, affording peak power factor (PF) of 21.7 ± 0.8 μW m^{-1} K^{-2} at room temperature. After chemical doping of SWCNTs with mixed acids of sulfuric acid and nitric acid, together with the preparation of PPy through electropolymerization of pyrrole, the room temperature PF of the nanocomposites jumped to 240.3 ± 5.0 μW m^{-1} K^{-2}.

The PEDOT/SWCNT nanocomposites prepared by dynamic 3-phase interfacial polymerization and subsequent physical mixing exhibited maximum power factor of 253.7 ± 10.4 μW m^{-1} K^{-2} at room temperature. By chemical doping of SWCNTs, the power factors of such composites can be further improved to even higher values, 350.0 ± 47.6 μW m^{-1} K^{-2} at room temperature and 510.2 μW m^{-1} K^{-2} at 412 K. Similarly, PEDOT/Te/SWCNT composites were prepared with room temperature PF of 169.8 ± 7.8 μW m^{-1} K^{-2}. After further improvement in the TE performance of such nanocomposite materials, they will be promising in the fields of self-powered electronics and wearable devices.

Construction of High-performance Electromagnetic Shielding Materials Based on Nano-carbon Fillers and Silicone Rubber

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Abstract: With the rapid progress of electronic technology, electronic devices are growing in number, getting smaller and more complex, and operated at higher speed, accordingly causing much increase of the electromagnetic interference (EMI). If no any measures are taken, the increased EMI may pose great adverse effects on device performance, human health, and surrounding environment. In this context, the EM shielding (EMS) materials achieve the rapid and persistent development. Compared with conventional metal-based materials, the polymer composite enhanced with the functional fillers is considered as a promising candidate for its excellent combination of many merits, including light-weight, low-cost, easy-to-fabricate, and anti-corrosion. [1,2] Among various fillers, the nano-carbon ones, particularly graphene (G) and carbon nanotube (CNT), have attracted great attention owing to their high aspect ratio together with prominent thermal/electrical conductivity and mechanical property.

As a meaningful attempt for the development of high-performance EMS materials, this report presented the design and preparation of several nanocomposites, based on nano-carbon fillers and silicone rubber, with excellent EMS performance. Despite the filler content down to only 0.6 wt%, the resultant composites still realize >30 dB of absorption-dominated (>90%) average EMS effectiveness in X-band and exhibit high elasticity, excellent fatigue durability, and good mechanical strength. [3-5] In other words, the composites simultaneously acquire the functions of EMS, environmental sealing, and vibration damping, being a typical structure-function integrated material.

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Development of Gold Nanoflowers and Quantum Dots Based Impedimetric Aptasensor for 3,4-Methyl enedioxy Methamphetamine (MDMA) Detection

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Abstract: The 3,4-Methylenedioxymethylamphetamine (MDMA) is a major drug that comes under the category of Amphetamine-like substances (ATS) and was initially used as appetite suppressor. But hallucinogenic and stimulant properties of this drug increased its misuse across the globe, which also has the risk of depression, insomnia, impulsive behavior, irritability, impaired cognition, arrhythmia, and ultimately death. Increasing graph of MDMA/ ecstasy abuse calls for reliable, rapid, economical, and on-spot detection assay, in which chromatography and spectroscopy-based techniques fail. With this aim, we have designed gold nanoflowers (AuNFs) and silicon quantum dots (SiQDs) based electrochemical aptasensor for direct MDMA detection in biological samples. In the present study, the sensing platform was sequentially fabricated with AuNFs and SiQDs which further characterized morphologically and electrochemically. Subsequently, MDMA-specific aptamer (*MDMA-Apt*) was covalently attached to SiQDs/AuNFs@Au electrode and impedance spectroscopy was performed. The SiQDs/AuNFs@Au electrode exhibited ~20 times higher electroconductivity and provided a large surface area in comparison to the bare electrode. The *MDMA-Apt*/SiQDs/AuNFs@Au exhibited an increase in impedance with increasing MDMA concentration in a wide linear range. The developed sensing platform also exhibited a low limit of detection along with excellent sensitivity, high precision, and stability. This aptasensor displayed excellent analytical performance in MDMA spiked urine samples, which will support their practical implementation in real-world use. This novel sensing device can be further used for other ATS-based recreational drugs determination in forensic science.

Flexible and Tough Thermoelectrochemical Cells for Low-grade Heat Harvesting

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Abstract: Traditional solid thermoelectric materials are far from satisfaction. Firstly, their application in low-grade heat harvesting is substantially hindered by the relatively low Seebeck coeffient (S_e) near room temperature (on the order of $\mu V\ K^{-1}$). Secondly, their mechanical rigidity, high cost and toxicity further hamper their development in flexible and wearable applications. While the booming of wearable electronics has stimulated the urgent demand for flexible, efficient and robust energy supply systems. Fortunately, Thermoelectrochemical Cells (TECs) offer a cost-efficient and scalable route for direct heat-to-electricity conversion based on thermogalvanic effect. A TEC comprises two electrodes and an electrolyte containing a redox couple, providing a much higher S_e compared to traditional solid thermoelectrics (on the order of $mV\ K^{-1}$). By taking the advantage of hydrogel electrolytes, the problems of electrolyte leakage and complicated packaging issues that exist in conventional liquid-based TECs can be addressed. Herein, we utilize Fe^{3+}/Fe^{2+} redox couple to simultaneously regulate the thermoelectrochemical performance and mechanical robustness of flexible quasi-solid-state TECs. The hydrogel electrolyte constructed in this work demonstrates a high thermoelectrochemical S_e together with an impressive fracture toughness at the optimized Fe^{3+}/Fe^{2+} concentration, thus exhibiting stable thermoelectrochemical performance against various harsh mechanical stimuli. The flexible quasi-solid-state TEC based on the mechanically robust hydrogel electrolyte offers a novel route to promote the development of wearable electronics.

Graphene/Gold Nanoparticles Electrochemical Enzyme Biosensor

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Abstract: Organophosphorus (OPs) pesticide used as insecticides are widely used in agricultural pest control, household and storage deworming. The detection of pesticides needs more simple and efficient methods. One of the best ways is to make electrochemical enzyme biosensor. Acetylcholine esterase (AChE) can be used to detect organic phosphorus in the environment. Based on strong specific biometric components and high sensitivity electrochemical analysis techniques, electrochemical acetylcholinesterase sensors were constructed, and their sensing properties and sensing mechanisms were studied. RGO-PDA and AuNPs and AgNPs nanomaterials were prepared first and then characterized by UV-Vis, SEM and TEM. The nanomaterials and AChE were composited and fixed on the GCE surface to construct the sensor GCE/RGO-PDA-AuNPs-AgNPs-AChE-CS in the presence of CS to optimize the structure and test conditions of the sensor. The results show that the sensor can achieve a detection limit of 9.1 pM for methyl parathion and a wide linear detection range of 76 pM~3.04 μM, indicating that the sensor has practical value. The results show that the electrochemical acetylcholinesterase sensors have excellent stability, good anti-interference ability and excellent preservation performance.

High Performance Conductive Nanocomposite Hydrogels for Monitoring Organ Motions

Jun Fu

Sun Yat-sen University

Abstract: Hydrogels have been important candidate materials for wearable and implantable flexible electronics. For implantable applications, both high sensory performances and device-tissue interface are critical for stable, reliable, and durable applications under complicated loadings or movement. It is desired to prepare conductive hydrogels with high conductivity, linear sensing behavior, and broad working range. On the other hand, tissue adhesive hydrogels are needed to form a robust hydrogel-tissue adhesion.

In this talk, recent progress in nanocomposite hydrogels with outstanding conductivity and sensory performances are presented. Structure designs at the molecular level and micro-scale are performed to significantly improve the mechanical properties, conductivity, and sensory performance of the hydrogels. Conductive polymer/hydrophilic polymer double network hydrogels are prepared to show a low percolation conduction at very low conductive polymer content, which provides a high conductivity and outstanding mechanical strength, toughness, and fatigue resistance. 3D printed structures further enhance the sensitivity. Moreover, zwitterionic moieties and dopamine are used to entitle robust adhesion between hydrogels and biotissues or organs. Organ motions are monitored by using the high performance and adhesive conductive hydrogel sensor through remote transmission.

Highly Compressible Thermoelectric PEDOT-Tos/SWCNT Hybrid Aerogel Generator for Thermoelectric Application

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Abstract: The aerogel has been regarded as a promising thermoelectric (TE) candidate with a large surface area and high porosity that can significantly suppress thermal conductivity and hence improve TE performance. However, the aerogel is rarely assembled into TE generators (TEGs) to harvest heat. Herein, we report the TE performances of an elastic TEG assembled with vertical-type architectures consisting of poly(3,4-ethylenedioxythiophene)-tosylate (PEDOT-Tos)/single-walled carbon nanotube (SWCNT) aerogels. The present TE aerogel was prepared by chemical oxidative polymerization, physical mixing, and subsequent freeze-drying process. The assembled TEG not only inherits the merits of ultralight weight and compressibility of aerogels, but also displays significant enhancement of TE performance with compression strain. The TEG has a maximum output of 1967 nW with 10 aerogel legs, a temperature difference of 50 K and a compression strain of 50%. In addition, the TEG shows unique heat harvesting capability under vertical temperature differences in versatile application scenarios (such as hot oil, flat plate and human foot as a cushion).

Improved Methods of Silver Nanoparticles Biosynthesis Using Laggera Crispata (Vahl) Hpper and J.R l Wood Leaves Extract, Characterization, and Application

Bulcha Belay Etana

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Abstract: In this research work we chosen a simple approach for the synthesis of AgNPs using Laggera crispata (Vahl) Hpper and J.R l Wood, leaves extract for reducing and stabilizing agent of silver nano particles for textile electrode application. Laggera crispata (Vahl) Hpper and J.R l Wood, isolated from Jimma University ,Jimma institute of technology (JiT) around work shop center ,Jimma ,Oromia,Ethiopia , has promising ability when synthesized with silver nanoparticles. We have developed a rapid, single-step, cost-effective and eco-friendly method for the synthesis of AgNPs using aqueous leaves of (Laggera crispata (Vahl) Hpper and J.R l Wood) extract at room temperature. The AgNPs began to produced just after the reaction was initiated. Leaves of Laggera crispata (Vahl) Hpper and J.R l Wood were collected and washed by tap water and rinsed with distilled water to remove dusts from the surfaces of leaves not to contaminated the aquas extract that used as reducing and stabilizing agent. 500 mL of DI water was added to the washed leaves and mixture was exposed water bath for 20 min at 60 C. Different amount of plant extract was added dropwise to silver nitrate solution of 100 mL, 200 mL, 300 mL to 0.3 mM aqueous solution of silver nitrate (AgNO3). The reaction was kept overnight until incubation Ag^{+} ions in AgNO3 solution were reduced to Ag atoms by the extract. Silver nanoparticles were obtained in powder form and the precipitated solution have been centrifuged. All reaction has been done at room temperature. and comparatively analysed using Match3 soft analysis from XRD result. Synthesis of colloidal AgNP was controlled by UV-Visible spectroscopy, The UV-Visible spectrum showed a peak between 350 and 600 nm corresponding to the Plasmon absorbance of the AgNPs were used for characterization of synthesized silver nanoparticles whereas XRD investigation confirmed the presence of Ag^{0} in the nanoparticles, and interactions between the bioactive compounds of the plants and the produced AgNPs were evident in the FTIR spectra. FTIR is used for determination of the bonds starching vibration present in the AgNPs. Size of the AgNPs crystallites were determined using powder X-ray diffraction (XRD) pattern of the prepared sample using Match3 software analysis. Three peaks have been identified corresponding to (hkl) values of silver. The XRD study confirms that the resultant particles are silver nanoparticles having FCC structure. The average crystalline size D, the value of the interplanar spacing between the atoms, d, lattice constant a and cell volume V have been estimated using match3 software licensed by Dr. Parabal Dasgupta. Thus, silver nanoparticles with well-defined dimensions could be synthesized by reduction of metal ions using plant extract while FTIR analysis of AgNPs shows its stability after storage and no noticeable change in peaks location was observed. Size of the AgNPs lies in range ranged from 38 to 100 nm.

Ionic Liquid-Modulated PEDOT:PSS-based Thermoelectric Composites

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Abstract: In the recent decade, polymer thermoelectric (TE) composite has achieved significant progress in harvesting low-quality/waste heat. Intrinsically conducting polymers, such as poly(3,4-ethylenedioxythiophene) (PEDOT), polypyrrole and polyaniline are usually selected as the organic polymer components of composites, in which PEDOT is perhaps the most successful one with the high TE performance and the commercial availability in the form of PEDOT:polystyrenesulfonate (PSS) solution. Herein, the synergistically boosting TE properties of PEDOT:PSS/single-walled CNT (SWCNT) composites by the ionic liquid (IL) are reported. The IL additive has two major functions, i.e. inducing the phase separation of PEDOT:PSS and a linear quinoid conformation of PEDOT and promoting the SWCNT dispersion. The maximum power factor reaches 182.7 ± 9.2 μW m^{-1} K^{-2} for the flexible PEDOT:PSS/SWCNT film with the IL at room temperature. Besides, polyvinyl alcohol (PVA) is added to the PEDOT:PSS/SWCNT system with IL to modulate the mechanical performance. The resultant PEDOT:PSS/PVA/SWCNT composite shows a high TE performance with a power factor of 106.1 ± 8.2 μW m^{-1} K^{-2} at room temperature, and strong mechanical robustness with a tensile modulus of 4.2 ± 0.5 GPa and fracture strength of 136.5 ± 10.6 MPa. The present study provides a promising way to enhance TE performance and help address the inferior mechanical performance of TE composites without significantly compromising TE performance for PEDOT:PSS-based TE composite.

Metallic Nanoparticles from Plant Extracts: a Green Alternative to Conventional Synthesis

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Abstract: Green synthesis has become a suitable alternative to conventional synthesis of metallic nanoparticles due to its environmental and economic benefits. Compared to classic chemical and physical methods, green synthesis is cost-effective, reproductible and the resulted metallic nanoparticles are in most cases more stable than those obtained via classical routes. This method involves the use of microorganisms or different plant extracts in a one-pot reaction that does not require toxic catalysts and no hazardous by-products are formed. Therefore, numerous researchers are shifting to this green alternative especially since plants and their aqueous extracts are able to form even more stable metallic nanoparticles than their conventional or microorganisms' counterparts. This research paper presents the green synthesis of silver (AgNPs), gold (AuNPs) and iron oxide (magnetite, FeONPs) nanoparticles from the aqueous extracts of different medicinal plants such as: Elderflower (Sambucus nigra), Cornflowers (Centaurea cyanus), Sea buckthorn (Hippophae rhamnoides), Lungwort (Pulmonaria officinalis) and Ramson (Allium ursinum). All the aqueous extracts are analysed by means of qualitative assays of different phytocomponents and quantitative spectrophotometric determinations of total content of phenols, flavonoids, tannins, terpenoids and carotenoids. The kinetics of all three metallic nanoparticles is investigated using UV-Vis recordings at different time intervals and the presence of functional groups is studied via FTIR techniques. In order to determine the size distribution of the colloidal metallic nanoparticles, dynamic light scattering (DLS) is used and, also, the zeta potential is recorded for all the studied samples. Also, studies concerning the ability of AgNPs and FeONPs in the degradation of different azoic dyes are undertaken and the potential antimicrobial capacity of AgNPs and AuNPs is studied.

Microfluidic Flow Synthesis of Mesoporous Metal-Organic Frameworks with Structural Defects

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Abstract: Metal-organic frameworks (MOFs), composed by metal ions/ion clusters and organic ligands, have attracted considerable attention from both research and industry community as a class of highly porous and ordered crystalline materials since emerged in 1990s. Variable compositions and structures endow MOFs with different morphology, size, and chemical properties. Nevertheless, defect engineering opens up opportunities to tailor unique features due to the defective structures-induced mesopores, and thus extends their applications, like improved adsorption capacity, and enhanced catalytic activity.1,2 However, the synthesis of mesoporous MOFs via controllable creation of defects on the parent MOFs is still challenging. In the present study, we use microfluidic laminar flow synthesis to introduce structural defects into MOFs, generating mesopores in MOFs. During the synthesis on-chip, the mixing of metal ions and organic linkers is stream-stream diffusion-dependent because of the laminar flows in the microfluidic channel. Under such continuously changed gradient concentration of MOF precursors, the resultant MOF products, zeolitic imidazolate framework (ZIF-8), exhibited structural defects and mesopores, compared with microporous crystal MOFs produced by conventional bulk solution synthesis approach. The defective structures and mesopore size distribution were further characterized by the X-ray diffraction (XRD) analysis and the Brunauer-Emmett-Teller (BET) analysis. Moreover, the defect-induced mesopores can be tuned by adjusting the flow rate of MOF precursors infused into the microfluidic channels. This study provides a simple and convenient method for controllable production of mesoporous MOFs on the basis of defect-engineering.

N doped Fluorescent Carbon Dots for Sensing, Bioimaging and Light-emitting Diodes

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Abstract: Carbon dots (CDs) have attracted widespread attention in the fields of fluorescence sensors, bioimaging, drug delivery and optoelectronic devices applications due to their easy processing, environmental friendliness, superior stability and unique optical properties. Herein, N-doped carbon dots (N-CDs) with an average size of 2.3 nm were successfully prepared *via* one-step hydrothermal carbonization using citric acid (CA) and tryptamine (Try). The obtained N-CDs exhibited excitation-independent, excellent resistance to pH change, high ion strength, UV irradiation and high oxidant concentration. It was found that the as-prepared N-CDs presented a sensitive response to Fe^{3+} based on nonradiative electron-transfer. Meanwhile, they were successfully applied for Fe^{3+} bioimaging in A549 cells thanks to their good biocompatibility. Furthermore, a blue light-emitting-diode was fabricated through mixing the obtained N-CDs with epoxy on the surface of gallium nitride (GaN)-based LED chips. The as-prepared LEDs showed outstanding color rendering properties (CCT of 1961 K, CIE coordinates of (0.31, 0.33), and CRI of 83.7). This research shows that the N-CDs are promising materials in sensing, bioimaging and LED illuminations.

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Nano-sized Polymer Supports Immobilizing Mono(phenoxy-imine) Metal Complexes for Ethylene Polymerization

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Abstract: Polyethylene (PE) is the world's most widely used polymer. Commercial PEs are produced by using heterogeneous Ziegler–Natta catalysts and metallocene catalysts supported by inorganic particles such as silica, clay, and magnesium chloride. Although highly active, the residual inorganic components in the final polyolefin products may be detrimental to the polymer properties, such as mechanical and optical performances, compatibility during the plastic recycling, and so on. Organic supports do not require fastidious pre-treatment and have little effect on the final PEs properties. Tailor-made nano-sized polymer supports are highly appreciated not only for a pure polymeric final product but also for a rationalized polymerization process. Herein, we synthesized three nano-supports with different topological structures (polystyrene (PS) nanosphere, molecular bottlebrush, and PS single-chain) immobilizing mono(phenoxy-imine) catalysts (FI catalysts) for ethylene polymerization. First, phenoxy-imine ligand was covalently immobilized on the surface of functionalized PS nanospheres. Pressure sensitive supported FI catalysts with high catalytic activity were successfully prepared. PEs with bimodal and broad molecular weight distritutions were prepared in one pot by shifting the polymerization pressure. Second, molecular bottlebrush supports were synthesized using grafting-through method. It is found that the ligand structure significantly affects the catalytic activity, PEs molecular weight, and PEs morphology. Bimodal PEs were prepared in one pot by combining two different ligands in one molecular bottlebrush. And third, FI catalysts immobilized on linear PS nano-supports were used to prepared disentangled polyethylene nanocrystals.

Observations and Hypotheses: A Journey in Expanding the Structural, Functional, and Mechanistic Scope of Synthesis

Jin Zhu

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Abstract: Observations and hypotheses are the two fundamental pillars of modern science. This talk will present our synthetic efforts in broadening the spectrum of observations and hypotheses. This translates to the expansion of the structural, functional, and mechanistic scope of synthesis. Key observations made in polymer and materials synthesis include low-temperature depolymerization of vinyl polymer, highly deliquescent property of polymer, and solvent-driven organogel shrinkage. In organic synthesis, formalization of observations and formulation of hypotheses have been practiced. A relay formalism is introduced to categorize the transition metal catalysis mechanisms; transition metal catalysis can be perceived as a continuous relay of the catalytic center from product (donor) to one reactant (acceptor) and can proceed by either dissociative relay or associative relay mode; the dissociative relay refers to a process of passing an innocent catalytic center, in an intermediate product-released and reactant-free state, to one reactant (acceptor), whereas the associative relay involves the passing of a non-innocent catalytic center through the competitive release of product by one additional reactant (acceptor). A reactivity relay cascade formalism is proposed to delineate the reactivity site transfer process; a reaction can encompass either one reactivity paradigm, identified as a reactivity site relay trajectory featuring reactivity initiation to termination by a discrete closed suite of electron pushing pathways (from the perspective of electron pushing formalism, each prior electron pushing pathway acting as a necessary condition for the ensuing electron pushing pathway), or multiple reactivity paradigms accommodated into a consecutive reactivity paradigm relay trajectory (from the perspective of electron pushing formalism, each prior reactivity paradigm acting as neither a necessary nor a sufficient condition for the ensuing reactivity paradigm). A polarity relay concept is used to generalize the observations of polarity matching-mediated ring-closure transformations. A skeleton-oriented synthesis concept is devised as a complementary thought framework for efficient synthesis as opposed to target-oriented synthesis and diversity-oriented synthesis; skeleton-oriented synthesis refers to a traceless appendage planning synthetic strategy for constructing molecular skeletons, with unintended appendages from the reactivity-assisting groups eliminated, and utilizing the accessible reactivity of ring atoms for attaching intended appendages. Forward reactivity analysis is emphasized as a useful tool for streamlining the synthesis by the forward synthetic planning of synergism in reactivity of coupling partners in a consecutive reaction. In biological synthesis, a decentralized approach for the formulation of hypotheses is proposed. The centralized hypothesis formulation approach, which exploits a primary phenomenon to extract a dominant hypothesis, has monopolized scientific thinking and practice for centuries. The major flaw of this essentially ad hoc approach is that it can constrict the conceivable experimental boundaries, thwart quest for alternative legitimate hypotheses, and ultimately hinder understanding of the system of interest. In contrast, our decentralized approach operates through preconception-free phenomenon accumulation and parallel, reticular logical reasoning processes, thus offering an objective, inclusive view of the system and allowing the derivation of a set of more coherent and tenable hypotheses. Through this approach, a hierarchical model has been established for a prion self-assembled structure, enabling comprehensive insight into hitherto elusive static and dynamic aspects of this intriguing system.

Organic Thin Film Thermoelectric Material and Device

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Abstract: Thermoelectric device is one critical technique of energy harvesting from the environment. Flexible thermoelectric thin films have received increasing attention due to their ability to generate power in wearable electronics and internet-of-things (IoT) sensors. In this talk, synergistic enhancements in both the thermoelectric and mechanical performance of poly(3,4-ethylenedioxythiophene) (PEDOT)-based flexible thermoelectric thin films were obtained by utilizing the modulation effect of an ionic liquid (IL), i.e. bis(trifluoromethane) sulfonimide lithium salt (LiTFSI). The power factor increased from 1 $\mu W \cdot m^{-1}K^{-2}$ to 117 $\mu W \cdot m^{-1}K^{-2}$, while the strain increased from 5% to >35%. For the energy harvesting application, one of the challenges is to build up the temperature difference in conventional in-plane architecture. We get an idea from the condensation of dewdrops on the leaf tip and design a vertically free-standing leaf-inspired (leaf-TEG) by using the as-fabricated IL/PEDOT films. We proof-of-concept wearable 100-leaf-TEG (100 leaves, L = 10 mm) standing on silicone rubber substrate generated 1, 4, and 11 μW in the palm touching, mouth blowing, and arm wearing scenes in an indoor environment, respectively. The proposed leaf-TEG should be a promising candidate solution for thermal energy harvesting from the environment, particularly for scenarios with limited temperature differences and convection heat transfer conditions.

Rapid and Sensitive Aging Evaluation of Polyolefin Nanocomposites and Correlation to Natural Aging

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Abstract: Stability evaluation is very important for long-term performance of structural and functional polymer materials. However, it is still a challenge to correlate conventional accelerated aging behavior to practical appearance. A novel rapid and sensitive aging evaluation method of polymer materials was developed and an experimental apparatus was set up based on detection of trace gaseous degradation products (e.g. CO_2) at very early stage. Aging conditions such as UV irradiation, temperature, humidity and oxygen content can be adjusted to simulate various climates conditions. By this method, the stability of polyethylene (PE) nanocomposites and polypropylene (PP) nanocomposites was evaluated within hours, much shorter than general months or even years evaluation that needed for conventional aging evaluation. Natural exposure of PE and PP nanocomposites were also carried out. The results demonstrated a linear relationship between the generation rate of CO_2 by the new method and natural logarithm of the carbonyl index during natural aging. The effects of aging conditions and fillers were investigated. The activation energy was calculated and showed good correspondence to literature data. This method is proved to be a efficient and powerful tool for stability evaluation and lifetime prediction of polymer materials.

Session 7: Structure Materials and Application

Atomic Scale Study of Compositional and Structural Evolution of Early-Stage Grain Boundary Precipitation in Al-Cu Alloys through Phase-field Crystal Simulation

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Abstract: Grain boundary (GB) precipitation alters the compositional partitioning, interface structure and phase constitution in GB regions, thus affecting the chemical and mechanical properties of materials. Since continuum models cannot capture the atomic details of these phenomena and molecular dynamics cannot span the time scales required for precipitations studies, here, we use phase-field crystal simulations to study the atomic-scale structural and compositional evolution during GB precipitation in Al-Cu alloys. The composition evolution is dominated by solute segregation at the very beginning and then by confined spinodal decomposition which results in steep increase of concentration and the formation of disorder clusters at nucleation sites acting as the precursor of nuclei, just like in the bulk where decomposition and Gunier-Preston zones are the precursors of the Al_2Cu phase. We find that the clusters on low-angle GBs nucleate at the dislocations through local spinodal decomposition, while amplitude-modulated decomposition drives the formation of compositional precursors and subsequent nucleation on high-angle GBs globally, leading to distinct differences in the nucleation mode between low-angle and high-angle GBs. Interestingly, nucleation can be substantially promoted by rotating the GB plane from the symmetric position by a very small angle, especially for low-angle GBs. These results not only shed light on atomic scale early-state precipitation process and nucleation mechanism at GBs in Al-Cu alloy systems but also help to under the GB phase transformation in other alloy systems.

Multifunctional Mesoporous Carbon Materials Assambly from Nanoemulsion

Peng Liang

City University of Hong Kong

Abstract: Carbon-based mesoporous materials are popular mesoscopic structural materials, which have great application potential. This is mainly because mesoporous carbon materials not only have the properties of general mesoporous materials, such as adjustable pore size of 2-50 nm, large pore volume, high specific surface area, etc., but also have their own unique properties, such as light weight, rigid skeleton, good electrical conductivity and chemical stability. It has a broad prospect in catalysis, hydrogen storage, separation and electrochemistry. So far, many methods have been developed to regulate the morphology and structure of carbon-based mesoporous materials, including spraying, drip, Stober method, colloid assisted assembly, confined assembly and solid state reaction.However, the morphology and mesoscopic structure of mesoporous carbon nanospheres synthesized by the above methods still cannot meet the needs of the development of The Times.At the same time, the research on the synthesis mechanism of mesoporous carbon nanospheres is not profound enough, and the application research is also very limited.Therefore, it is of great significance to further develop a simple and feasible synthesis method to construct functional mesoporous materials, to conduct in-depth research on its synthesis mechanism, and to give full play to its application potential.After a long period of exploration, we found that the introduction of hydrophobic organic small molecules into micellar synthesis system, namely the construction of nano-microemulsion system, can give the synthesis method more powerful functions.Based on this idea, systematic studies have been carried out on the development and synthesis of novel mesoporous carbon materials, the design of novel morphologies, the regulation of mesoscopic structures and the functionalization of carbon skeletons.Meanwhile, the applications of these materials in energy storage and catalysis are studied.

Superlubricity of Fullerene Derivatives Induced by Host-guest Assembly

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Abstract: Fullerenes have been recognized as good candidates for solid lubricants. In this study, the microscale superlubricity of fullerene derivatives was accomplished by the construction of regular host-guest assembly structures. Herein, the host-guest assembly structures of fullerene derivatives were successfully constructed on a highly oriented pyrolytic graphite (HOPG) surface by introducing the macrocycles as the templates and were explicitly revealed by scanning tunneling microscopy (STM). Meanwhile, the nanotribological properties of the host-guest assemblies were measured using atomic force microscopy (AFM), revealing ultralow friction coefficients of 0.003-0.008, which could be attributed to the restriction on removal of fullerene molecules after introducing the templates. The interaction energies were calculated by density functional theory (DFT) method, which indicates the correlation between friction coefficients and interaction strength in the host-guest assemblies. The effort on fullerene-related superlubricity could extend the solid superlubrication systems and provide a novel pathway to explore the friction mechanisms at the molecular level.

Developing of Preceramic Paper-Derived SiCf/SiC Composites and Characterizing of Properties

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Abstract: Composites based on silicon carbide (SiC) as structural components are interesting for applications with high irradiance flux and high temperature conditions. The addition of SiC fibers can be used to reduce the density and to improve the mechanical properties. This work describes the processing and characterization of novel preceramic paper-derived SiC laminated composite with Hi-Nicalon SiC fibers fabricated by Spark Plasma Sintering. The content of fibers in the composites was 10 wt.%. The sintering temperature and pressure were 2100 ~ 2200 °C and 20 ~ 100 MPa, respectively. In sintering processing, the organic components in preceramic paper decompose and the SiC filler are sintered together with SiC fibers to form composites. In the small punch strength test, the loading curve of composite shows step-like fracture after reaching the highest loading point: the fracture mode of the composite materials exhibits quasi-ductility rather than pure brittleness. The nanoindentation indenter is pressed along the fiber axis in composites, and the hardness and elastic modulus of the fiber under different sintering conditions have almost the same values of ~ 38 GPa and ~ 420 GPa, respectively, which approaching to that of the original fiber. The results of microstructural analysis show that longer sintering time causes the increase of the proportion of the 6H-SiC; the higher sintering temperature (2200 °C) leads to partial transition of 4H-SiC to 6H-SiC during the sintering process, with observing of the long-life component of positrons corresponds to Si vacancies. The composite sintered at 2200 °C has the approaching S-parameter of Doppler broadening spectrum but significantly higher W-parameter, which is the contribution of anti-site defects C_{Si} formed by carbon atoms occupying silicon vacancies. Because high temperature sintering accelerates the diffusion of carbon atoms. The analysis of the difference in W-parameters can be confirmed by comparing the energy spectra or the ratio curve of graphite, SiC, and Si. The Raman characteristic peaks of turbostratic graphite appear in the fiber area, this is caused by the diffusion of carbon from the preceramic paper during the high-temperature sintering process. The S-parameter of the composite irradiated by Si ions at 400 °C reached the highest at 10 dpa, and then decreases with increasing dose, which exhibit to have recrystallized. For the composites pre-injected with 10 000 appm He, the S parameter increased with the increasing of Si ion irradiation dose, indicating that He combined with vacancy-type defects and inhibited the recovery of defects.

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Flexible Wearable Sensors Triggered by Liquid Metal for Environmental Acid Detection

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Abstract: Wearable flexible devices for monitoring acidic environments are essential for human health and environmental friendliness. However, how to demonstrate changes quickly and intuitively in acidic environment is more appropriate for practical applications. Herein, the acid visualization sensor triggered by gallium-based liquid metal (LM) was designed and fabricated. The sensor composed of the liquid metal fluid, tungsten trioxide sheet (WO_3), and the flexible substrate (PDMS) can achieve a fast yellow- blue color-switching when the acid spray contacts the WO_3-LM through the hole-columnar structure of the flexible substrate. The reaction mechanism is that there is a redox reaction between WO_3 and liquid metal at the presence of acidic condition, in which hydrogen ions (H^+) enter the lattice of WO_3 to generate hydrogen tungsten bronze heteropoly blue ($H_{0.23}WO_3$), and the color-switching increased with the increasing of concentration of hydrogen ions in the solution. Finally, a scenario for simulating different acidic environments and concentrations was established to illustrate the detection performance of the sensor. The experimental results showcased that the prepared sample can well realize the monitoring of different acid concentrations, which provides new possibilities for visual reminders and early warnings of acid environments.

High Static Magnetic Metallurgy and Processing of Metallic Alloys

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Abstract: Electromagnetic processing of materials has been developed for decades. During the solidification process of metallic alloys, their microstructure will be affected by the melt flow, the distribution of solute and phase, the evolution of solid-liquid interface morphology and the crystal orientation. The application of the high static magnetic field (HSMF) to control the microstructure in metallic materials has attracted more attention for its green, non-contact, strong magnetic orientation and high energy density. In our studies, we have successfully carried out solidification experiments under the HSMF up to 30 T. It is found that the melt convection and the phase segregation can be effectively suppressed in such a strong field. Such as, for Zn-Bi immiscible alloy, the HSMF can suppress the collision and coagulation between droplets in the immiscible gap as a result of micro-nano second phases homogeneously dispersed in the matrix. The directional solidification experiments of immiscible Zn-Bi alloy under a 5 T HSMF show that the HSMF was can improve the stability of the fibre by reducing the matrix/fibre interfacial energy. Besides, we also found that the HSMF can reduce the effective diffusion coefficient by suppressing the melt convection in Al-Cu liquid melt. As a result, the HSMF can effectively influence the growth kinetics of solid-liquid interface and modify the dendritic morphology.

Irradiation Hardening of the 304NG and 304L SS after the Triple Beam Irradiation

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Abstract: Types 304 SS suffers from inter-granular stress corrosion cracking (IGSCC) in boiling water reactors. Lower carbon 304L SS reduces IGSCC. By adding of nitrogen and further limiting the contents of phosphorus and sulfur impurities, the nitrogen-strengthened nuclear grade 304NG stainless steels (SS) have been developed in the past several decades as the new generation of internal structural materials in light water reactors. The irradiation effects of 304NG and 304L SS were simulated by the triple ion beam irradiation including the heavy ion, hydrogen and helium, with various doses and temperatures. The depth-sensing nanoindentation with the continuous multi-cycle measurement was employed to characterize the mechanical property changes due to the ion irradiation. It is observed that 304NG shows less hardening than 304L exposed to the same amount of irradiation damages. The dose and temperature dependence of irradiation hardening was discussed. The hardness generally increases with the increasing dose for the specimens irradiated at 300 °C, and the hardening decreases with increasing irradiation temperature. However, it seems the hardening of 304NG SS did not reaches the saturation even for the peak dose reaches 150 dpa. One possibility is that the implanted interstitial atoms with large concentration have a significant role in the hardening.

Metal-organic Frameworks (MOFs) for Superlubricity

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Abstract: According to statistics, the energy dissipated by friction accounts for more than one-fifth of the total primary energy in that year. Therefore, it is urgent to achieve energy efficiency by overcoming friction, and solid superlubricity technology is dedicated to reducing friction to negligible levels. Most of the reported microscopic friction mechanisms are related to the intrinsic structural parameters of lubricating materials, such as surface deformation capacity and surface adhesion. But conventional materials can't overcome these friction mechanisms at the same time. Inorganic materials have high surface stiffness, but it's high inherent surface energy cause strong surface adhesion. Polymer material has the characteristics of low surface energy, but its surface is easy to deform that lead to puckering effect. The emerging inorganic organic hybrid materials may have the advantages of both inorganic and organic materials, and metal-organic framework (MOFs) is a typical representative of this kind of materials. Our Friction Force Microscope (FFM) experimental results confirm that MOFs is a promising new generation of superlubricating materials, whose inorganic organic hybrid structure and microporous surface contribute to extremely low friction.

Numerical Study on UnequalLlateral Impact Behavior of CFRP Reinforced Concrete Square Members

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Abstract: Carbon fiber reinforced polymer (CFRP) sheets have been utilized to improve the impact resistance of reinforced concrete structures. The purpose of this study is to examine the response of CFRP reinforced concrete square members to an unequal lateral impact force. The drop-hammer impact test equipment was used to assess the impact performance of CFRP members. The significance of unequal lateral impact load was emphasized and addressed by determining CFRP members' failure mechanisms and dynamic response characteristics. A finite element (FE) modeling technique was developed and shown to predict the impact responses of CFRP members accurately. The influence of the number of CFRP layers, wrapping, impact location, height, and hammer mass on the dynamic response characteristics under an impact force was also evaluated. The numerical model's superior predictions regarding impact force history, deflection time history, and failure modes were verified by experimental findings, confirming the model's and parametric studies' validity. The experimental and numerical investigations may be used to help improve the impact resistance of structural elements.

Quantitative XRD Investigation of a First Order of External Applied Constraints Coupling on the Heavy Metal Cation Removal by Na Rich Montmorillonite

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Aims of the work: Nowadays, clay minerals are considered as a promising material in the context of geological barrier for the confinement of radioactive industrial waste which represents a real danger to the environment and humanity. Understanding the effectiveness of the smectite mineral use in this approach remains insufficient and need more explanation in relation with her response (e.g. structural, hydrous and cation exchange process) versus external applied constraints.

Methods: A reference Na-rich montmorillonite (SWy-2) is used as a starting material. To investigate the cation exchange process, diffusion, permeability and the removal possibility, three heavy metal cation are used (Ba^{2+}, Cu^{2+} and Co^{2+}). The first order of external applied constraints coupling is realized (at laboratory scale) and assured by simultaneously varying the intensity of the geochemical and thermal stress. To evaluate the mineral fraction response, quantitative XRD analysis and porosity measurements are used. The quantitative XRD analysis, based on the comparison of the experimental 00*l* reflections with those calculated, allows rebuilding of theoretical model describing the layers stacking at the crystallite level according to c* axis.

Results: The qualitative XRD investigation of the external applied constraints coupling strength on cation exchange process properties shows an interstratified hydration character for all complexes probably attributed to the incomplete or partial interlamellar space saturation. The XRD modelling approach shows: (i) Whatever the constraint strength and the exchangeable cation type the sample exhibits a heterogeneous hydration behavior traduced by the coexistence of 0W, 1W, 2W and 3W hydration states within the crystallite. (ii) The theoretical decomposition of the experimental XRD profiles allowed us to identify all existing different layer populations and their stacking mode. (iii) A domination of the segregated stacking mode trends by increasing constraint strength. (iv) The layer interstratification was approved by the coexistence of the four hydration states (i.e., 0W, 1W, 2W and 3W). (v) There is coexistence within the crystallite of different kinds of layer populations stacked according to a specific set of junction probabilities. In addition, the XRD modelling approach allowed us to assign a hydration footprint response and to map the interstratification of the different populations of layers, for the corresponding constraints value. The adsorption measurement results based on BET and BJH pore size distribution analyses confirm the exfoliation process versus applied constraint.

Conclusion: Structural properties (e.g. layer composition, interlamellar space content, layers stacking mode, crystallite size, interlamellar space hydration state, cation exchange process) evolution was investigated as a function of the applied external constraint strength using XRD profile modeling approach. Obtained results demonstrate the existence of a direct link between the stress intensity (which increases with coupling) and the response of the stressed material as a pure cation exchanger for further environmental use.

The Properties of High Strengthening and Toughening B_4C-SiC Ceramics

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Abstract: In this work, boron carbide (B_4C)–silicon carbide (SiC) ceramic matrix composites were designed to improve the strength and toughness of B_4C ceramics. B_4C–SiC ceramic matrix composites with high strength and toughness and the bending strength of 476 MPa could be obtained through the addition of 10 vol.% SiC. The bending strength and fracture toughness of the B_4C–SiC ceramic matrix composites had greatly improved compared with those of pure B_4C ceramics under the condition of similar density. The results indicated that the uniform distribution of ceramic powder had a great influence on the improvement in the performance of the B_4C–SiC ceramics. The fracture toughness of the ceramics reached 11.2 $MPa \cdot m^{1/2}$. The B_4C–SiC composite material had a good comprehensive performance and was highly beneficial for improving ballistic resistance properties. Such an improvement is conducive to the engineering application of composite materials.

Utilization of Eco-sustainable and Cost-efective Volcanic Condensed Pyroclastic Flow from Tungurahua Vulcano as Catalyst in Organic Reactions

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Abstract: The condensed pyroclastic flow from Tungurahua volcano, CPF-Tungurahua, Ecuador, was collected during the 2015 eruption. The PCF-Tungucat was characterized by physicochemical procedures (adsorption isotherms, TEM-SEM, chemical-mineralogical composition) and its catalytic capacity, in several chemical synthesis processes, was evaluated. Tungucats materials (volcanic catalysts) have satisfactory catalytic properties in heterogeneous and biphasic conditions, in processes of oxidation-aromatization of dihydropyridines, acetoxylation of alcohols I and II and constitute an excellent carrier for advanced oxidation processes via Fenton-H_2O_2 and in combinations with TiO_2 during the oxidative treatment of organic wastes. The chemical and phases composition were determained in a volcanic catalyst, Tungucats, with the use of different analytical techniques. The adsorption isotherm of nitrogen was correlated with the BET, Langmuir and Dubinin ecuations. These three models combined with mercury porosimetry showed that the mineral is essencially a mesoporous-macroporous material, with a significant surface área. These materials are eco-sustainable, low cost, easy to handle and can be used without previous thermal, acid-base treatments for several catalytic cycles.

Session 8: Materials Simulation and Design

On the Application of Time-temperature Equivalent Formulation for the Description of Thermorheologically Complex Material Behaviour

Linan Qiao

BAM

Abstract: In materials physics, the creep or relaxation behaviour of processes or materials that are time- and temperature-dependent can be characterised with simplified theoretical or complex phenomenological models. For example, for polymers, time-temperature superposition principle (TTS formulation) based on Williams-Landel-Ferry or Arrhenius equations was used for the description of thermorheologically simple behaviour. In contrast, for metals, many thermorheologically complex behaviours were described using an individually adapted time- temperature equivalent parameter. That means, in most of the cases, the time-temperature equivalent formulation (TTE formulation) is used without detail theoretical explanation. Fundamental works are these of LARSON and MILLER, MANSON and HAFERD, ORR, SHERBY and DORN et al. In this presentation an overview of them is given. Furthermore, a conceptual framework for both thermorheologically simple as well as complex behaviours by using just one approach is suggested in this presentation. For this purpose, as an example, the power law formulation was used for the TTE formulation. Results show, with additional normalisation conditions, most of the developed phenomenological time- temperature parameter models can be treated as special cases of the new formulation. After the theoretical introduction, the new power law time-temperature equivalent formulation with a generalized analytic stress/rupture time function was used for the rupture time analyses of 8 different metals under different isotherm conditions come from the original work of Larson and Miller. Different results of Larson-Miller parameter approach and the new method are compared and discussed. Finally, in the aspect of the arrow of time, the new defined time-temperature equivalent variable can be described as a bended arrow of time, which can help us to understand corresponding physical meaning of the suggested method.

Finding Li-ion Solid-state Electrolytes with First-principles Calculations

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Abstract: All solid-state batteries (ASSLBs) have attracted tremendous attention because of ever-increasing concern about safety issues in using lithium-ion batteries. The ASSLBs require solid-state electrolytes (SSEs) that exhibit good Li-ion conductivity and electrochemical stability. While compared to the liquid electrolyte (LE), the overall rate performance of inorganic solid-state electrolytes (ISSEs) in a state-of-the-art ASSLBs setup is not satisfactory because of three main obstacles:1) ionic conductivity less than 10^{-4} S cm^{-1} at room temperature, 2) electrode-electrolyte interfacial incompatibility, and 3) a narrow electrochemical stability window. Therefore, searching for new ISSE materials with large bandgap, high Li-ion conduction, and good electrochemical stability is an urgent need for the ASSLBs field. And the demand for Li-ion solid-state electrolyte materials design, materials optimization, and materials understanding, are at an all time high. We will discuss some materials can be used to explore ISSEs materials, and first-principle calculations how can be used to accelerate the search for good ISSEs materials.

A Multiscale-simulation and Data-driven Study of Lithium Battery Electrolytes

Xiang Chen

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Abstract: Lithium metal batteries are considered as promising next-generation energy storage devices due to their ultrahigh energy densities. However, the high reactivity of lithium metal toward organic solvents and salts renders inevitable side reactions, which further leads to undesirable electrolyte depletion, cell failure, and the evolution of flammable gas. Tremendous efforts from experiments have been devoted to the exploration of advanced electrolytes mainly through trial-and-error approaches, which are both time-consuming and cost-expensive. Herein, the ion–solvent chemistry was developed to prove the intrinsic instability of normal organic electrolytes towards lithium metal anodes through multiscale calculations and in situ microscopic observations. Based on the ion–solvent model, several strategies were further proposed to build stable electrolytes for alkali metal anodes, including additive design and regulating anions in electrolyte solvation shells. Finally, a big-data paradigm was established to achieve the rational design of advanced electrolytes through the combination of high-throughput calculations and machine-learning studies.

Recycling of Solid Wastes (Low-grade Diatomite, Steel Slag) for Water-cleaning

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Abstract: Advances in materials science and technology are providing unprecedented opportunities to treat pollutants in water. It is emphasized that during treating pollutants in practical waste water by using these developed materials, the following precedent conditions should be met: low cost, high treatment efficiency, environment security, and reuse of treatment agents. Low-grade diatomite and steel slag are promising raw materials for the removal of heavy metal ions. The main component of diatomite is amorphous SiO_2 with Si-O tetrahedral interconnection nets. It consists of abundant coordination and oxygen bridge defects, forming numerous Si-OH groups on the surface. The raw diatomite, however, has a low specific surface area (15-20 m^2/g), giving rise to a low adsorption capacity. Therefore, it is highly desirable to modify the surface of diatomite to improve its performance for water-cleaning applications. Steel slag is mainly composed of element Fe, Ca, Si, Mg, etc., endowing it with great potentials to make reusable materials for detailed requirements alternative. Especially, the utilization of these chemical compositions for constructing low-cost and multifunctional materials for water remediation has also been investigated to promote recycling and reutilization of discarded steel slag resources. However, there is still a lack of a simple strategy for full use of steel slag to design and construct visible light photocatalysts with optimized composition and structure. By tuning the crystallization kinetics in solution phase using various chemical routes, solid wastes(low-grade diatomite, steel slag, etc.) can be recycled as useful resource. These obtained composites combine the high surface area of a porous skeleton with high adsorption or catalysis activity of loaded particles. Such hybrid materials thus offer new opportunities to achieve multifunctionality and the resultant synergistic effects for water purification. These developed materials in our group have been applied for treating waste water from many industries, such as textile, dyeing, paper and pulp, petrochemical, electroplating, leather tanning, metallurgy, etc.

A Rational Design for the Separation of Metallic and Semiconducting Single-walled Carbon Nanotubes using a Magnetic Field

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Abstract: The separation of metallic (m-) and semiconducting (s-) single-walled carbon nanotubes (SWNTs) without causing contamination and damage is a major challenge for SWNT-based devices. As a facile and nondestructive tool, the use of a magnetic field could be an ideal strategy to separate m-/s-SWNTs, based on the difference of magnetic susceptibilities. Here, we designed a novel magnetic field-assisted floating catalyst chemical vapor deposition system to separate m-/s-SWNTs. Briefly, m-SWNTs are attracted toward the magnetic pole, leaving s-SWNTs on the substrate. By using this strategy, s-SWNTs with a purity of 99% could be obtained, which is enough to construct high-performance transistors with a mobility of 230 cm2 V−1 s−1 and an on/off ratio of 106. We also established a model to quantitatively calculate the percentage of m-SWNTs on the substrate and this model shows a good match with the experimental data. Furthermore, our rational design also provides a new avenue for the growth of SWNTs with specific chirality and manipulated arrangement due to the difference of magnetic susceptibilities between different diameters, chiralities, and types.

Beyond Mean-field: Location Specific Precipitation Kinetics

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Abstract: The prediction of precipitation kinetics is of great significance in the study of micro-structure of materials to further analyze and understand the mechanical properties. Mean-field modelling has become an established modelling method to capture the behavior of precipitation particles in precipitate strengthened engineering materials. The approximations given by the mean-field model are based on the assumption of weak interaction between precipitate particles, whilst this approach has many applications in non-dilute precipitate dispersion. Considering the overlapping of diffusion fields between the neighboring particles, correction factors have been introduced to describe the accelerated rate of diffusion to improve the accuracy of the predictions. In this project, a modified discrete model has been proposed to explicitly account for the competitive growth of particles with a quasi-static method. The model has been applied to evaluate different mean-field correction factors to account for competitive growth which has been derived following similar assumptions. As a result, the mean-field method with different correction factors manage to capture the behavior of precipitation particles with a volume fraction up to 20% accurately, however fail to predict the precipitate kinetics at 40%. Then the discrete model has been applied to predict the kinetics in the engineering nickel-based super-alloys 738LC and RR1000 for further evaluation. In the comparison between the measured experimental data and predictions given by a conventional mean-field method, this modified discrete model gives better predictions in IN738LC in the transition of a bimodal particle radius dispersion to a unimodal dispersion. However, when applied to RR1000, the results are less satisfying, as significant heterogeneity in particle matrix has been observed and the model needs further refinement to improve its ability to capture the precipitate kinetics in more complicated conditions for materials during service with reliability and accuracy.

Decarbonising Data Science to Reveal the Dependency between Material Formulation and Battery Property

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Abstract: Battery manufacturing plays a direct and pivotal role in determining battery performance, which, in turn, significantly affects the applications of battery-related energy storage systems. As a complicated process that involves material, chemical, and electrical operations, effective battery property predictions and reliable analysis of strongly-coupled battery material formulation become the key but challenging issues for wider battery applications. This paper scrutinizes the effects of five material formulation variables on the resulted Li-ion battery properties via decarbonising data science solution. Specifically, an effective RUBoost based ensemble learning framework is proposed to compensate for class imbalance issue and well classify three key quality indicators including the electronic conductivity, thickness, and half-cell capacity for both LFP and LTO-based battery electrode. Experimental results reveal that the proposed models could well handle the class imbalance issues and accurately classify/predict the battery properties at the early material preparation stage. Moreover, the importance weights of material variables and the correlations of material variable pairs could be effectively quantified. This could assist engineers to obtain critical insights to understand the underlying complicated non-linear battery material and manufacturing behavior. Due to the superiority in terms of accuracy, interpretability and decarbonising nature, the proposed data science solution could not only help to conduct reliable multi-classification of manufactured electrode but also benefit battery material selection and smarter manufacturing.

Design Pinciples and High-throughput Screening of Supports Boosting the Stability of Metal Nanocatalysts

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Abstract: The stability of supported nanocatalysts is crucial to meet environmental and energy challenges; however, the lack of a fundamental theory on their stability necessitates trial-and-error experimentation and delays lab-to-fab translation. Here, we report the Sabatier principle of MSI for the stability of supported NPs against sintering based on a linear scaling relationship between the MSI descriptors that govern the OR and PMC processes. Sintering kinetic simulations of 10 transition metals (TMs) and 91 supports (323 metal–support pairs in total) using 1252 energetics data were conducted, and a universal volcanic dependence of the sintering kinetics on MSI was revealed. The optimal MSI corresponding to the highest stability on homogeneous supports should be neither too strong nor too weak. Too strong of a MSI triggers rapid OR, whereas too weak of a MSI stimulates facile PMC, both of which are detrimental to the stability. For supports with the optimal MSI to NPs, the sintering onset temperature is approximately half of the melting temperature of the bulk metal for 3 nm NPs, substantiated by the long-reported empirical Tammann temperature. The revealed Sabatier principle enables the high-throughput screening of heteroenergetic supports to break the scaling relationship and boost the sintering resistance of the supported NPs far beyond the Tammann temperature. The theory substantiated by molecular dynamics (MD) simulation based on the first-principles neural network potential and available experiments may pave the way for the design of ultrastable supported nanocatalysts.

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DFT Guided Catalyst Design for Photocatalytic HER

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Abstract: While the precise design of catalysts is one of ultimate goals in catalysis, practical strategies often fall short, especially for complicated photocatalytic processes. Taking the hydrogen evolution reaction (HER) as an example, we found that the electron transfer from TiO_2 oxide to the metal cocatalysts is significantly boosted by the adsorption of proton on the metal, which is otherwise endothermic without the presence of proton. Further by systematically investigating the energetics of the directional electron transfer and the surface H-H coupling reactions on a variety of Pt nanoparticles with different size, we determined that the quasi two-Pt-layer particles, corresponding to ~1 nm size, are the best catalyst for photocatalytic HER. Moreover, we developed a function-oriented optimization approach for designing robust metal cocatalysts supported on TiO_2, and successfully determined and verified bimetallic $Pt/Rh/TiO_2$ and $Pt/Cu/TiO_2$ catalysts to be robust substitutes for conventional Pt/TiO_2. The right metal type as well as the proper stacking sequence are demonstrated to be the key to boosting the performance. Besides, we tentatively identify the tunneling barrier height as an effective descriptor for the important electron transfer process in photocatalysis on metal/oxide catalysts.[3] These results push forward the frontier of photocatalyst design towards higher water splitting efficiency.

Electrocatalytical Mechanism of FeCoNiCuPd High-Entropy Alloy for Nitrogen Reduction Reaction: A Density Functional Theory Study

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Abstract: To search excellent catalyst for electrocatalytic nitrogen reduction reaction (eNRR) is important for the alternative to the traditional Haber-Bosch process. Herein, based on density functional theory (DFT) calculations, we systematically investigated the activation mechanism of N_2 and catalytic pathway of NH_3 electrosynthesis of different proportions of high-entropy alloy (HEA) FeCoNiCuPd. Through formation energy calculations, the stability of HEA is dependent on the ratio of constituents, uncovering the high thermal stability of $Ni_{0.3}(FeCoCuPd)_{0.175}$. Gibbs free energy results indicated crystal plane (111) of $Ni_{0.3}(FeCoCuPd)_{0.175}$ features excellent performance of electrocatalytic nitrogen reduction reaction with the lowest overpotential of 0.34eV. A series of catalytically kinetic mechanism calculations reveal that $Ni_{0.3}(FeCoCuPd)_{0.175}$ thermodynamically follows the distal pathway with the rate-determining step of $*N_2 \rightarrow *NNH$ with the barrier of 0.50 eV. Relative to the secondary reaction of hydrogen evolution reaction, such catalyst has excellent selectivity of 99%. Detailed electronical calculations results uncover the dependence between catalytic activity and *d*-band center, shedding light on the critical role of Ni element ratio in the catalytic performance.

Interface Regulation for High-performance Sodium Metal Batteries

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Abstract: The rapid development of electric vehicles, communication stations, renewable energy, and aerospace fields urgently requires large-scale energy storage devices with high safety and high energy density. Sodium metal has extremely high theoretical capacity, low oxidation-reduction potential, earth-abundance, and low cost. Thus, the high specific energy sodium metal battery (SMBs) is one of the ideal choices for large-scale energy storage systems. Similar to lithium metal, the practical application of sodium metal batteries needs to solve two major problems, including the side reaction between sodium metal and electrolyte and Na dendrites during the electro-deposition of Na, which not only shorten the lifespan of SMBs, but also may cause security risks. Multiple approaches have been developed to address above challenging problems, mainly including making initial Na nucleation layers, constructing artificial solid electrolyte interface (SEI) films, and developing new electrolytes and additives. Based these strategies, our group has devoted considerable effort for long-term stable sodium metal electrodes. Specifically, i) Initial Na nucleation layers: we inhibited dendrites by constructing a nano-structured sodium metal nucleation buffer layer in the ether electrolyte system, achieving extremely high coulombic efficiency in the high-capacity long cycle of sodium metal (***Nano Lett.*** 2020, 20, 4464; ***Nano Energy*** 2021, 79, 105457; ***J. Mater. Chem. A***, 2021, 9, 13200-13208; ***Small*** 2021, 17, 2007578), also confirming that the side reaction between ether and sodium is small. These research results have opened up a promising avenue to stable SMAs by designing alloy-based nucleation layers. ii) Artificial SEI protective layers: we report a protective layer rich in sodium salt of organic sulfur on the surface of sodium, inhibiting sodium dendrites in carbonate-based electrolyte, achieving excellent cycle stability. (***Angew. Chem***. 2020, 59, 6596; ***Nano Lett.*** 2021, 21, 619). These results provide a good basis for further research on the artificial SEI protective layer of organic sulfur sodium salt. iii) Electrolyte optimization: To mitigate the safety concerns of organic flammable ether and the serious side reactions of carbonate-based electrolyte, we report a non-flammable phosphate-based electrolyte, promoting dendrite-free plating/stripping of Na metal with high safety and reversibility. (***Energy Storage Mater.*** 2021, 42, 145–153).

Molecular Dynamics Simulations on Boron-containing Oxide Glasses

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Abstract: Boron-containing oxide glasses are with both technological and industrial interests, ranging from cook and lab wares, optical components, bio-active glasses, to nuclear waste disposal. However, complicated structure features, such as boroxol rings, boron coordination conversion, and the so-called "boron anomaly" phenomenon, lead to the difficulties to fully understand this kind of systems. In this work, various boron-containing glass systems have been investigated using the newly developed potentials. Structures and properties, such as density, pair distribution function, bond angle distribution function, mechanical properties etc., have been carefully calculated and show good agreement with the experimental and theoretical findings. Both the boron coordination conversion and boron anomaly phenomenon have been well reproduced. In addition, the effects of the system size and cooling rate have been studied to provide a guide to future simulations of boron-containing glass systems. Furthermore, the structures of multi-component glass, including boron-containing bio-active glass and the simplified French Nuclear Waste glass, have been well simulated. This work helps understand the structure and properties of the boron-containing glass systems and benefits future composition design of this kind of systems.

Next Generation Batteries System: Low Cost and In-situ Recycling

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Abstract: Next-generation energy system with unlimited energy source and low cost is promising candidates towards society.[1-3] Rechargeable Aluminum-ion batteries (AIBs) are considered as a new generation of large-scale energy storage device due to their attractive features of abundant aluminum source, high specific capacity and energy density.[2] However, the AIBs suffer from the lack of suitable cathode materials with desirable capacity and long-term stability, which severely restrict the practical application of AIBs. Herein, we report a binder-free and self-standing cobalt sulfide encapsulated in carbon nanotubes as a novel cathode material for AIBs.[4-5] The binder-free and self-standing electrode effectively eliminate the side-reactions and material disintegrations in AIBs. In the meanwhile, the electrode exhibits not only high discharge capacity (315 mA h g^{-1} at 100 mA g^{-1}), enhanced rate ability (154 mA h g^{-1} at 1 A g^{-1}) but also extraordinary cycling ability (maintain 87 mA h g^{-1} after 6000 cycles at 1 A g^{-1}). The new findings reported here highlights the possibility for designing high performance cathode materials for scalable and flexible AIBs.[4] Besides that, we also proposed a new kind of solar-rechargeable batteries, in which perovskite solar cell shared the dual-function aluminum electrode with AIBs. Benefit from the ultra-fast rate-capacity, this device boosted the performance of solar-rechargeable batteries.[2]

O-MXenes for Electrochemical Nitrogen Reduction

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Abstract: Ammonia (NH_3), as a crucial chemical in industry and agriculture, have contributed greatly to the development of our economy and society. Currently, NH_3 industry heavily depends on energy- and capital-intensive Haber-Bosch process, which leads to serious energy and environmental issues. Thus, NH_3 electrosynthesis under ambient conditions has received wide attention. The key issue is how to develop efficient electrocatalysts with the improved performance. In this work, we theoretically designed various O-MXenes for electrochemical nitrogen reduction via density functional theory (DFT) calculations and least absolute shrinkage and selection operator (LASSO) regression. Through a three-step screening method, $Nb_3C_2O_x$ has been regarded as the promising candidate for the nitrogen reduction reaction (NRR) with high stability, activity and selectivity. According to the free energy profile, the potential-determining step of $Nb_3C_2O_x$ is $*NH_2$ hydrogenate into $*NH_3$ with limiting potential of -0.45 V, which is lower than that of the Ru (0001) stepped surface. Furthermore, LASSO analysis has been employed to develop accurate descriptors from the list of varibles for predict G_x value of NRR. LASSO method have provided some analytical expressions for regression with good fitting effect ($R^2 > 0.8$). The descriptors composed of adsorption energy have been proved as an important varible to describe the G_x, compatible with previous work. This work not only provides a strategy to understand NRR activity of catalysts, but also provides new insights into the catalysts design of NRR and other similar reaction.

Phase Field Simulations Accelerated Heterogeneous Microstructure Design and Mechanical Properties Optimization in Titanium Alloys

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Abstract: The design of alloys with simultaneous high strength and high ductility is still a difficult challenge. Here, we propose a new approach to design multi-phase alloys with a synergistic combination of strength and ductility by engineering heterogeneous precipitate microstructures through the activation of different transformation mechanisms. Using a two-phase titanium alloy as an example, phase field simulations are carried out firstly to design heat treatment schedules that involve both conventional nucleation and growth and non-conventional pseudospinodal decomposition mechanisms, the calculated microstructures have been evaluated by crystal plasticity finite element modeling. According to simulations, we then set a two-step heat treatment to produce bimodal $\alpha + \beta$ microstructure in Ti-10V-2Fe-3Al and Ti-5Al-5Mo-5V-3Cr-1Zr. Further mechanical testing shows that the ductility of the alloy is increased by ~50% and the strength is increased by ~10% as compared to its unimodal counterpart. Our work may provide a general way to improve the mechanical properties of alloys through multiscale microstructure design.

Point Defect-induced Dielectric Response Mechanism of RECOB Crystals

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Abstract: The dielectric performance of RECOB-type (Re: rare earth ions) crystals is vital for modulating their electro-elastic properties and improving the sensing capabilities of such high temperature piezoelectric sensors. In general, the dielectric permittivities d_{22} of RECOB crystals are found to be increased with increasing RE^{3+} ion radius, whereas LaCOB exhibits an abnormal drop in the dielectric permittivity d_{22}. This presents an obstacle to the component design and optimization of the dielectric and piezoelectric properties of RECOB crystals. Thereby we investigated the dielectric mechanism of RECOB crystals by combining first-principle calculations and experiments. It is found that both electronic hybridization and bond vibrations contribute to the dielectric permittivity of RECOB crystals. A significant decrease in dielectric permittivity d_{22} for LaCOB can be attributed to the distinct reduction in the ionic displacement polarization due to the decrease of La_{Ca} and Ca_{La} antisite defects concentrations. Charged La_{Ca}^{+} antisite defects play an important role in improving the dielectric properties of LaCOB by changing the polarization direction (Fig. 1). This suggests that it would be useful to increase the dielectric permittivity d_{22} of LaCOB by increasing La_{Ca} antisite defect concentration, such as via partially replacing La^{3+} with smaller ions like Y^{3+}, Er^{3+}, and Tm^{3+}.

Quantitative Insights into the Reaction Mechanism for the Direct Synthesis of H_2O_2 over Transition Metals: Coverage-dependent Microkinetic Modeling

Zihao Yao

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Abstract: The direct synthesis is the most promising alternative method for the production of hydrogen peroxide, and bottleneck is still unsolved. The breakthrough lies in elusive reaction mechanism issues. In this work, an advanced coverage-dependent kinetic modeling is combined with the energetics from first principles calculations to investigate the formation of H_2O_2 over transition metals. We show that the adsorbate-adsorbate interactions considerably affect the reaction mechanism of synthesis of hydrogen peroxide on Pd(111). Without the coverage effect, O_2 is likely to go through the direct dissociation mechanism, and water is the major product. When the coverage effects are included, the dissociations of O-O and O-OH bonds are significantly inhibited, and on the contrary, the hydrogenations of O_2 and OOH are promoted, leading to production of H_2O_2. We demonstrate that the reaction temperature induces strong variations in the coverage of intermediates, which in turn causes changes in product selectivity. Being consistent with operando experiment, our kinetic simulations indicate that the H_2/O_2 partial pressure ratio has great effects on H_2O_2 selectivity and the reaction rate of H_2O_2 is lower under the conditions of hydrogen-rich (oxygen lean) and oxygen-rich (hydrogen lean), which is highly related to the intermediate coverage. The same approach is also applied to other important relevant metals, i.e. Cu(111), Au(111), PdAu and PdHg alloys, and the trends of activity and selectivity have been obtained.

Rational Materials Design for Gas Molecule Capture and Utilization

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Abstract: Gas molecules such as oxygen, hydrogen and carbon dioxide play an essential role in many chemical processes as they can provide abundant active substances and raw materials during chemical reactions. However, due to the high dispersion of gas molecules, lower gas concentrations are not conducive to chemical reactions. The capture of gas molecules using porous materials can significantly increase the gas concentration in the pore channel due to the pore enrichment effect, thus accelerating the reaction process. On this basis, the introduction of different catalytic active centres enables the efficient implementation of various catalytic processes. In the process of material design, we have carried out a series of research works using large-scale screening and machine learning methods. 1. We designed and screened porous materials capable of capturing and converting CO_2 at room temperature and pressure by constructing a material structure database. 2. We designed efficient electrocatalytic oxygen evolution reaction (OER) catalyst materials using density functional theory calculations and machine learning methods.

Rational Screening of Non-Noble-Metal-Based CN Catalysts for Dehydrogenation of Formic Acid

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Abstract: Formic acid (FA) is a safe, renewable and promising hydrogen carrier. A critical challenge is the effective screening of the suitable non-noble-metal-based catalysts for FA dehydrogenation to substitute expensive noble-metal-based ones. Here, a rational screening of all possible catalysts with M-N-C structures (among 12 common transition metals) over N-doped graphene-like surface for FA dehydrogenation has been conducted using density functional theory (DFT) and followed by experimental analysis. Based on the adsorption energy of key intermediates, preliminary screening suggests Co as a possible active metal for M-N-C. Experimental analysis and further DFT calculations suggest that atomically dispersed Co with two-coordinate nitrogen atoms and two-coordinate carbon atoms (Co-N2-C2) are preferable for FA dehydrogenation. The appropriate N contents inside catalysts are critical to catalytic activity, whose amount can be tuned by the choosing of different types of sacrifice template and the pyrolysis temperature. This work develops an effective screening method for catalysts avoiding tedious trial and error.

Simulations of Plasmonic Nanoparticles and Molecular Response

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Abstract: The plasmonic response of quantum-sized nanoparitcles exhibiting interesting features attracts much attention. In this region, the near-field properties are drastically modified and depend strongly on the geometric arrangements. However, simulating realistically sized systems remains computational challenges. On the other hand, the chemical environments modify the near-field distributions of plasmonic nanoparticles, and the fields in turn break the traditional selection rule of molecular spectroscopy. For example, the tip-enhanced Raman spectroscopy exhibits quite different spectral structures and subnanometer spatial resolution. We developed an atomistic electrodynamics model to sufficiently simulate the plasmonic responses of metal nanoparticles. The atomistic electrodynamics model provides a unified description of bare and ligand-coated nanoparticles, as well as strongly interacting nanoparticle dimer system in the quantum size regime where traditional classical models fail. Incorporating with quantum mechanics approaches, it allows us to understand the origin of high-resolution near-field spectroscopy which reflects the molecule's local polarizability density changes. Moreover, it provides practical strategies in manipulating plasmonic response at the atomic level.

The High Activity and Selectivity on Ni Catalyst Loaded Defect-graphyne in Explicit Aqueous Media for 2e- oxygen Reduction Reaction: Density Functional Theory Calculations

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Abstract: Hydrogen peroxide (H_2O_2) has a key position in the global industry. To achieve greener and more efficient H_2O_2 synthesis, the design of high-performance single atom catalysts (SACs) is vital. Herein, through density functional theory (DFT), we build a three-step screening strategy to identify the optimal SAC from 174 transition metal (TM = 3d, 4d, 5d transition metal) SACs with pure graphyne (γ-GY) and defect-graphyne (V-γ-GY). It is found that a single Ni atom loaded on γ-graphyne with carbon vacancies (Ni@V-γ-GY) displayed remarkable thermodynamic stability, excellent selectivity, and high activity with an ultralow overpotential of 0.03 V. Furthermore, based on ab-initio molecular dynamic (AIMD) and DFT calculations under the explicit H_2O solvent, the hydrogen-bond framework plays an beneficial role in the high performance of H_2O_2 synthesis via the H transfer from water on Ni@V-γ-GY. This work will provide one way to better design the high-performance SACs for H_2O_2 synthesis effectively.

Theoretical Studies of Photocatalysis with Metal–organic Frameworks

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Abstract: Separation of photo-excited charges (electrons and holes) can exert important control over the lifetimes of photoexcited states. We address this issue in metal–organic frameworks (MOFs), which are potential photocatalysts due to their tunability that provides greater photoredox possibilities and their porosity that facilitates the diffusion of reactants, with the potential to overcome the low charge mobility of many nonporous semiconductors. By using Kohn-Sham density functional theory (KS-DFT), we have studied a series of MOFs in recent years. In particular, we studied UiO-66, which is built from $Zr_6O_4(OH)_4$ nodes and 1,4-benzene-dicarboxylate linkers, because it has superior tunability, such as complete or partial metal (Hf, Th, Ti, U, Ce) substitutions in the nodes and a variety of possible linker functionalizations. Ligand-to-metal charge transfer (LMCT) can lead to separation of photo-excited charges in the MOF, and with pure metals (Zr, Hf, Th, Ti, U, or Ce) in the nodes that LMCT is favorable only for Ce, where it is promoted by the low-lying empty 4f states of Ce^{4+}. Time-dependent density functional theory (TD-DFT) calculations suggest that excitations are more likely to occur in the linker of UiO-66(Ce) upon light absorption. Therefore, in UiO-66(Ce), the photogenerated charges via linker-localized excitations can be separated effectively through LMCT, prolonging the lifetime of the photoexcited states. We predict that incorporating Ce^{4+} (f^0 metal ion) into the node of a MOF is an effective way to stabilize the LMCT excited states and increase the photocatalytic activity. We also found that linker functionalization is possible to engineer the electronic structure of the Ce-MOF for a desired reaction (e.g., CO_2 reduction) while preserving favorable LMCT.

Theoretical Study on Degradation Mechanism of Hybrid Perovskite

Xiao Wang

Abstract: A promising breakthrough in the photovoltaic industry was realized with the emergence of organic-inorganic hybrid perovskite (OIHP) semiconductors. Incorporation of methylammonium lead halide ($MAPbI_3$) perovskites into solar cells has demonstrated power conversion efficiencies up to most recent 25.5%, highlighting the potential as inexpensive and solution-processable alternatives to silicon solar cell technologies. However, its widespread use is still limited by poor chemical stability: perovskite degrades rapidly under moisture, UV exposure, extreme temperatures, oxygen and bias voltages. Many efforts have been made to reveal the final decomposition products and pathways of $MAPbI_3$. However, the general decomposition pathway and the crucial degradation products of OIHPs are still opaque due to the difficulty in obtaining intrinsic structure evidences during decomposition. Combined the first-principles calculations and in-situ selective regional electron diffraction (SAED) for controllable low-dose electronic lighting, the crystal structure of perovskite intermediates found in the experiment was analyzed with further verification of its rationality and stability, and the effect on photovoltaic performance was studied as well. On this basis, we studied the degradation mechanism of OIHP and proposed an energy-driven degradation pathway. Based on the proposed path, we put forward a feasible scheme to inhibit degradation, which provides theoretical guidance for the stabilization of OIHP-based solar cells.

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Understanding the Effect of Water Molecule on Electrocatalytic Hydrogen Peroxide Synthesis

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Abstract: Two–electron (2e–) oxygen reduction reaction (ORR) shows great promise for on–site electrochemical synthesis of hydrogen peroxide (H2O2). However, it is still a great challenge to understand the effect of water molecule on electrocatalytic H2O2 synthesis. By density functional theory (DFT) and ab initio molecular dynamics simulations (AIMD), the nature of O2 activation and 2e- ORR mechanism have been studied in the aqueous solution. In the presence of water, the adsorption energy of O2 were further enhanced compared with gas phase due to the formation of hydrogen bonds with the surrounding H2O molecules. And the hydrogen bonding promoted the stabilization of the *OOH intermediate by the H2O molecule, which significantly facilitated the electrochemical hydrogenation process. 2e- ORR has more competitive than hydrogen evolution reaction (HER) in the aqueous solution. This work reveals the crucial role of water molecule in the activation and hydrogenation of O2 in the aqueous 2e- ORR process.

Theoretical Design and Simulation of Acid Electrolysis Water Catalyst

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Abstract: By converting renewable electricity into hydrogen fuel through electrolysis, we hope to promote the use of new energy and achieve the goals of "peak carbon dioxide emission" and "carbon neutrality". Compared with the conventional water electrolysis devices with alkaline electrolyte, the polymer electrolyte membrane (PEM) electrolysis device using acidic electrolyte is more compact and efficient. However, there is a lack of stable anode materials under acidic condition. By combining theoretical calculations with experimental synthesis and characterization, we have explored a series of ruthenium dioxide based electrode materials. Transition metal dopants and surface defect are introduced to reduce the amount of precious metals and regulate the chemical environment of the surface. As a result, the overpotential of the anode reaction is significantly decreased and the stability is also improved. These RuO2-based materials can be used in future acidic electrolysis device.

Session 9: Multiscale Analysis and Characterization of Materials

Crystal Grwoth and Characterization of Several NLO and Laser Crystals

Kunpeng Wang

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Abstract: A series of lithium-based rare earth phosphate monocrystallines were grown, mass characterization of crystals was carried out, wafers in various crystallography directions were oriented, processed and polished, and conventional structural characterizations such as single crystal structure analysis, elemental analysis, XRD phase purity analysis were carried out, and magnetic properties and lithium-ion isotropic insidation were tested using methods such as cp, muSR, SQUID, ESR, neutron dissidation, Yana, b, c, and so on. A single crystal-based LiMn0.95Ni0.05PO4/Li semi-battery model is designed for anisotropic lithium ion diffusion and conductivity characterization, and more than 20 new oxide crystals, such as high purity positive LiMn, are also grown PO4 crystals, magnetic resistance Li2CuZrO4 crystals, poly-iron LaSrFeO3 crystals, solid-state electrolyte Li7La3Zr2O12 crystals, high-purity positive LiFePO4 crystals, as well as a number of high-temperature superconducting monocrystalline. At the same time, the basic physical parameters such as low temperature thermal expansion are also tested.

Mechanism and Control of Negative Thermal Expansion in Metal-based Magnetic Materials

Yuzhu Song

University of Science and Technology Beijing

Abstract: A minute shape change, caused by the normal thermal expansion on heating, may degrade the excellent performance of solids. The mismatch of thermal expansion coefficients has an important impact on materials, aerospace, precision instruments and other fields. Negative thermal expansion (NTE) has attracted extensive attention in basic research and application fields due to its unique advantages on compensating and controlling positive thermal expansion (PTE). Here, a variety of new magnetic NTE systems and excellent zero thermal expansion materials were found; based on the advanced large-scale scientific facility, the NTE mechanisms induced by magnetic order-to-disorder transition and the reduce of intrinsic magnetic moment were revealed, which covers almost all the common magnetic transitions, such as FM-PM, FIM-PM, AFM-PM, FM-FM, Canting-PM and short-range magnetic order. The new methods of controlling NTE on magnetic materials have been developed, including the coexistence of magnetic phases and in-situ external magnetic field. It is helpful to reveal the complex mechanism of magnetic NTE, develop and design new NTE materials and promote its application in high-tech field.

Using Fourier Transform IR Spectroscopy to Analyze Bio-chemical Contaminants on Composite Materials based on Recycled PET

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Abstract: Aimed at developing accurate, reliable and cost-saving analytical techniques for bio-chemical contaminants screening on composite materials based on recycled PET, we evaluated in this paper the potential of Fourier transform infrared (FT-IR) spectroscopy as a measurable approach for the rapid identification of IR signatures. Various composite materials based on recycled PET in different amounts of aluminum and iron nano-powders obtained using an injection-molding machine has been used as contaminants support. The contamination was performed using quantified protein solution added in droplets on the clean, decontaminated PET samples, oven dried and kept in protective environment until the analysis. IR spectroscopy (using Spectrometer FT-IT Nicolet Summit Pro equipped with Everest attenuated total reflectance accessory) has been used to analyze the bare composite materials and the protein solution contaminated samples. The results showed consistent modifications between bare and contaminated materials. The corresponding IR spectral profiles were assumed to represent the used bio-chemical contaminants, indicating that FT-IR is a promising technique for the identification of potential biochemical contaminates on recycled PET.

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A Novel Antiferroelectric Dipoles Configuration

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Abstract: Due to their unique crystal structure and field-induced strain behavior, antiferroelectrics have important potential applications in displacement actuators, pyroelectrics, energy storage and other fields. The most widely studied $PbZrO_3$-based antiferroelectric, which always have complex crystal structure, its microscopic antiferroelectric nature and structure-properties relationship are still controversial. Combining the advantages of electron diffraction, high resolution neutrons and high resolution synchrotron radiation diffraction techniques in precise structure analysis, we reveal the incommensurate characteristics of micro-polarization configurations in antiferroelectric. Different from the strict antiparallel arrangement of electric dipoles in traditional cognition, the $PbZrO_3$-based antiferroelectric presents a special dipoles arrangement, generated by the superposition of different sine waves, which is classified as the Ising- Neel mixed polarization configuration. In addition, positive and negative polarization cannot be completely offset on the long range scale, and there is obvious net polarization. The peculiar electric polarization configuration is caused by the modulation of the A position Pb^{2+} shift and the distortion of the oxygen octahedra in the local sublattice. This polarization configuration acts as a bridge in the transition from classical antiferroelectric to classical ferroelectric, and is the result of the competition between this two energy states. It is well known that the concepts of ferroelectric and antiferroelectric are derived from ferromagnetism and antiferromagnetism, and there is always a one-to-one correspondence between them in physical terms. However, in terms of the arrangement of microscopic dipole configurations, ferroelectric materials have long been limited to parallel or antiparallel arrangement. In this work, this unique polarization configuration changes the traditional cognition of the two simple ways of limiting dipole arrangement in ferroelectric materials, deepens our understanding of antiferroelectric theory, and makes an important supplement to the unity of electricity and magnetism in microstructure.

A review on Effect of Weldmetal Chemistry on Stress Corrosion Cracking (SCC) in Dissimilar Weldments of Duplex and Austenitic Stainless Steels

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Abstract: Stress Corrosion Cracking (SCC) is an environmental degradation process and the resistance to SCC depends upon metallurgical characteristics of materials. Though stainless steels possess high resistance to corrosion however they mostly suffer from SCC in aggressive environments. At preeminent temperature applications, duplex stainless steel (DSS) is preferred over austenitic stainless steel (ASS). So it becomes indispensable to join DSS with ASS components operating at high temperatures. In dissimilar stainless steel weldments (DSSW), there are different chemical compositions of base metals, filler metals, elevated temperature in welding process and thereafter non-uniform cooling rate cause formation of different welding zones across the weld line. These zones exhibit different resistance to SCC due to difference in microstructures. Different filler metals are used to weld DSS and ASS so it is important to characterize these filler metals based on their chemical composition. In this paper a review on the study of weldmetal chemistry and its effect on formation of different heat affected zones (HAZs), which alter the resistance to SCC of DSSW involving DSS and ASS is carried out. It is found, HAZ associated with DSS is more susceptible to SCC and it is attributed to presence of delta ferrite network (δ-Fe) and intermetallic secondary (Fe-Cr-Mo) phases.

Application of Focused Ion Beam in Atom Probe Tomography

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Abstract: APT (Atom Probe tomography) is currently the most advanced technology for atomic distribution of different elements at the quantitative analysis nanometer scale. It works by applying a forward voltage to the sample, the tip atoms leave the surface in a positive ion state and are picked up by the detector under the action of extremely high pulsed negative electric field. At first, the needle tip was prepared by two times common electrolytic polishing, but the diameter of the needle tip was too large to meet the test requirement of APT, which led to the low success rate of electropolishing. With the development of focused ion beam (FIB) technology, its excellent etching accuracy has also been applied to the preparation of needle-tip samples, and it can be used in conjunction with the Scanning electron microscope to visually monitor the milling process, therefore, it can be used for sample preparation at a specific site. In this review, we will introduce the advantages of FIB and APT, FIB sample preparation process, and the latest development of APT sample preparation based on FIB, its applications in alloy grain boundaries, multilayer film materials, microelectronic device structures and nanowires are discussed. At last, we describe the challenge of FIB sampling and the future development of APT.

Atomic Insights into the Growth and Self-assembly of Ultrafine Cerium Oxides Nanocatalysts

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Abstract: The fabrication of metal oxides nanocrystals (NCs) possessing with morphology, narrow size distribution, and active exposing facets attracts the extensive attention in the field of nanomaterials and surface chemistry. Among all the chemical approaches, supercritical water for nanoparticle synthesis has been showing a superior ability for aiding the spontaneous nucleation and controlled growth process because of the unique medium. In comparison with commonly used two-phase hydrothermal reaction under the moderate temperature (100-200°C), the organic surfactant is miscible with the inorganic metal oxides precursor solution in supercritical condition, leading to the in-situ surface modification of nanocrystal during the growth process [1]. Thus, by fine-tuning the synthetic conditions in supercritical water, the morphologies, size, exposed facets, and the distribution of as-synthesized NCs can be adjusted properly. Cerium oxide (CeO_2) has been recognized as one of the best candidates in applications as diverse as solid oxide fuel cells, catalytic antioxidants for treating oxidative stress-related diseases, and catalytic converters for cleaning vehicle exhaust gas. Most of its interesting properties, including its extraordinarily high capacity to store oxygen, stem from the flexible valence switching between cerium cations (Ce^{4+} and Ce^{3+}). For years, tremendous efforts have been made to investigate the valence state variation and oxygen vacancies in CeO_2 NCs. In this regard, we have systematically explored the morphology evolution of CeO_2 NCs by fine-tuning the addition of surfactant ligand in supercritical water, and the effect of exposing facets on the catalytic performance, and the formation mechanism of cubic CeO_2 NCs with mostly {100}facets exposure is also discussed [2, 3]. Moreover, regarding the valence state variation of Ce cations, the effect of size and exposing facet on the reduction of CeO_2 NCs are fully studied [2, 4]. Furthermore, one kind of active dopants of Cr cations is also introduced to cubic CeO_2 NCs in supercritical water, and its effect on the Ce valence states and the presentative oxygen storage capacities is investigated as well [5]. Therefore, we have obtained the substantial evidences on the growth and self-assembly process of ultrafine CeO_2 NCs in supercritical water, the underling formation mechanism of cubic CeO_2 NCs, and subsequently the atomic-scale insights have been paid to the size, exposing facets, and active dopants dependent valence state variation of Ce cations, and related oxygen storage performance, which provides a basis for understanding the intrinsic features of cerium oxide nanocrystals, and it will further provide critical guidance for designing and fabricating novel oxygen-storage materials that can be used as catalysts and solid electrolytes.

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Boosting Lithium-ion Storage of Misfit-Layered Sulfide by Pre-lithiation as Free-standing Anode

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Abstract: Layered metal sulfides have attracted increasing attention for next-generation energy storage systems due to their high energy density and abundance resources.[1] Misfit layer sulfides $PbTiS_3$ (PTS) and $SnTiS_3$ (STS) are assembled by two different layers which stack alternately and orderly via van der Waals force. The structure changes of PTS and STS were evaluated through *in-situ* powder X-ray diffraction studies, revealing the reversible conversion-alloying reaction with Li^+.[2, 3] Herein, STS embedded in pre-lithiated graphene oxide sheets can exhibit low strain and fast reaction kinetics, which delivers a specific capacity (635 mA h g^{-1}) after 500 cycles at 1.0 A g^{-1}, demonstrating an excellent application prospect.

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Crystal Growth, Morphologies, Optical and Thermal Properties of Co-doping Sulfamic Acid

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Abstract: We successfully grew the crystals of the Cobalt doping sulfamic acid by the aqueous solution method. The stoichiometric aminosulfonic acid, cobalt chloride and deionized water were placed in a clean 5 ml beaker, and stirred with a glass rod to dissolve all the solid in the beaker. There was no granular solid in the beaker, and the liquid in the beaker was clear and transparent purple liquid. The beaker was placed in an oven at 55℃ to evaporate deionized water in the solution. After 72 hours, several centimeter-level sulfamic acid crystals doped with cobalt were obtained. The surface of the crystal was covered with purple cobalt chloride and cobalt oxychloride solids. The crystal was washed with deionized water to remove the purple solid on the surface of the crystal, and a colorless and transparent sulfamic acid crystal doped with cobalt element was obtained. The crystal was analyzed by powder X-ray diffraction, EDS elemental analysis, infrared, Raman and fluorescence spectra. In addition, the thermal analysis of the crystal and the surface morphology characteristics were analyzed by scanning electron microscopy.

Crystal Phase-controlled Synthesis of Noble Metal Nanocrystals for Electrocatalytic Applications

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Abstract: Crystal phase-controlled synthesis of noble metal nanocrystals provides new opportunities to modulate their physiochemical properties. However, it still remains a significant challenge to fine-tune the crystal phase, because noble metals tend to crystalize into their thermodynamically stable phases due to the strong metallic interactions between atoms. In this presentation, we will introduce a series of the developed synthetic strategies for the preparation of noble metal-based catalysts with tunable crystal phases. For example, we developed a general wet-chemical method to obtain *hcp* PtBi nanoplates, *fcc* Pd_3Pb nanocubes and *hcp* $Pd_{2.5}Bi_{1.5}$ intermetallic nanoparticles with assisted by Br^- ions. And in this method, Br^- ions could coordinate with the metal ions and decrease their reduction potential thus reduction kinetics, meanwhile, Br- ions could combine with molecular oxygen (i.e. Br^-/O_2) to generate oxidative etching effect thus reconstruct the atom arrangement. These two factors are beneficial for the formation of intermetallic structure with tunable crystal phases. These synthesized noble metal nanomaterials could be used as electrocatalysts and exhibited excellent electrochemical performance towards hydrogen evolution and ethanol oxidation reactions.

Defect Structures and Ionic Transporting Mechanisms in Two New Families of Oxide Ion Conductors: Melilite La1+xCa1-xAl3O7-0.5x and Ruddlesden-Popper Perovskite La2-x(Ca/Sr/Ba)xBaIn2O7-0.5x

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Abstract: Oxide ion conductors are attracting more and more attentions due to their widespread applications in developing technologies including solid oxide fuel cells (SOFCs), oxygen sensors and pumps, oxygen separation membranes, and so on. The defect structures and transporting mechanisms studies are vital to well understand the electrical behaviors. Herein, we showcase complementary characterizations for the crystal structure invsetigations, and the computer simulations for the defect formation and transporting mechanisms in the melilite-structured La1+xCa1-xAl3O7+0.5x materials and Ruddlesden-Popper perovskite La2-xBa1+xIn2O7-0.5x mateirals. In the former case, interstitial oxygen defects were comfirmed based on the Rietveld structural refinement against the neutron diffraction (ND) data, and multiple interstitial defect positions within the pentagonal ring were revealed, demonstrating the diversity of local structures around the oxygen interstitial defects in La1+xCa1-xAl3O7+0.5x. Variable temperature solid-state 27Al nuclear magnetic resonance (NMR) spectroscopy measurements demonstrate the existence of 5-coordinated AlO5 polyhedra and dynamic exchange processes between these 5-coordinated Al sites, representing the first example of evidence for the migration mechanism of interstitial oxide ions in melilites by NMR. For the later case of La2-x(Ca/Sr/Ba)xBaIn2O7-0.5x mateirals, XRD and ND Rietveld structural refinements, combined with defect formation energy calculations based on the interatomic potential approach, revealed the doping mechanism. In addition, molecular dynamic (MD) simulations were applied to study the ionic transporting mechanisms for both La1+xCa1-xAl3O7+0.5x and La2-x(Ca/Sr/Ba)xBaIn2O7-0.5x mateirals.

Diffraction Grating and Its Application in Spectral Measurement

Xiaotian Li

Changchun Institute of Optics, Fine Mechanics and Physics, Chinese Academy of Sciences

Abstract: Diffraction grating is the core optical element of spectrometer, and its performance will affect the measurement accuracy of spectrometer. Firstly, this report will focus on the progress in the development of large grating ruling machine and mechanical ruling grating, including grating ruling error correction technology, grating ruling knife active control technology and control method combining software and hardware in Changchun Institute of Optics, Fine Mechanics and Physics, Chinese Academy of Sciences in China; In addition, the research progress of holographic grating and scanning exposure grating will be briefly introduced. Finally, the research progress of mosaic-grating and echelle-grating spatial heterodyne Raman spectrometer, transmission grating spectrometer, grating diffraction efficiency measuring instrument,Fluorescence spectrometer, echelle grating spectrometer and so on will be introduced. We will focus on the mosaic grating and echelle grating spatial heterodyne Raman spectrometer， which have the advantages of high throughput, high resolution, wide band, compact structure, no moving components and strong robustness. It has a good application prospect in the field of material chemical analysis.

Electrolyte and Interfacial Model

Jun Ming

State Key Laboratory of Rare Earth Resource Utilization, Changchun Institute of Applied Chemistry, Chinese Academy of Sciences

Abstract: Electrolytes play a critical role in controlling metal-ion battery performance. However, the molecular behavior of electrolyte components and their effects on electrodes are not fully understood. Herein, three important theories were proposed for the first time in the field of metal-ion battery electrolyte: i) the Li^{+} solvation structure prevails over solid electrolyte interphase layer (SEI) to determine graphite electrode performance; ii) the discovery of the coordination role of electrolyte additives, that is, the additives can change the coordination environment of Li^{+}; iii) construction of a molecular/ion interfacial model instead of the SEI layer to explain the electrochemical behaviors of graphite (i.e., Li^{+} (de-)intercalation or Li^{+}-solvent co-intercalation). The applicant also introduced the “solvation structure theory” and the “solvation structure formula" to analyze the electrolyte qualitatively and quantitatively in an imaginative way. Then, the "Li^{+}-solvent interaction strength concept" and "molecular/ion interface arrangement theory" were further presented to explain the difference in electrode (e.g., graphite, metal anode, alloying anode, cathode) performance.

Experimental Determination of Magnetic Anisotropy in Lanthanide Metallocene Single-molecule Magnet

Yin-Shan Meng

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Abstract: Lanthanide metallocene compounds have attracted extensive interest because of not only their novel structures and reactivities but also their outstanding single-molecule magnet (SMM) performance. Previously, we demonstrated that the equatorial ligand field has great impact on the QTM and blocking barriers of dysprosium metallocene and proposed that the isolated dysprosium metallocenes are promising SMMs. This have been proven by the isolated $[(Cp^{ttt})_2Dy]^+$ and $[(Cp^{iPr5})Dy(Cp^*)]^+$ whose blocking temperature have reached a milestone and surpassed liquid nitrogen temperature. However, their magnetic anisotropy properties have not been fully understood at experimental or theoretical levels due to the air- and moisture- sensitivity and crystalline symmetry limitation. Now we report a family of dinuclear dysprosium metallocenes. Their magnetic easy axes were determined by temperature-dependent angular-resolved magnetometry. Their electronic structures and magnetic properties were investigated by multi-techniques. Our results provided the first experimental evidences for the magnetic anisotroy of lanthanide based single molecule magnets.

Green Printing Technology for Manufacturing Functional Devices

Yanlin Song

Institute of Chemistry, Chinese Academy of Sciences

Abstract: Based on the droplet drying process on the surfaces of different wettability, controllable nanoparticles assembling and stereo structures patterning could be achieved. Through controlling the droplet spinning motion and movement of the vapor-solid-liquid three phase contact lines, the basic units (dot, line, plane and stereo structures) via the printing technology can be precisely controlled. Significantly, we achieved the silver nanoparticles assembled conductive patterns with single nanoparticle resolution. Our further work on assembling metal nanomaterials or graphene via printing process, patterned various linear or curved 1D/2D structures on diverse substrates. The desirable conductive patterns contribute the remarkable application on sensitive electronical skin, transparent touch screen, multi-layer circuits, ultra-integrated complex circuits, solar cells and soft actuators. Moreover, stereo structures can be prepared through manipulating the solid-solid interface, which contributes to a versatile additive manufacture procedure. This achievement on printed electronics and additive manufacture are benefited from the fundamental researches on interfacial wettability manipulation, morphology control of drying droplets, as well as functional nanomaterial fabrication, which constructs the theoretical and technical system of Green Printing Technology.

Highly Stable and Efficient Copper-based Perovskite Scintillators

Yuntao Wu, Guohao Ren

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Abstract: Low-dimensional metal halide perovskites with excellent luminescent properties have become leading candidates for optoelectronic and radiation detection applications. Here, we incorporated Tl cation into zero-dimensional perovskite $Cs_3Cu_2I_5$ host and develop an ultra-bright and efficient scintillator for X-ray and g-ray detection. The Tl-doped $Cs_3Cu_2I_5$crystals exhibit a high photoluminescence luminescence quantum efficiency of 79.2%. The radioluminescence emission of $Cs_3Cu_2I_5$:Tl crystal under X-ray excitation consists of a self-trapped exciton emission peaking at 440 nm and a Tl-related emission peaking at 510 nm at room temperature. With optimized Tl doping, our $Cs_3Cu_2I_5$ not only demonstrates about five-times enhanced steady-state scintillation yield up to 150,000 photons/MeV and an improvement of X-ray detection limit from 103.6 to 66.3 nGy/s, but also maintains an extremely low afterglow of 0.17% at 10 ms after X-ray cut-off. The $Cs_3Cu_2I_5$:Tl also possess an excellent energy resolution of 3.4% at 662 keV and an ultra-high light yield of 87,000 photons/MeV under ^{137}Cs g-ray radiation.

Host-guest Complexation for Efficient Formamidinium-Based Perovskite Solar Cells

Hong Zhang

Swiss Federal Institute of Technology Lausanne (EPFL)

Abstract: The use of molecular modulators to reduce the defect density at the surface and grain boundaries of perovskite materials has been demonstrated to be an effective approach to enhance the photovoltaic performance and device stability of perovskite solar cells. Herein, we employ crown ethers to modulate perovskite films, affording passivation of undercoordinated surface defects [*J. Am. Chem. Soc.* 2020, 142, 19980; *Nat. Commun.* 2021, 12, 3383]. This interaction has been elucidated by solid-state nuclear magnetic resonance and density functional theory calculations. The crown ether hosts induce the formation of host–guest complexes on the surface of the perovskite films, which reduces the concentration of surface electronic defects and suppresses nonradiative recombination by 40% while minimizing moisture permeation. As a result, we achieved substantially improved photovoltaic performance with power conversion efficiencies exceeding 24%, accompanied by enhanced stability under ambient and operational conditions. This work opens a new avenue to improve the performance and stability of perovskite-based optoelectronic devices through supramolecular chemistry.

In-Situ Environmental TEM for Probing the Dynamic of Catalysts at High Temperature

Feng Yang

Southern University of Science and Technology

Abstract: Revealing the catalyst structure and chemistry in the reactive environment at the atomic scale is imperative for the rational design of catalysts and the exploration of reaction mechanism. However, direct access of such information at atomic resolution under reactive environment, especially at high temperature is still very challenging. The role of carbon atoms in the near-surface of catalysts is widely concerned in many catalytic processes such as the synthesis of carbon nanotubes (CNTs). Tracking intermetallic Co_7W_6 nanocrystals with a defined structure and a high melting point by environmental aberration-corrected transmission electron microscopy (ETEM) in combination with *in-situ* synchrotron X-ray absorption spectroscopy, we directly revealed the structural and chemical stability of the intermetallic nanocrystals at atomic level when catalyzting CNT growth at high temperature. The nucleation of CNTs from transition monometal was linked with an alternating dissolving and precipitating cycle of carbon in catalysts close to the nucleation site. The strong metal-support interaction (SMSI) has long been a hot topic in heterogeneous catalysis. We tracked at atomic-scale the interfacial reaction induced SMSI between SiO_2 and Co nanoparticles as well as evolution under reactive conditions by ETEM. Such SMSI in metal-SiO_2 system was also found to greatly boost the catalytic hydrogenation. Understanding the dynamics of foreign atoms in catalysts brings deeper insight into the structure evolution of catalysts and facilitates inferring mechanisms of catalysis.

In-situ Study of Structure-activity Relationship of Molybdenum Carbide-based Methanol Hydrogen Production Catalyst

Lili Lin

Zhejiang University of Technology

Abstract: Methanol, a high-density hydrogen energy carrier, solves the problem of inefficient and expensive hydrogen storage and transport and has a significant potential of promoting the H_2 application. The development of high-efficiency catalyst for hydrogen production from methanol reforming is the key to the implementation of this indirect hydrogen storage strategy. The atomically dispersed M/α-MoC (γ-Mo_2N) catalysts we developed exhibit unprecedented hydrogen production activity, which is 1-2 orders of magnitude higher than that of traditional M/oxide catalysts. The structure and electronic properties of the M/α-MoC catalyst were characterized by a variety of in-situ techniques (XAFS, XPS, XRD, ESTEM) from multiple scales and dimensions to clarify the relationship between the hydrogen production performance and the structure in depth. Furthermore, the positive electronic properties of M/α-MoC was applied to other reactions to prove the reliability of structure, and expands its utilizations. The structural evolution of single atomic dispersion of metal over the carbide substrates are also monitored and studied by operando techniques and theoretical methods.

Interfacial van der Waals Engineering and Atomic-scale Characterization of Low Dimensional Materials

Shao-Chun Li

National Laboratory of Solid State Microstructures, School of Physics, Nanjing University

Abstract: Low-dimensional materials, particularly at the 2D limit, exhibit versatile properties different from their bulk counterparts, and can find great application potentials in various fields such as electronics, catalysis, energy etc. The van der Waals interactions, even though weak, plays a vital role in the epitaxy of these materials. On the other hand, to characterize the electronic structure at atomic-scale provides the direct and significant information to fully understand their physical properties. In this talk, I will present how we employed vdW interactions to discover a series of new 2D materials, and to finely tune their electronic structures. The puckered honeycomb antimonene (PHA) is the structural analog of black phosphorene, which however doesn't exist in nature. We successfully realized the monolayered PHA, with a precisely control of thickness. [1] In combination with scanning tunneling microscopy (STM), we found it hosts the linearly dispersive band structure across the Fermi level. Through tuning the interfacial vdW interactions, we were able to tune a narrow band gap, thus realizing both metallic and semiconducting PHA monolayers. [2] To engineer the interlayer vdW interaction in stacked hetero-bilayers can induce more exotic phenomena. We focused on the 1T phase of transition metal dichalcogenides (TMDs) that usually exhibit rich physical phenomena, [3] and successfully grew 1T-TiSe2/1T-TiTe2 bilayers with controllable twist angle through sophisticated epitaxy control. We discovered a moiré enhanced charge density wave state at small twist angles. [4]

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Ligand Engineering of Nanocrystal Assembly Advanced by in Situ Liquid-cell TEM

Yu Wang

South China University of Technology

Abstract: Nanocrystal superlattices are usually constructed through assembling nanocrystals into designated topology for the emergent properties in physics and chemistry. During nanocrystal assembly, surface ligands are pivotal for scaffolding the mesostructured superlattices and their presence at superlattice interfaces can dramatically alter the physical and chemical properties. Here we use in situ liquid-cell TEM to investigate nanocrystal assembly during the superlattice formation and transformation with a focus on ligand engineering. We find the versatile deformability of PbSe or PbS semiconductor nanocrystals under different ligand controlling environments and its profound effect on the formation of superlattice defects. The dynamic deformability of semiconductor nanocrystals revealed in this work is significant not only for the designing of nanocrystals and nanocrystal architectures with desired properties for various applications, but also for controlling the physical and chemical processes of a wide range of matter at the atomic or nanometric level.The knowledge of ligand engineering gained from in situ study enables us to construct strong coupled moiré superlattices with unique electronic properties, such as the formation of mini-bands.

Line-rotated Remapping for High-resolution Electron Backscatter Diffraction

Yongzhe Wang

Shanghai Institute of Ceramics, Chinese Academy of Sciences

Abstract: A novel line-rotated remapping high angular resolution electron backscatter diffraction (LRR-HR-EBSD) was proposed to effectively measure the elastic strain with the presence of lattice rotation as large as ~34°. The finite rotation matrix for remapping the test patterns to the similar orientation of reference pattern was determined using the parameters (slopes and intercepts) of Kikuchi lines, which was accurately located by the combination of pattern rotation and gray gradient detection. Thus, the displacements during the first pass cross-correlation were modified to a function of corresponding Kikuchi lines and points only on the reference Kikuchi lines. Consequently, the related points in the test patterns could be negligible, which would inevitably cause in the disastrous decrease of correlation coefficient with the large lattice rotation. This might be the essential issue for the largest angle limitation of the stranded cross-correlation algorithm. Subsequently, the second sub-pixel cross-correlation was executed using the remapped test patterns, and the resolution could be ~7.0×10^{-4} when the lattice rotation was about ~34°. Furthermore, the new LRR remapping method was applied to the experimental evaluation of strain under the nano-indentations and the tension measurement on the same Ni single crystal.

Multiple Length Scale Investigations on Multifunctional Oxides for Electronic Device Applications

Changjian Li

Southern University of Science and Technology

Abstract: Due to the strong correlation among charge, spin, orbital and lattice, complex oxides exhibit various interesting properties, including superconductivity, ferromagnetism, antiferromagnetism, ferroelectricity, etc. Interface, strain and defects provide additional freedom to manipulate the physical properties of complex oxides. Here I show by combining atomic controlled pulsed laser deposition, macroscopic physical property engineering and atomic-scale characterization via scanning transmission electron microscopy is effective to understand the functional oxide thin film physics and developing novel device applications. In LaMnO3/SrTiO3 heterostructures, we observed a unit cell sensitive antiferromagnetic to ferromagnetic phase transition and revealed the atomic scale origin of ferromagnetism. In BaTiO3 based ferroelectric tunnel junctions, through interface engineering, we showed an enhancement of On/off ratio by two orders of magnitude and 400% tunnel electroresistance ratio at room temperature for 2 unit cell of BaTiO3. Furthermore, we realized three-state nonvolatile memory in a single Pt/BaTiO3/Nb:SrTiO3 device by combining both oxygen vacancy migration and ferroelectricity switching.

New High Entropy Alloys (HEA) with Small Additions for Possible Use as Biomaterials

Pedro Pablo Socorro-Perdomo [1], Nestor Ruben Florido-Suarez [1], Julia C. Mirza Rosca [1], Ionelia Voiculescu [2]

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[2] Politehnica University of Bucharest

Abstract: New class of materials has been developing in the last years and the materials from this class have unique structural properties that open up a wide range of possibilities for the creation and development of novel materials for specific applications. In the medical field, HEAs have been developed for metallic medical devices, in various alloy systems, where biocompatibility and mechanical properties are essential conditions. First, a base alloy was designed, a high entropy equiatomic multicomponent alloy with pure elements (99.95%) as Cr, Co, Fe, Mo and Ni (named LAS1) and from this alloy two other alloys are obtained by adding another alloying component. In one alloy, Ti is added (LAS2) and in the other Zr is added (LAS3) in order to study the mechanical behavior that allows us to consider its use as a biomaterial. An ingot of each of these alloys is fabricated by vacuum arc melting in an inert argon atmosphere and six remeltings are carried out to ensure their homogeneity. By means of a three-point bending test, the modulus of elasticity E is calculated. The fatigue experiments were carried out. For this purpose, filaments are cut and tested in an Electroforce_3100 machine that applies a maximum load of 22 Newton. At least 10 tests are performed with each of the designed alloys and the mean,

Organic Cation Intercalation in Reduced-dimensional Perovskites: The Influences on the Crystal Orientation and the Bandedge Integrity

Zhenyu Yang

Sun Yat-sen University

Abstract: Metal halide perovskites exhibit outstanding photovoltaic properties due to their superior charge carrier mobilities, low densities of deep trap states, and low-temperature solution processability. The introduction of bulky organic cations, causing the formation of reduced-dimensional (RD) perovskite structures, makes up the average dimensionally tuned perovskite in a solid-state material that could be used as a means to enhance the materials stability against irradiation, heat, and moisture. However, the widely-used organic cations, such as phenylethylammonium (PEA) and butylammonium (BA), are intrinsically non-conductive. The incorporation of the large organic end groups also cause the change of the crystal orientation that impairs the carrier separation and transport within the RD perovskite active layer. Recently, we investigated several new classes of bulky organic cations that can effectively tailor the near band-edge states of the RD perovskite thin films. Inspired by the high conductivity of conjugated ligands (e.g., thiophene- and pyridine-based organic cations), we investigate RD perovskites incorporating an electron-rich π functional group. Due to the high polarizability of the conjugating structures, the valence π electrons are more loosely bound to the aromatic rings, resulting in higher charge mobility. As a result, the power conversion efficiency of the new RD perovskite devices is more than a 10% relative improvement compared to conventional PEA-based devices. In this talk, we will also demonstrate multifunctional ligands that can effectively tailor the orientation of the inorganic components within the RD perovskite structures, which improves the charge extraction and transport in the optoelectronic devices, such as solar cells and light-emitting diodes.

Partial Lattice Ions Substituted by Aluminum Ions in Sepiolite

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[2] Shenzhen Institute of Advanced Technology, Chinese Academy of Sciences

Abstract: Sepiolite was modified with Al^{3+} via hydrothermal reaction. The substitution amount of Al^{3+} for Mg^{2+} and Si^{4+} located at sepiolite lattice and the influence of substitution amount on the structure, specific surface area, and surface acidity of Al-modified sepiolite were investigated. On this basis, indigo–sepiolite composite pigments were prepared by Al-modified sepiolite and indigo via grinding method to evaluate the influence of Al-modified sepiolite on the structure, bonding strength, and weather resistance of composite pigment. The crystal structure of Al-modified sepiolite had no obvious change after modification. Al^{3+} mainly substituted Mg^{2+} located at the octahedron of the sepiolite lattice, and the substitution amount was positively related to the dosage of Al^{3+}. The specific surface area of Al-modified sepiolite decreased and the distribution of channel size became wider after Al modification. In addition, the absolute value of zeta potential decreased as well as the solid acid sites increased with the increase of Al substitution in Al-modified sepiolite. For indigo–sepiolite composite pigments, the structure of Al-modified sepiolite had no obvious change as well. The adsorption amount of indigo in composite pigment after treating by DMSO and Al content as well as weak acid amount in Al-modified sepiolite presented linear correlation, indicating that Al modification could enhance the bonding strength between indigo and Al-modified sepiolite by increasing the amount of coordinated water with Al. For indigo, Al-modified sepiolite could brighten the color and reduce the weather resistance of the prepared composite pigment. The results of this study provide a new idea and basis for regulating the structure and properties of clay and for studying the preparation of composite pigment and clay functional materials.

Probing and Modulating the Interactions of the DNAzyme with DNA-functionalized Nanoparticles

Yuqiang Hu, Zhen Zhang, Tongbo Wu

Huazhong University of Science and Technology

Abstract: DNA-functionalized gold nanoparticles are one of the most versatile bionanomaterials for biomedical and clinical diagnosis. Herein, we discovered that the performance of DNAzyme cleaving the substrate is highly related to its length. This intriguing phenomenon only appears at the interfaces of DNA-functionalized gold nanoparticles. We systematically investigated the causes of this phenomenon. We conjectured that the DNAzyme with extended nucleotides that do not match its substrate strand is vulnerable to non-specific adsorption, electrostatic repulsion, and steric hindrance. Based on our improved understanding of this phenomenon, we have successfully developed a highly sensitive and specific amplifiable biosensor with a DNAzyme motor. The DNAzyme motor could be used to detect human apurinic/apyrimidinic endonuclease 1 (APE1) and DNA mutations. The designing and validating of the APE1 and DNA mutation detection biosensor suggest that the improved understanding of the interaction between the analyte and HS-ssDNA functionalized AuNPs may promote the development of biosensors and nanodevices in the future.

Probing the Optoelectronic Properties of Semiconductors via Time-resolved Microwave Conductivity (TRMC)

Qianqian Lin

Wuhan University

Abstract: Along with the remarkable progress in the field of organic, quantum dots based and recently emerged perovskite optoelectronics, solution-processable semiconductors have shown unprecedented successes. However, the characterization of these novel semiconductos is very challenging due to the highly disordered structure, low conductivity and relatively short carrier lifetimes. In this talk, I will present the optoelectronic characterization of these novel materials systems, mainly via time-resolved microwave conductivity (TRMC) - an non-contact technique and do not require any electrodes. I will start with the basic principle and the set-up of the TRMC technique. Then, I will focus on the optoelectronic properties obtained from the TRMC decays, including real and imaginary conductivity at GHz region, mobility, recombination rates, shallow trap density and carrier lifetime. At the end, I discuss the key challenges facing this technique. I will also point out the opportunities, which are promising to explore and may require more research activities.

Realization of Quasi-1D Materials via Chemical Strategy

Shu Guo, R.J. Cava

Department of Chemistry, Princeton University

Abstract: The structural dimensionality of materials plays an important role in their physical properties. Structurally, frustrated magnetic materials could be classified into quasi-1D (chains or ribbons), 2D (layered sheet), and 3D (framework) structural motifs. Specifically, quasi-1D materials, in which the crystal structures are highly anisotropic, and the physical properties are closely related to the spin-orbit coupling, are very rare and deserve further study. Recently, some interesting physical properties such as spin-Peierls transitions, superconductivity, and the quantum spin liquid state have been reported in the quasi-1D system. Here, a family of previous unreported quasi-1D materials with different 1D chain fragments are designed via chemical strategy. Their crystal structures are analyzed via single-crystal X-ray diffraction. These quasi-1D materials exhibit different 1D chain fragments along their c axes. The flatness of the electronic bands is suggested by the density functional theory calculations. Our results might be helpful for understanding the structure-properties relationship among quasi-1D materials.

Single Crystal Growth and Characterization of the Nickel doped Thiourea CH4N2S

Longyu Cao, Kunpeng Wang, Hongbin Chen, Qilin Cui, Xuejiao Wang, Xiangyu Han

Zaozhuang College

Abstract: In this study, nickel doped thiourea single crystal was grown by traditional aqueous solvent method. The raw materials NiCl2·6H2O and CH4N2S were placed in a beaker containing 5ml distilled water at a certain stoichiometric ratio and stirred until the two substances were completely dissolved. After the solvent was completely volatilized, a green nickel dithiourea hexahydrate single crystal was obtained. By powder X - ray diffraction (XRD) measurement and Rietveld refinement, the details of atomic positions occupying of nickel ion and its effect on lattice were carefully studied. The peak broadening and intensity variation of some frequency regions in the crystal structure were studied by IR and Raman spectra, and the atomic structure of the crystal was explored. At the same time, the surface morphology, composition and element analysis of the crystal were studied by scanning electron microscopy (SEM). We also tested the hardness properties and physical properties of the crystal along the different crystalline directions, in addition, we measured the refractive index and dielectric constant of the crystal.

Studies on the Smart Luminescent Materials Based on Rare Earth Complexes

Yu Tang

Lanzhou University

Abstract: Rare earth complexes have very important application value in optical information storage and life science. Focused on the key scientific problem about how to precisely control the function of luminescent material based on the rare earth complexes at the molecular level, we have carried out a series of research work. On the basis of the properties of molecular design and the characteristics of the rare earth luminescence, we used interfacial effect, in-situ coordination and energy transfer, to establish a new strategy of the molecular regulation of luminescent material based on the rare earth complexes. And the strategy has been applied in the optical information storage and biological probes. By means of stimulus responsive design of ligands, the collaborative modulation of rare earth fluorescence spectra and life in a material system has been realized and the two-photon excited smart probes for diagnosis and therapies are constructed. And the studies provide a new idea and perspective for the creation and manufacture of the smart luminescent materials based on rare earth complexes.

Study of the Synthesis Mechanism of Heterogeneous Catalytic Materials at the Atomic Level by In-situ Characterization

Siyu Yao

Zhejiang University

Abstract: The performance of heterogeneous catalytic materials is determined by the microscale geometric and electronic structure. Synthesis methods have been extensively demonstrated to be an effective way to tune the structural properties of catalytic active species, including the composition, crystal structure, exposing facet as well as particle size. Despite the success obtained, the atomic level understandings of the mechanism of catalyst synthesis are still limited, due to the complexity of the synthesis systems, lack of in-situ/operando researches, and the poor spatial/temporal resolution of characterization methods. In this presentation, I will present the study of the synthesis mechanism of quasi-homogeneous metal and metal carbide particles using wet chemical synthesis and the high temperature stable single atomic catalyst fabrication using strong metal-support interaction (SMSI) effect at the atomic level using advanced synchrotron-based in-situ X-ray absorption fine structure spectroscopy and X-ray diffraction methods. Comments on the potential and limitations of the in-situ characterization methodology will also be presented.

Synthesis of Active Bimetal Oxide by Calcination followed by Alkaline Activation and Its Application for Chloride Adsorption from Simulated Concrete Pore Solution

Ji-Hua Zhu, Xianyang Wu, Ibrahim M. A. Mohamed, Feng Xing

Guangdong Province Key Laboratory of Durability for Marine Civil Engineering, Shenzhen University

Abstract: Calcination followed by alkaline activation using aqueous hydroxide solution was utilized to chemically prepared active Mg/Al layer double oxide (ALDO) and investigated to stabilize the pH on the simulated concrete pore solution (SCPS) in addition to adsorb chlorides from the SCPS. The synthesized ALDO material was investigated in terms of FESEM, XRD, and XPS techniques. The effect of ALDO on the pH of SCPS was studied and the pH was successfully stabilized. The SCP solution without HDMO had a lower initial pH of 11, and that of SCP/HDMO started at 12.45. A 13 % increase in the pH of the SCP solution can be due to the release of hydroxides from the HDMO structure. The as-prepared ALDO demonstrated improved Cl^- adsorption in SCPS with maximum Cl^- uptake capacity at 0.204 mmoles/g using 20 mmol/l as initial concentration. The Langmuir isotherm model provided a better fit to the experimental adsorption data than Freundlich isotherm. This may be attributed to the unique nature of ALDO, which has bonds between Lewis acidic metals and Lewis basic oxide. In short, ALDO material can be applied as an interesting material in civil engineering towards stabilize the pH on the SCPS and chloride adsorption.

Synthesis, Crystal Growth and Morphologies of the Co-doping NH4VO3

Qilin Cui, Hongbin Chen, Xuejiao Wang, Xiangyu Han, Longyu Cao, Kunpeng Wang

Zaozhuang University

Abstract: We synthesized the polycrystals and successfully grew the centimeter sizes of the single crystals of the Cobalt doping ammonium metavanadate NH4VO3 by the traditional aqueous evaporation method. The single crystals with red brown color are totally transparent, and no obvious micro defects were observed. Large amount of micron-sized triangle growth hills on the surfaces along the different crystalline directions were observed by the polarizing microscope. Based on the polarized images, we found that the crystals were grown by the two-dimension nuclei (2D) growth mechanisms on the (001) and (010) miller faces, and however, the spiral dislocation growth mode was dominated on the (100) and (110) faces. The discovered 2D nuclei were accumulated mainly on the center of the (110) surfaces, but extended primarily to the edges of the (010) surfaces. The sizes of the 2D nuclei are from 2-30 um, and the height of the nuclei is from 0.5-15 um. Regarding the spiral dislocations, we found that all of them are developed from the center of the surfaces.

Synthesis, Crystal Growth, and Characterization of the Nickel doped NH2SO3H

Xuejiao Wang

Zaozhuang University

Abstract: Nickel doped NH2SO3H polycrystals have been synthesized, and the single crystals with centimeter sizes have been successfully grown by the traditional solvent evaporation method. The stoichiometric raw chemicals were totally dissolved into a 5ml breaker, and evaporated for 10 days in a cabinet. Afterwards, several centimeter sized single crystals with no obvious micro defects were obtained. We washed carefully the crystals with deionized water in order to clean all kinds of the impurities attached to the surfaces. The phase has been determined by powder X - ray diffraction (XRD) and the single crystal structure has been solved by the FullProf code based on the Rietveld refinement technique. The occupation of Nickel atoms was investigated. In addition, we have studied the surface morphology by polarization microscope and the scanning electron microscope. Some special growth nucleus and spiral dislocations were observed. The hardness, infrared (IR), Raman, and the Ultraviolet-Visible (UV-VIS) Spectroscopy have also been measured.

The Borate Optical Crystals with Anomalous Thermal/Mechanical Properties

Xingxing Jiang, Zheshuai Lin

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Abstract: Borate is an optical materials family with high structural anisotropy. Apart from the excellent optical performance, the high structural anistropy could also lead to anomalous thermal/mechanical properties, which, combined with the good optical properties, could bring the new application in the special optical apparatus operated in complex/extreme condition. Aiming at the exploration of optical materials with anomalous thermal/mechanical properties, we carried out systematic study in borates and made the following achievement: 1) We discovered the deep-ultraviolet optical crystals $KBe_2BO_3F_2$ (KBBF) with two-dimensional negative compressibility, and proposed the application in ultra-sensitive stress converting and acoustic-optic device; 2) Put forward the stratgy to reduce thermal expansion via introducing strong electronegativity atom, and discovered the near-zero thermal expansion crystal $Zn_4B_6O_{13}$ (ZBO); 3) Proposed the "Lu-Ban stool" -like model for the exploration of linear incompressibility, and discovered the first zero linear compressibility crystal AEB_2O_4 in non-dense material system; 4) Discovered the $LiBO_2$ crystal that can "squeeze" volume compressibility onto one dimension, which can be utilized to stabilize the transmission system under high-pressure condition.

Thermoelectric Properties of Nano-grained Mooihoekite $Cu_9Fe_9S_{16}$

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Abstract: Cu-Fe-S-based compounds have received a lot of attention in thermoelectricity because of the non-toxic nature of the constituent elements and the abundance of reserves. Compared with CuFeS2 and Cu5FeS4, the current research on the Mooihoekite mineral Cu9Fe9S16 is very little, and its electrothermal properties and transport mechanism are still unclear. In this work, a series of Cu9-xFe9+xS16 (x=0, 0.5, 1.0, 1.5, 2.0) samples were synthesized by the conventional melt annealing sintering process, and the phase composition, microstructure, and electrothermal transport mechanism of these samples were systematically investigated. The XRD refinement results showed that the synthesized phases were pure phases with a tetragonal space group structure. The cell parameters are a = b = 10.608 Å, c = 5.353 Å, $\alpha = \beta = \gamma = 90°$. Transmission electron microscopy shows that the grain size of the Cu9Fe9S16 compound is in the nanometer range. Compared with other Cu-Fe-S compounds, Cu9Fe9S16 has a lower intrinsic lattice thermal conductivity of 1.28 W m-1 K-1 at room temperature, and many nano-grain boundaries and low-frequency optical branches in the material should be responsible for the low intrinsic thermal conductivity. Introducing Fe doping at the Cu site can significantly increase the carrier concentration and thus change the electrical transport properties of the material. At 800 K, the highest zT value of the Cu9Fe9S16 material is 0.21, which is comparable to that of the CuFeS2 compound.

The Origin of the Forbidden Reflection in Black Phosphorus

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Abstract: Black phosphorus (BP) has attracted considerable attention in recent years for its extraordinary optoelectronic properties including a tunable direct bandgap from 0.33 eV to ~1.5 eV, high carrier mobility up to 1000 $cm^2V^{-1}s^{-1}$, and highly anisotropy both in-plane and out-of-plane. In addition, the BP monolayer is predicted to have extremely high hole mobility in the order of 10000 $cm^2V^{-1}s^{-1}$, which shows great promise in electronic devices. To determine if a BP flake is monolayer or multilayer, the frequently used approach is to measure its electron diffraction. A strong (101) reflection in the electron diffraction pattern is generally accepted as a signature of the BP monolayer since this reflection should be forbidden in bulk and few-layer BP. Interestingly, we have observed a strong (101) reflection in BP multilayers flake. Besides, its reflection intensity increases when the BP flake is tilted away from the zone axis. To understand this result, we have simulated the Scanning Transmission Electron Microscopy (STEM) of BP flake using a multislice approach. The (101) reflection is found to be negligible in the Fast Fourier Transform of the STEM of BP flake without sample tilt and becomes remarkable when the BP flake is tilted. This work improves the understanding of the forbidden reflection in BP and demands a better reliable approach to unambiguously determine the BP monolayer.

Session 10: Manufacturing Processes and Systems

Organ manufacturing equipment and technology

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Abstract: Organ manufacturing is expected to solve the problem of clinical tissue and organ shortage. Bioprinting is a promising technology focusing on organ manufacturing. The key problem is the precise assembly of multiple bioinks and biomaterials. We systematically studied the rheological properties of bioink and regulated the printability and biocompatibility of collagen biomaterials under the extrusion process. Complex tissue construction is studied based on extruded multi-material printing. We will present our serialized organ-manufacturing equipment and processes based on novel extrusion processes. As the primary solution, the extrusion-based multi-printhead bioprinting method requires printhead switching during the printing process, which induces inefficient motion time and material interface defects. We present a valve-based consecutive bioprinting method to resolve these problems, containing a precise integrated switching printhead and a well-matched voxelated digital model. As an exemplar, we fabricate a multimaterials complex structure tissue with a vascular tree, then placed it in complete medium with continuous perfusion for 5 d. Our study suggests that the valve-based consecutive bioprinting method is sufficient to fabricate heterogeneous tissues with complex multimaterial interfaces.

Construction and Application of Femtosecond Laser Two-Photon Polymerization Additive Manufacturing System

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Abstract: Using a small domestically developed femtosecond laser, a femtosecond laser two-photon polymerization additive manufacturing system including optical unit, control unit, monitoring unit, and test unit was built, and related control software was independently developed. The entire system integrates spot detection, interface search, micro-nano manufacturing, and performance testing. The problems that may occur in the process of two-photon polymerization additive manufacturing from platform construction to resin preparation to actual polymerization were described in detail, and the causes of the problems were analyzed. The effects of different powers and scanning speeds on the degree of polymerization were compared, and the effect of objective lens magnification on line width was analyzed in detail, a qualitative analysis model was established, and the concepts of threshold expansion effect and focus reduction effect are proposed, and the influence and synergy between these two concepts are discussed. Successfully manufactured a linear structure with micrometer precision and millimeter scale.

Design and Additive Manufacturing of High Performance Porous Ceramics

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Abstract: Porous ceramics, be them with micro pores or macro structs, either in a lattice or an irregular form, have been extensively used in advanced applications, ranging from bone implants, catalytic filters, to functional device components, due to their promising chemical and biological stability, and robust physical properties such as electrochemical, acoustic, optical, and magnetic characteristics. In this presentation, we report current advances of structural and functional ceramic components prepared with an integrated design and 3D printing approach in our institute (AMI-SZU). Honeycomb structures of cordierite are fabricated using DLP polymerization-based 3D printing technique for gas purifier use. Ordered lattice structures of polymer-derived ceramics, such as ZrOC and SiOC, are fabricated via DLP 3D printing technique as well for structural uses and microwave absorption uses. Lattice structures of Li_4SiO_4 are fabricated for tritium breeding used in fusion reactors. Porous thin layers of perovskite LSCF are fabricated using inkjet printing as electrodes used in SOFCs. Porous Li-based structures are fabricated using low temperature direct ink writing as electrodes used in LIBs. The principle, advantages and drawbacks of each 3D printing techniques involved are described in detail and the performance and properties of relevant ceramic components fabricated are discussed.

Design and Fabrication of Soft Materials with Unprecedented Mechanics

Ji Liu

Southern University of Science and Technology

Abstract: The human tissues and organs are mostly soft, wet and bioactive; however, machines are commonly hard, dry and biologically inert. Bridging human-machine interfaces is of importance to address those grand challenges in health, energy and suitability. Functional soft materials emerging at the interface between engineering and biological systems are challenging our fundamental knowledges, motivating technological innovations, and enabling impactful applications. Inspired by the nature's design principles, a great variety of functional soft materials with emerging properties and functions could be readily manufactured. In this talk, I will mainly focus on how to engineer soft materials with unprecedented mechanics, such high toughness and fatigue-resistant properties, by rational control of the multi-length scale structure. Such emerging soft materials could be further engineered as the ingestible electronics for long-term monitoring important physiological conditions and biomarkers, important loading bearing components for soft robots or hydrogel armours. Moreover, fatigue-resistant adhesion between soft materials and engineering matrix, i.e. metals, ceramics, elastomers, will also be discussed.

Effect of Al_2O_3 Content on the Crystallization and Properties of Transparent Glass-Ceramics with High-Fracture Toughness for Mobile Terminals

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Abstract: The mechanical properties of transparent glass-ceramics are greater than that of high-alumina glass, and it is an important protective material for mobile terminals. Among all kinds of transparent glass ceramics, Li_2O-Al_2O_3-SiO_2 (LAS) glass ceramics have excellent mechanical and optical properties. However, LAS glass-ceramics will precipitate many kinds of crystals, which will cause huge changes in performance. For each composition, the content of Al_2O_3 have an dominant effect on the glass structure and crystallization, which in turn affects the later ion strengthening process and mechanical and optical properties, and affects the application of glass-ceramics. Therefore, in this paper, LAS glass-ceramics were prepared by a melt quenching method. Effect of different Al_2O_3 content on the structure, crystallization, transmittance and fracture toughness of LAS glass-ceramics was investigated by means of XRD, FESEM and other methods as well. The results show that the glass transition temperature and crystallization temperature of the glass increase as the content of Al_2O_3 increases, which restrains the precipitation of lithium disilicate crystals. The main crystalline phase of glass-ceramics changes from lithium disilicate and petalite to silicon dioxide, which reduces the fracture toughness of glass-ceramics. When the Al_2O_3 content of is 7.1 wt%, the specimen has outstanding transmittance and fracture toughness. The transmittance is 90.32%. The fracture toughness is 1.13 $MPa \cdot m^{1/2}$. Compared with high-alumina glass, the glass have greatly improved fracture toughness and can be used as a new protective material for mobile terminals.

Effect of Shape on the Mechanical Property of Porous Ti-24Nb-4Zr-8Sn Alloy Fabricated by Electron Beam Melting

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Abstract: In this paper, the porous Ti-24Nb-4Zr-8Sn (Ti2448) alloy with unit cell of rhombic dodecahedron structure and topology optimized structure were fabricated by electron beam melting. The influence of cell morphology on the microstructure, static compressive property and fatigue properties of porous Ti2448 alloy were studied and the internal mechanism was discussed. The results showed that the topology optimized structure had higher compressive strength than rhombic dodecahedron structure for Ti2448 cellular structure. Whilst rhombic dodecahedron structure had smoother compressive curves, this was the typical deformation behavior of ductile metal porous materials. Under the strain-controlled fatigue (low cyclic fatigue), the fatigue life of Ti2448 cellular structure decreased with the increase of applied strain. For the same rhombic dodecahedron cellular structure, Ti2448 alloy had better fatigue resistance than Ti-6Al-4V alloy. Firstly, porous Ti2448 alloy had lower accumulation of plastic strain, so the fatigue cracks initiation life was prolonged. Secondly, fatigue cracks of Ti2448 porous specimens were deflected at the grain boundaries, which increases the fatigue crack propagation life of the material. Under the stress-controlled fatigue (high cyclic fatigue), the fatigue strength of porous structure is proportional to the static compressive strength. The static compressive strength can be improved by adjusting cell shape, further to improve the high cyclic fatigue property.

Fabrication of 3D Printed Hydrogel Scaffolds and Their Application in Tissue Regeneration and Repair

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Abstract: Tissue engineering scaffolds with host tissue mechanical and biological properties provide a new therapy for the regeneration of damaged tissues or organs. 3D printing technology enables the scaffold to have more controllable structure and morphology, which can accurately replicate the structure and function of natural tissues. Our team, starting from the design of material chemistry and material structure, is committed to the development of bio-inks to construct scaffolds with natural tissue structures and functions. In terms of the construction of bionic blood vessels, we designed the 3D printed scaffolds to form a vascular network with a bifurcated structure by the "dynamic sacrificial printing"; combined with the droplet microfluidic technology, we prepared the hollow hydrogel fibers with vascular barrier function in the 3D printed microfluidic chip. In order to reconstruct cartilage, we fabricated a microporous hydrogel scaffold through horseradish peroxidase-mediated crosslinking of silk fibroin and tyramine-substituted gelatin by low-temperature 3D printing, followed by seeding stem cell aggregate. In terms of simulating bone structure, we prepared a double-crosslinked 3D printed hydrogel scaffold loaded with copper-doped bioactive glass, which owns the function of promoting osteogenesis and angiogenesis. In addition to the hydrogel bio-inks, we have prepared a new type of microgel bio-ink. The ink not only has good printability, but also has injection protection and microporosity. It protects cells from the damage of shear force and ensures that cells have high activity after printing. Meanwhile, the connected microporous structure is conducive to cell infiltration and extracellular matrix deposition.

Functionalized Biofabrication Technologies for Tissue Regeneration

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Abstract: Damages of cartilage, tendon, and other soft tissues are common sports injuries, which cover a wide range of patient ages. 3D bioprinting has the ability to prepare artificial tissues, which can control the distribution of cells, extracellular matrix, and other bioactive compounds in different locations of the engineered tissues. In a series of studies, we focus on the development of bioprinting techniques such as extrusion-based bioprinting, aspiration-assisted bioprinting, and electro-hydrodynamic jet printing, etc. We have investigated the major issues on biofabrication, including 1) the control and optimization of the bioprinting processes, 2) preparation and characterization of bioink with high cell density, 3) fabrication of artificial tissues with anatomically relevant structures and functions, 4) induction of bioprinted tissue in terms of biological functions and physical properties, 5) multi-scale biofabrication and regeneration of soft tissues. Regarding biomedical applications, we explore the biofabrication of zonally-stratified cartilage with high cell density, which imitates the collagen and cellular organization of the native tissue, and possesses similar mechanical properties of the human cartilage. In addition, we develop a novel fabrication process to generate porous tissues with controllable porosities, which can be differentiated into cartilage and bone tissues. In another case, tendon scaffolds with fibrous structure and enhanced mechanical properties are also developed, in which the cellular organization can be regulated. Through these studies, we use different biofabrication technologies creatively to construct artificial tissues that can be potentially applied for the repair of human tissue defects, which aims to realize the integration of structural mimicry and bio-functionalization.

Microstructure and Mechanical Properties of Beta-Type Ti-24Nb-4Zr-8Sn Porous Structure Fabricated by Electron Beam Melting

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Abstract: Porous titanium and its alloys have been considered as promising replacement for dense implants, considering they possess low elastic modulus matching to that of human bone and are capable of providing space for in-growth of bony tissue to achieve a better fixation. Recently, additive manufacturing (AM) using the electron beam melting (EBM) method has been successfully applied to fabrication of Ti-6Al-4V cellular meshes and foams. However, the toxicity of elements (i.e. Al, V) and low fatigue strength of EBM-produced Ti-6Al-4V components has been pointed out. To avoid these shortcomings, fabrication of low-modulus non-toxic b-type titanium alloy cellular structures is good choice. In this talk, electron beam melting (EBM) is applied to manufacture β-type Ti-24Nb-4Zr-8Sn porous components with 60–90% porosity. Microstructures, defects and mechanical properties of EBM-produced components are investigated. The processing-microstructure-property relationship and deformation behavior of EBM-produced components are detailed discussed.

Material Characterisation and Multi-Physics Computational Modelling of Electron Beam Powder Bed Fusion Additive Manufacturing of Ti2448 Titanium Alloy

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Abstract: The metastable b-type Ti-24Nb-4Zr-8Sn (Ti2448) alloy has been successfully manufactured by electron beam powder bed fusion (PBF-EB) technique, which is currently receiving extensive attention in the field of processing and manufacturing. In this work, cylindrical samples of Ti2448 alloy have been successfully manufactured by using electron beam powder bed fusion (PBF-EB) technique. Thermal history and microstructure of manufactured samples are characterised using computational and experimental methods. To analyse the influence of thermal history on microstructure of materials, the thermal process of PBF-EB has been computationally predicted using the layer-by-layer modelling method. The microstructure of the Ti2448 alloy mainly includes orth phase and β phase. The profile of orth phase along the radius of manufactured samples is different from that along the height of samples. By comparing the experimental results of material microstructure with the computational modelling results of material thermal history, it can be seen that aging time and aging temperature lead to the variation of orth phase content in manufactured samples. Variation in thermal history from location to location of a manufactured sample results in nonuniform profile of grain size. The computational modelling proves to be an effective tool that can help experimentalists to understand the influence of macroscopic processes on material microstructural evolution and hence potentially optimise the process parameters of PBF-EB to eliminate or otherwise modify such microstructural gradients.

Near Net Forming Research for Fin-Typed LED Radiator

Ni Ly

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Abstract: Pure aluminum radiator is the best choice for heat dissipation of various LED products at present. Its forming methods include common extrusion forming, die casting forming, forging forming and so on. Compared with other forming technologies, the LED radiator formed by cold forging has good heat dissipation performance, but there are some disadvantages in the forming process, such as uneven deformation, large material consumption and low die life. Taking fin-typed radiator as an example, the cold forging process of pure aluminum radiator is analyzed by finite element method. The calculation results show that improper die structure may lead to serious uneven flow velocity distribution of aluminum in the cold forging die, inconsistent fin length and warpage tendency. The equal hole diameter structure of radiator cold forging die is modified to gradient hole diameter. Numerical simulation and production test show that the modified structure design can improve the significant uneven metal flow rate in the die. The extruded fins have uniform length, which is conducive to reducing subsequent machining and production cost.

Study on Annular Laser Cladding Process with Small-Spot Powder Stream Coaxially Feeding into the Center of the Focused Laser

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Abstract: Annular laser metal deposition (ALMD) is a typical metal material processing technology using annular focused high-energy laser beam coaxially coupled with the deposited material transported in the laser for substrate surface. Compared with other existing laser metal deposition technologies, it has a significant improvement in laser energy utilization, material deposition rate, laser and material coupling accuracy, deposition process stability, processing freedom and deposition layer bonding quality. Based on the above advantages, the technology is widely used to repair worn parts, for instance, aircraft engine, corroded hull surface and mechanical equipment commonly used in the mining industry, and gradually applied to additive manufacturing (AM) of precision parts. In this paper, a high-precision powder deposition processing head with an annular laser beam (ALB) was proposed, which includes an energy excitation unit, a beam shaping & focusing unit and a powder feeding unit. Compared with conventional annular laser cladding processing heads, it can produce a cladding layer with narrower melt path and better quality on the substrate surface. The article explored the influence of the focusing lens' type (spherical lens & aspherical lens) on the spot size and energy distribution of the annular focused beam by means of optical model simulation and beam quality testing. The influence of the above factor combined with different powder feeding tube diameters (0.8 mm, 1.0 mm, 1.2 mm and 1.6 mm) on the cladding process has been characterized based on the geometry and porosity of the cladding layer. The results showed that an aspheric lens with a smaller spot diameter in the optical path of the processing head can produce deposition spots with higher accuracy and better quality when it was combined with the small diameter of the powder feeding tube in the powder feeding unit.

Study on Machining Process for Inner Surface of SUS Pipeline Used in Hydrogen Flow System by MAF Process

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Abstract: In this paper, we study on the machining process for inner surface of SUS pipeline used in hydrogen flow system by MAF process. Various SUS pipelines are generally applied for the transporting of high purity substances such as hydrogen gas used in many applications for semiconductors, LEDs, displays, and other photovoltaic segments. But, the limitations of these components, e.g., bad surface quality, low precision/accuracy, and dirty surface are demanded to be enhanced before they have been used. Thus, this paper studies the new application of magnetic abrasive finishing process (MAFP) for generating the smoothness surface of SUS pipeline in hydrogen flow system. This process used a strong flux density of magnets with unbonded magnetic particles to remove the foreign particles and rough part from the surface of SUS pipeline, helping in decreased the friction coefficient and wear resistance, and reduced the hydrogen gas waste during the transporting process. The results indicated that this new machining process for inner finishing of SUS pipeline used in hydrogen flow system are feasible to achieve good quality and high efficiency of SUS pipe line in which the surface accuracy is down from 0.24 μm to 0.05 μm within the short machining time.

Study on the Multiple-Ram Forging Technology of the High Temperature-Pressure Valve Body

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Abstract: The study on the multiple-ram forging of the high temperature-pressure valve body is intended to meet the technical requirements for the valve body sustaining high steam parameters in thermal power generation units. The multiple-ram forging of a 3-inch gate valve body was used as an example to demonstrate the features of the multiple-ram forging, in which principles and methods of multi-ram forging was elaborated through the die design of the 3-inch gate valve body. Numerical simulation was used to investigate the influence of the tool's movement sequence on the forming load, clamping force, the horizontal punch load, the vertical punch load and the temperature distribution on the tools. The experiment on a 40 MN multi-ram hydraulic press produced a 3-inch gate valve body forging with required dimensions. In compliance with national technical requirements, mechanical properties test and the forging flow line observation were done with the multi-ram forged valve body, which indicate that: the multi-ram forged valve body achieved better technical qualities than those required by the national standard.

Exploring on Functional Bioinks for 3D Bioprinting of Tissue-engineered Constructs

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Abstract: The emerging 3D bioprinting technique that is strongly dependent on the development of bioinks offers a promising opportunity to customize personalized bioscaffolds for precision and individualized therapy of tissue defects [1-5]. The biomaterials which can be used as bio-inks for tissue regeneration should satisfy the following basic requirements: (1) extrusion properties – suitable rheology for bioprinting; (2) stability – the printed scaffolds should not collapse before solidification or crosslinking; (3) biocompatibility and porosity – high cell viability after printing, with optimal avenues for the adequate diffusion of nutrients and oxygen to facilitate cell proliferation or differentiation in the short term; (4) appropriate mechanical properties; and (5) tissue inducing capability to promote cell differentiation and new tissue formation in the long term. On basis of these requirements, we currently developed a series of functional bioinks for facile extrusion bioprinting, include the modification of alginate/gelatin-based bioinks, high strength hydrogel-based bioinks and so on.

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