

# Phase Engineering of Nanomaterials

📅 20 - 22 November 2024

📍 Wong Cheung Lo Hui Yuet Hall  
Floor 5, Lau Ming Wai Academic Building  
City University of Hong Kong  
Tat Chee Avenue, Hong Kong



*Register Now*

## Scientific Committee

Prof. Freddy Boey, *CityUHK*  
Prof. Chun-Sing Lee, *CityUHK*  
Prof. Mengsu (Michael) Yang, *CityUHK*  
Prof. Shuk Han Cheng, *CityUHK*  
Prof. Jian Lu, *CityUHK*  
Prof. Xin Wang, *CityUHK*  
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Dr. Kristina Karez, *Nature*  
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Dr. Alexander Rosu-Finsen, *Nature Reviews Chemistry*  
Dr. Xin Li, *Nature Materials*  
Dr. Lu Shi, *Nature Nanotechnology*  
Dr. Davide Esposito, *Nature Catalysis*  
Dr. Ali Stoddart, *Nature Synthesis*

# Nature Conference on Phase Engineering of Nanomaterials 2024 | Nov 20-22, 2024

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## Nature Conference on Phase Engineering of Nanomaterials 2024

### Background

Organized by City University of Hong Kong, Hong Kong Institute for Clean Energy, Department of Chemistry, Department of Material Science and Engineering, Hong Kong Branch of National Precious Metals Material Engineering Research Center, Nature, Nature Communications, Nature Reviews Materials, Nature Review Chemistry, Nature Materials, Nature Nanotechnology, Nature Catalysis and Nature Synthesis.

After the success of the inaugural Nature Conference on "Chemistry of 2D materials" in 2022, held virtually, we are pleased to announce the upcoming Nature Conference on "Phase Engineering of Nanomaterials". This on-site conference aims to gather renowned international experts for in-depth discussions and knowledge sharing on the phase-dependent properties of different nanomaterials. Topics to be covered include chemical synthesis, processing, characterization, and phase engineering of transition metal dichalcogenides and other nanomaterials, as well as their applications in advanced electronics and catalysis.

The Conference will consist of a series of plenary talks from world-leading scientists sharing sessions featuring the following areas:

- I. Phase engineering of transition metal dichalcogenides
- II. Phase engineering of metallic nanomaterials and In-situ studies of phase transformation
- III. Phase-dependent electrocatalysis and photocatalysis
- IV. Phase-dependent wet-chemical synthesis
- V. Phase-based heterostructures for electronics and catalysis

## **Nature Conference on Phase Engineering of Nanomaterials 2024 | Nov 20-22, 2024**

**Organiser:** City University of Hong Kong  
Hong Kong Institute for Clean Energy, City University of Hong Kong  
Department of Chemistry, City University of Hong Kong  
Department of Materials Science and Engineering, City University of Hong Kong  
Hong Kong Branch of National Precious Metals Material Engineering Research Center, City University of Hong Kong  
Nature  
Nature Communications  
Nature Reviews Materials  
Nature Reviews Chemistry  
Nature Materials  
Nature Nanotechnology  
Nature Catalysis  
Nature Synthesis

**Date:** November 20-22, 2024

**Venue:** Wong Cheung Lo Hui Yuet Hall  
Floor 5, Lau Ming Wai Academic Building  
City University of Hong Kong  
Tat Chee Avenue, Hong Kong

**Language:** English

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Prof. Jian LU, City University of Hong Kong  
Prof. Xin WANG, City University of Hong Kong  
Prof. Xiaocheng ZENG, City University of Hong Kong  
Prof. Hua ZHANG, City University of Hong Kong  
Kristina KAREH, Nature  
Antonio FORNIERI, Nature Communications  
Silvia MILANA, Nature Communications  
Charlotte ALLARD, Nature Reviews Materials  
Alexander ROSU-FINSEN, Nature Reviews Chemistry  
Xin LI, Nature Materials  
Lu SHI, Nature Nanotechnology  
Davide ESPOSITO, Nature Catalysis  
Ali STODDART, Nature Synthesis

### **Coordinator:**

Prof. Zhanxi FAN, City University of Hong Kong  
Prof. Qiyuan HE, City University of Hong Kong  
Prof. Thuc Hue LY, City University of Hong Kong  
Prof. Zonglong ZHU, City University of Hong Kong

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### Organisers



City University of Hong Kong (CityUHK) is a world-class institution ranked among the best universities internationally and is committed to nurturing and developing the talents of students, and creating applicable knowledge to contribute to social and economic advancement. CityUHK puts particular emphasis on professional education and research, covering different disciplines, namely business, creative media, data science, energy and environment, engineering, humanities and social sciences, law, science and veterinary medicine, and life sciences. Our 30th-anniversary celebrations, which begin in January 2024, will feature events that highlight our accomplishments, our exceptional students, our faculty's world-class research, and our extensive local and international network of friends and supporters, all of whom have contributed to CityUHK's standing as an outstanding higher education institution.



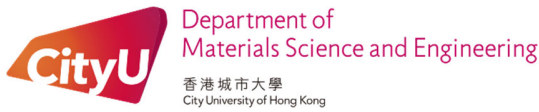
The Hong Kong Institute for Clean Energy (HKICE) aims to be a global leader in promoting cutting-edge research, education, and technology development in clean energy to tackle the grand challenges on achieving global net-zero carbon emission. It provides a vibrant platform to integrate diverse background professionals working in clean energy to train next-generation leaders and generate sustainable environmental solutions for creating societal impacts.



The Department of Chemistry at City University of Hong Kong is a vibrant hub where research and education thrive, united by a commitment to excellence in all its endeavours. Our ambition is to be recognized as a leading chemistry department in the Asia-Pacific region, both within Hong Kong and on the global stage. This vision is driven by our dedication to providing high-quality professional education that equips students with the skills and knowledge to succeed, conducting cutting-edge research that advances scientific understanding, and using our knowledge and expertise to address societal needs and promote sustainable development. We are committed to nurturing and developing our students, transforming research output into knowledge and technologies that benefit society, the region, and the world. By fostering a culture of excellence, innovation, and social responsibility, we strive to make a significant contribution to the advancement of chemistry and the betterment of humanity.

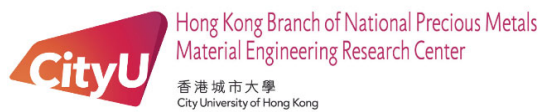


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Being the first of its kinds in Hong Kong, the Department of Materials Science and Engineering was established in 2017 with the aims to develop internationally competitive and leading-edge research and to provide a professional education curriculum that equips graduates to contribute to Hong Kong, the Greater China, and the whole world in materials science and engineering and related sectors.

The Department aspires to become one of the world-leading departments in research and professional education with a focus on four targeted areas, namely, 1) Computational materials science; 2) Functional materials; 3) Structural materials; 4) Materials characterization.



The establishment of the Hong Kong Branch of National Precious Metals Material Engineering Research Center (NPMM) at City University of Hong Kong (CityU) was approved by the Ministry of Science and Technology (MOST) of the People's Republic of China in November 2015. The core objective of setting up the branch is to strengthen the national center's overall capacity by developing the research of precious metals and nanomaterials, as well as the relevant devices.

Precious metal elements (gold, silver, platinum, palladium, rhodium, iridium, osmium and ruthenium) because of the particularity of atomic structure, showed excellent physical and chemical properties (such as high temperature oxidation resistance and corrosion resistance), electrical properties (excellent electrical conductivity, high temperature thermoelectric performance and stable temperature coefficient of resistance, etc.), high catalytic activity, strong coordination ability and therefore have a wide use in industry and are closely related to the development of modern high-tech.

NPMM positions itself to carry out fundamental and applied research to develop new precious metallic materials and upgrade conventional precious metallic materials and to fulfill the need of precious materials for the development of national economy, high-tech industrial development and national defense.

## **nature**

A weekly, international journal, publishing papers from any area of science with great potential impact and whose importance extends well beyond the confines of the specific discipline concerned. Nature has the highest impact factor of any journal publishing basic scientific research. Nature also publishes Reviews, as well as a broad range of informal material in the form of Editorials, News and News Features, Correspondence, Opinion, News and Views, Books and Arts, Futures (the award-winning science-fiction series) and NatureJobs (articles on careers and recruitment). The journal also publishes regular supplements, including Insights, Outlooks and Technology Features. Nature publishes much online-only information, including the award-winning daily Nature News, blogs, regular web focuses (collections of topical material, often from the journal's archive) and other web-only special features.

## **nature communications**

Nature Communications is an open access journal that publishes high-quality research from all areas of the natural sciences. Papers published by the journal represent important advances of significance to specialists within each field.

## **nature reviews materials**

Nature Reviews Materials is an online-only journal for the weekly publication of Reviews, Perspectives and Comments in all scientific disciplines within materials science.

Our Reviews aim to be balanced and objective analyses of the selected topic - with descriptions of relevant scientific literature and discussions that are easy to grasp for recent graduates in any materials-science related discipline, as well as informing principal investigators and industry-based research scientists of the latest advances. Reviews should provide the authors' insight into future directions and their opinion of the major challenges faced by researchers in the field.

## **nature reviews** chemistry

Nature Reviews Chemistry is an online-only journal for the weekly publication of Reviews, Perspectives and Comments in all disciplines within chemistry.

Our Reviews aim to be balanced and objective analyses of the selected topic – with descriptions of relevant scientific literature and discussions that are easy to grasp for recent graduates in any chemistry-related discipline, as well as informing principal investigators and industry-based research scientists of the latest advances. Reviews should provide the authors' insight into future directions and their opinion of the major challenges faced by researchers in the field.

## **nature** materials

Nature Materials is a monthly multi-disciplinary journal aimed at bringing together cutting-edge research across the entire spectrum of materials science and engineering. Materials research is a diverse and fast-growing discipline, which has moved from a largely applied, engineering focus to a position where it has an increasing impact on other classical disciplines such as physics, chemistry and biology. Nature Materials covers all applied and fundamental aspects of the synthesis/processing, structure/composition, properties and performance of materials, where "materials" are identified as substances in the condensed states (liquid, solid, colloidal) designed or manipulated for technological ends.

## **nature** nanotechnology

Nature Nanotechnology is an interdisciplinary journal that publishes papers of the highest quality and significance in all areas of nanoscience and nanotechnology. The journal covers research into the design, characterization and production of structures, devices and systems that involve the manipulation and control of materials and phenomena at atomic, molecular and macromolecular scales. Both bottom-up and top-down approaches — and combinations of the two — are covered.

Nature Nanotechnology also encourages the exchange of ideas between chemists, physicists, material scientists, biomedical researchers, engineers and other researchers who are active at the frontiers of this diverse and multidisciplinary field. Coverage extends from basic research in physics, chemistry and biology, including computational work and simulations, through to the development of new devices and technologies for applications in a wide range of industrial sectors (including information technology, medicine, manufacturing, high-performance materials, and energy and environmental technologies). Organic, inorganic and hybrid materials are all covered.

## **nature catalysis**

Launched in January 2018, Nature Catalysis is a monthly, online-only journal incorporating the best research from all areas of catalysis. Our broad scope, drawing from the work of scientists, engineers and researchers in industry and academia, ensures that published work reaches the widest possible audience.

Nature Catalysis brings together researchers from across all chemistry and related fields, publishing work on homogeneous catalysis, heterogeneous catalysis, and biocatalysts, incorporating both fundamental and applied studies. We have a particular interest in applied work that advances our knowledge and informs the development of sustainable industries and processes. Nature Catalysis provides coverage of the science and business of catalysis research, creating a unique journal for scientists, engineers and researchers in academia and industry.

## **nature synthesis**

Nature Synthesis is a new online journal, launched in January 2022. The journal is interested in all aspects of synthesis, from making discrete molecules to extended materials, as well as technological innovations leading to significant advances in synthetic methods and processes.

Nature Synthesis aims to bring together researchers from all areas of chemical and materials synthesis, publishing work based on organic, inorganic, organometallic and materials chemistry, as well as interdisciplinary studies at the interfaces between these disciplines. The journal will focus on the development of new synthetic methods and approaches, together with the preparation of molecular- or materials-based products that have practical value in research and society or extend our conceptual understanding of chemical or material systems.

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**Event Programme**

**Wednesday, November 20, 2024 (Day 1)**

**AM Session**

**08:00 – 08:30**

**Registration and Welcome Reception**

**08:30 - 09:00**

**Opening Ceremony**

**Welcoming Address**

Prof. Freddy BOEY, President of City University of Hong Kong

**Opening Remarks**

Dr. Antonio FORNIERI, Editor of Nature Communications

**Photo-taking**

**Session I: Phase engineering of transition metal dichalcogenides**

**09:00 - 09:30**

Session Chair: Hua ZHANG

**Talk 1: Recent Studies on 2D Hybrid Perovskites**

Kian Ping LOH

National University of Singapore, Singapore

**09:30 - 10:00**

**Talk 2: Phase-Controlled Synthesis of Ultra-Thin Transition Metal Chalcogenides**

Liying JIAO

Tsinghua University, China

**10:00 - 10:30**

**Talk 3: Phase Engineering of 2D Materials**

Heejun YANG

Korea Advanced Institute of Science & Technology (KAIST), South Korea

**10:30 - 11:00**

Tea Break

**11:00 - 11:30**

Session Chair: Antonio FORNIERI

**Talk 4: Super Graphene-Skinned Materials: Concept, Synthesis and Applications**

Zhongfan LIU

Beijing Graphene Institute (BGI) & Peking University, China

**11:30 - 12:00**

**Talk 5: State-of-The-Art Processing of 2D Materials**

Thuc Hue LY

City University of Hong Kong, HKSAR, China

**12:00 - 12:30**

**Talk 6: Phase and Composition Controlled Syntheses and Magnetic Property Explorations of 2D Metallic Transition-Metal Dichalcogenides**

Yanfeng ZHANG

Peking University, China

**12:30 - 14:00**

Lunch (By Invitation)

PM Session

**Session II: Phase engineering of metallic nanomaterials and In-situ studies of phase transformation**

**14:00 - 14:30** Session Chair: Charlotte ALLARD

**Talk 7: Electron Microscopy Imaging of Electron Beam-Sensitive Crystalline Materials**

Yu HAN

South China University of Technology, China

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**14:30 - 15:00** **Talk 8: Platinum Group Metal-Based Solid-Solution Alloy Nanocrystals: Binary to High-Entropy Alloys**

Hiroshi KITAGAWA

Kyoto University, Japan

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**15:00 - 15:30** **Talk 9: The Role of Atomic Defects in Phase Engineering of 2D Van der Waals Structures and Nanoparticles**

Ute KAISER

University of Ulm, Germany

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**15:30 - 16:00**

Tea Break

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**16:00 - 16:30** Session Chair: Xin LI

**Talk 10: Crystal Nucleation and Growth in High-Entropy Alloy Nanoparticles Revealed by Atomic Electron Tomography**

Jianwei John MIAO

University of California, Los Angeles, USA

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**16:30 - 17:00** **Talk 11: Revealing Kinetically Tuned Atomic Pathways for Interfacial Strain Relaxation**

Haimei ZHENG

Lawrence Berkeley National Lab, USA

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**17:00 - 17:15** **Short Talk 1: Crystallinity Modulation and Catalytic Property Study of Pd-Based Nanomaterials**

Hongfei CHENG

Tongji University, China

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**17:15 - 17:30** **Short Talk 2: Synthesis and Phase-Dependent Catalytic Behaviors of Unconventional-Phase Noble Metal Nanomaterials With Facet Precision**

Ye CHEN

The Chinese University of Hong Kong, Hong Kong, HKSAR, China

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**18:00 - 21:00**

Conference Dinner (By Invitation)

Thursday, November 21, 2024 (Day 2)

AM Session

08:30 - 09:00

Welcome Reception

Session III: Phase-dependent electrocatalysis and photocatalysis

09:00 - 09:30

Session Chair: Zhanxi FAN

**Talk 12: Phase Engineering of Nanomaterials (PEN)**

Hua ZHANG

City University of Hong Kong, HKSAR, China

09:30 - 10:00

**Talk 13: L1<sub>0</sub>-Intermetallics: Structure Stability and Catalysis Enhancement**

Shouheng SUN

Brown University, USA

10:00 - 10:30

**Talk 14: Supported Metal Catalysts Powered by Interpretable Machine Learning**

Wei-Xue LI

University of Science and Technology of China, China

10:30 - 11:00

Tea Break

11:00 - 11:30

Session Chair: Alexander ROSU-FINSEN

**Talk 15: From N-Alkane to Conjugated Polyene and Their Aromatization  
Via On-Surface Chemistry**

Lifeng CHI

Soochow University, China

11:30 - 12:00

**Talk 16: Charge Separation in Photocatalysis for Solar Hydrogen Production from Water  
Splitting**

Can LI

Dalian Institute of Chemical Physics, Chinese Academy of Sciences, China

12:00 - 12:30

Poster session

12:30 - 14:00

Lunch (By Invitation)

PM Session

Session IV: Phase-dependent wet-chemical synthesis

14:00 - 14:30 Session Chair: Yu HUANG

**Talk 17: Phase-Controlled Synthesis of Noble-Metal Nanocrystals: Templating Effect versus Reaction Kinetics**

Younan XIA

Georgia Institute of Technology, USA

14:30 - 15:00 **Talk 18: Towards Precise Control of Chemical Reactions on Metal**

Nanfeng ZHENG

Xiamen University, China

15:00 - 15:30 **Talk 19: Electron Videography of Colloidal Nanoparticles**

Qian CHEN

University of Illinois Urbana-Champaign, USA

15:30 - 16:00

Tea Break

16:00 - 16:30 Session Chair: Qiyuan HE

**Talk 20: Unlocking the Future of Clean Energy: Predicting and Designing Durable Catalysts for Hydrogen Fuel Cells**

Yu HUANG

University of California, Los Angeles, USA

16:30 - 17:00 **Talk 21: Phase Engineering of Atomically Precise Gold Nanoclusters**

Rongchao JIN

Carnegie Mellon University, USA

17:00 - 17:30 **Talk 22: Synthesis and Catalytic Properties of Amorphous Nanosheets**

Xun HONG

University of Science and Technology of China, China

18:00 - 21:00

Conference Banquet for All



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Friday, November 22, 2024 (Day 3)

AM Session

08:30 - 09:00

Welcome Reception

Session V: Phase-based heterostructures for electronics and catalysis

09:00 - 09:30 Session Chair: Thuc Hue LY

**Talk 23: Contemporary Challenges in Van der Waals Layered Semiconductors**

Young Hee LEE

Sungkyunkwan University, South Korea

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09:30 - 10:00

**Talk 24: Metallic Two-Dimensional Transition Metal Dichalcogenides**

Manish CHHOWALLA

University of Cambridge, UK

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10:00 - 10:30

**Talk 25: Phase Engineering Of WS<sub>2</sub> And MoS<sub>2</sub> Monolayer Quantum Dots by Rhenium**

Hyeon Suk SHIN

Sungkyunkwan University, South Korea

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10:30 - 11:00

Tea Break

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11:00 - 11:30 Session Chair: Zonglong ZHU

**Talk 26: Solution-Processed Nanosheets for Electronic Devices: Towards Homo- and Hetero-Stacks with Controlled Interfaces**

Jonathan COLEMAN

Trinity College Dublin, Ireland

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11:30 - 12:00

**Talk 27: Van der Waals Superlattices: The Bo(u)ndless Frontier**

Xiangfeng DUAN

University of California, Los Angeles, USA

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12:00 - 12:30

Poster session

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12:30 - 14:00

Lunch (By Invitation)

PM Session

Short Talk Session

14:00 - 14:15 Session Chair: Kristina KAREH

**Short Talk Session II**

**Short Talk 3: Advanced Atomic Catalysts Design For Energy Systems**

Bolong HUANG

The Hong Kong Polytechnic University, HKSAR, China

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14:15 - 14:30 **Short Talk 5: Stories About Single Atom Catalysis**

Huabin ZHANG

King Abdullah University of Science and Technology, Kingdom of Saudi Arabia

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14:30 – 14:45 **Short Talk 6: Mass Transfer Enhanced Electrocatalytic CO<sub>2</sub> Conversion**

Guobin WEN

Hunan University

Panel Discussion

14:45 – 15:45 Session Chair: Hua ZHANG

**Perspective, Challenges, and Opportunities in Phase Engineering of Nanomaterials**

Manish CHHOWALLA, Thuc Hue LY, Silvia MILANA, Heejun YANG, Haimei ZHENG

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15:45 – 15:55 **Poster Award Ceremony**

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15:55 - 16:00

**Closing Remarks**

Prof. Hua ZHANG, Director, Hong Kong Institute for Clean Energy

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**Program Abstract**

**Session I: Phase Engineering of Transition Metal Dichalcogenides**

**[Session I] Talk 1: Kian Ping LOH**

**RECENT STUDIES ON 2D HYBRID PEROVSKITES**

Kian Ping LOH

Department of Chemistry, National University of Singapore

Department of Applied Physics, Hong Kong Polytechnic University

[kian-ping.loh@polyu.edu.hk](mailto:kian-ping.loh@polyu.edu.hk) ; [chmlohkp@nus.edu.sg](mailto:chmlohkp@nus.edu.sg)

**First report of charge-to-spin conversion and spin hall conductivity on 2D Hybrid Organic-inorganic perovskites.**

We demonstrate highly efficient electrically driven charge-to-spin conversion in enantiopure chiral perovskites  $(R/S\text{-MB})_2(\text{MA})_3\text{Pb}_4\text{I}_{13}$  ( $\langle n \rangle = 4$ ). We measured a spin Hall angle  $\theta_{sh}$  of 5% and a spin lifetime of  $\sim 95$  ps at room temperature in  $\langle n \rangle = 4$  chiral perovskites, which is much larger than its racemic counterpart as well as the lower  $\langle n \rangle$  homologues. In addition to current-induced transverse spin current, the presence of a co-existing out-of-plane spin current confirms that both conventional and collinear spin Hall conductivities exist in these low-dimensional crystals.

**First Synthesis of New Phase 2D All Organic Perovskites**

We report the synthesis of metal-free 2D layered perovskite with the formula of  $\text{A}_2\text{B}_2\text{X}_4$ , which we christened as Choi-Loh van der Waals phase (CL-v phase). CL-v phase is reminiscent of Ruddlesden-Popper phase in terms of having a van der Waals gap mediated by interlayer hydrogen bonding, and can be grown or exfoliated into 2D organic sheets. As a hallmark of layered materials with van der Waals gap, changes in interlayer sliding enables polymorphs to be synthesized. Use as ultrathin dielectric layer in 2D materials FET was demonstrated.

**Reference**

- [1] Molecularly thin, two-dimensional all-organic perovskites, HS Choi, J Lin, G Wang, WPD Wong, IH Park, F Lin, J Yin, K Leng\*, J Lin\*, **Kian Ping Loh\*** *Science* 384 (6691), 60-66 (2024)
- [2] Two-Dimensional Chiral Perovskites with Large Spin Hall Angle and Collinear Spin Hall Conductivity, Ibrahim Abdelwahab, Jun Yin\*, Hyun Soo Yang\* and **Kian Ping Loh\*** et. al. *Science*, accepted June 2024.

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Kian Ping LOH obtained his Bachelor degree (Hons) from the National University of Singapore, Chemistry department in 1994, and his Ph.D. from the Physical and Theoretical Chemistry Laboratory, University of Oxford in 1996. He is a professor of Chemistry at the National University of Singapore. He is the director of the Jockey Club STEM laboratory on Quantum Materials and Physics at Hong Kong Polytechnic University. LOH's recent research focuses on the growth, molecular chemistry, electronic material science, and devices of 2D materials, which include 2D covalent organic framework, 2D hybrid perovskites, and 2D Topological Quantum materials. He is on the Clarivate's list of highly cited scientists from 2018-2023. He is an Academician of the Asia Pacific Academy of Materials (2015) and also an Academician of Singapore's National Academy of Science (2024). He is the winner of Singapore's President's Science Award in 2014 and the American Chemical Society Nano lectureship award in 2013.

[Session I] Talk 2: Liying JIAO

PHASE-CONTROLLED SYNTHESIS OF ULTRA-THIN TRANSITION METAL CHALCOGENIDES

Liying JIAO

Department of Chemistry, Tsinghua University, Beijing, China

[lyjiao@mail.tsinghua.edu.cn](mailto:lyjiao@mail.tsinghua.edu.cn)

Two-dimensional (2D) transition metal chalcogenides (TMCs) offer a variety of ultrathin components for the construction of high-performance electronic devices and serve as promising platforms for investigating quantum phenomena. The properties of 2D TMCs are highly dependent on their phase states, making the phase-controlled synthesis of these materials essential for both property exploration and application development. Utilizing phase diagrams as a guide, we have developed phase-controlled synthesis methods for 2D TMCs through vapor phase deposition or interfacial reactions, successfully achieving the synthesis of various 2D TMCs, such as MoS<sub>2</sub>, MoTe<sub>2</sub>, PdTe<sub>x</sub>, FeCr<sub>2</sub>S<sub>4</sub> and so on. Building upon phase-controlled synthesis, we have investigated the superconductivity, ferromagnetism, and ferroelectricity of these 2D TMCs and have constructed devices such as ferroelectric field-effect transistors, logic and radio frequency components, and magnetic tunnel junctions.



Liying JIAO is currently a Professor in the Department of Chemistry, Tsinghua University. She received her B.S. from Shandong University in 2003, and her Ph.D. from Peking University in 2008. She performed postdoctoral research in Stanford University during 2008-2012. She joined the Tsinghua faculty in 2012 as an Associate Professor and was promoted to Full Professor in 2021. Her research is focused on the synthesis and electronic devices of low dimensional materials.

[Session I] Talk 3: Heejun YANG

PHASE ENGINEERING OF 2D MATERIALS

Heejun YANG

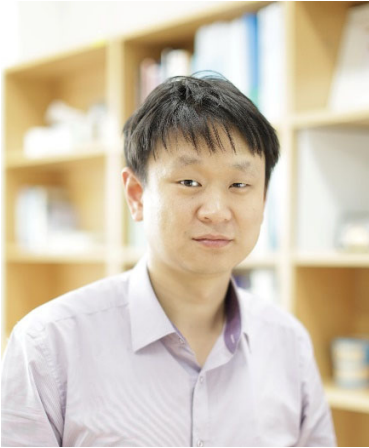
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Polymorphic 2D materials allow structural and electronic phase engineering, which can be used to realize energy-efficient, cost-effective, and scalable device applications [1-5]. Phase engineering covers not only conventional structural and metal-insulator transitions [1, 2] but also magnetic states, strongly correlated band structures, and topological phases in rich 2D materials [3]. The methods used for the local phase engineering of 2D materials include various optical, geometrical, and chemical processes, as well as traditional thermodynamic approaches. In this seminar, I will present our recent studies on the precise manipulation of local phases and phase-patterning of 2D materials, particularly with ideal and versatile phase interfaces for electronic and energy device applications [5, 6]. Polymorphic 2D materials and diverse quantum materials with their layered, vertical, and lateral geometries will be discussed, with an emphasis on the role and use of their phase interfaces. Various phase interfaces have demonstrated superior and unique performance in electronic and energy devices. The phase patterning leads to novel homo- and hetero-junction structures of 2D materials with low-dimensional phase boundaries, which highlights their potential for technological breakthroughs in future electronic, quantum, and energy devices.

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- [3] Structural and quantum-state phase transition in van der Waals layered materials, *Nature Physics* 13, 931 (2017)
- [4] Polymorphic spin, charge, and lattice waves in vanadium ditelluride, *Advanced Materials* 32, 1906578 (2020)
- [5] A polymorphic memtransistor with tunable metallic and semiconducting channel, *Advanced Materials* 2209089 (2023)
- [6] Phase-Engineering of 2D Materials, *Chemical Reviews* 123, 19, 11230 (2023)

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Heejun YANG received a B.S. in physics from KAIST in 2003 and a joint Ph.D. in physics from Seoul National University (Korea) and the University of Paris-Sud XI (France). He was awarded the IUPAP Young Scientist Prize (YSP) in Semiconductor Physics 2018 for his outstanding contribution to novel interface devices based on structural, electronic, and quantum-state control with van der Waals layered materials. His Ph.D. subject was graphene by scanning tunneling microscopy and spectroscopy (STM/STS), and he experienced industrial device studies in Samsung Electronics from 2010 to 2012. Then, he conducted his research on graphene spintronics in Albert Fert's (2007 Nobel laureate) group in CNRS/Thales as a postdoc from 2012 to 2014.

Based on his research background in molecular and nanometer-scale studies (in Seoul and Paris) and electric and spintronic device physics (in Samsung and CNRS/Thales), he moved to Sungkyunkwan University (2014~2021) and KAIST (2021~) and started original device studies with phase engineering of low-dimensional materials. He has proposed novel and conceptual interface devices such as 'Graphene Barristor' and 'Ohmic homojunction contact between semiconductor channels and metal electrodes.' In 2022, he gave an invited talk at the IUPAP centenary symposium as a representative YSP winner.

[Session I] Talk 4: Zhongfan LIU

**SUPER GRAPHENE-SKINNED MATERIALS: CONCEPT, SYNTHESIS AND APPLICATIONS**

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Super graphene-skinned materials describe a new type of graphene composite materials made by directly depositing continuous graphene layers on traditional materials via chemical vapor deposition (CVD) process. By growing high-performance graphene “skin”, the traditional materials are given new functionalities. The atomically thin graphene hitches a ride on the traditional material carriers to market. Beyond coating graphene powder on traditional materials, the directly-grown continuous graphene “skin” keeps its intrinsic excellent properties to a great extent, and holds the promise on future applications. Super graphene-skinned material is an innovative pathway for applications of continuous graphene films, which avoids the challenging peeling-transfer process and solves the non-self-supporting issue of ultrathin graphene film. The graphene skin almost has no influence on macroscale morphology of the supporting substrate, which leads to the high process compatibility of super graphene-skinned material in practical application scenarios. Therefore, graphene-skinned materials would exhibit their excellent performance without changing the processing of current engineering materials, and will be pushed to real industrial applications relying on the broad market of current engineering materials.

Super graphene-skinned materials can be categorized into graphene-skinned metallic materials and graphene-skinned nonmetallic materials. Depending on the different morphologies of supporting substrate materials including foil, fiber, powder, foam, etc., one can obtain graphene-skinned foil, graphene-skinned fiber, graphene-skinned powder, graphene-skinned foam, etc. Additionally, together with post-processing treatments and compositing with other materials, great versatilities can be expected for super graphene-skinned materials. A typical example is graphene-skinned glass fiber, which combines the excellent properties of graphene and glass fiber, such as the high electrical conductivity and thermal conductivity of graphene, along with the remarkable mechanical strength and flexibility of glass fiber. Graphene-skinned glass fiber presented wonderful electrothermal performances with fast heating rate and high heating uniformity, which has been successfully applied for the anti/deicing of aircraft and wind blade. The new concept of super graphene-skinned material opens up a new avenue for practical applications of continuous graphene films, strongly promotes the fusion of graphene and traditional materials, and provides new power for accelerating the graphene industry.



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Zhongfan LIU completed his PhD from University of Tokyo in 1990 and postdoctoral study from the same university and Institute for Molecular Science (IMS), Japan. His current research interests include CVD growth, mass production and equipment manufacturing, and unique applications of graphene. He is the founding Director of Beijing Graphene Institute (BGI) and a BOYA chair professor of Peking University. He is a member of the Chinese Academy of Sciences and a fellow of TWAS.

[Session I] Talk 5: Thuc Hue LY

STATE-OF-THE-ART PROCESSING OF 2D MATERIALS

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The scalable fabrication and integration of 2D devices require large-area synthesis and the state-of-the-art post-synthesis processing of 2D layers. Current challenges in processing 2D materials include: (1) Difficult to transfer the 2D materials without causing damage and contamination. (2) Challenges in effectively cleaning 2D materials. (3) Stress easily applied during processing, which can alter the phases and structures of 2D materials. (4) The patterning process for 2D materials is sophisticated, unrepeatable and non-reversible. To address these challenges, we have recently developed several innovative techniques: (i) We developed novel ice-aided transfer and ice-stamp transfer methods, in which water (ice) is the sole medium in the entire process. The adhesion between various 2D materials and ice can be precisely controlled by temperature. This controlled adhesion enables the transfer of ultrahigh-quality and exceptionally clean 2D flakes and continuous films, applicable across a wide range of substrates. (ii) Furthermore, beyond transfer, ice can also be utilized to clean the surfaces of 2D materials at higher temperatures. (iii) We can precisely control phases during transfer by relaxation of the growth strain on the substrate. For example, in 2D In<sub>2</sub>Se<sub>3</sub>, the intriguing ferroelectric phases can be obtained and show great promise for future neuromorphic computing. (iv) We developed a novel reversible, optical method for precise patterning of 2D ReS<sub>2</sub> materials, utilizing redox surface reactions. This technique allows for micrometer-scale patterning of 2D materials. (v) We also developed an atomic scale phase patterning technique by direct electron beam writing in 2D ReS<sub>2</sub>, achieving precision down to sub-1 nm. These state-of-the-art techniques enable the creation of unprecedented ultraclean and ultra-precise 2D structures and device performances, contributing significantly to the forthcoming technological revolutions associated with 2D materials.

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Prof. Thuc Hue LY obtained her Ph.D. degree in the department of Energy Science from Sungkyunkwan University under the supervision of Prof. Young Hee Lee, where she was working on 2D materials in 2015. In 2015 -2017, she worked as a research fellow in Center for Integrated Nanostructure Physics, Institute for Basic Science. She joined City University of Hong Kong in 2017 and was promoted to Associate Professor in 2023. Her main research area is two-dimensional (2D) materials. She has synthesized a variety of 2D materials through chemical vapor deposition (CVD) methods, studied the grain boundary (GB) structures, their electrical property, the interfacial strains between 2D materials and substrates which are critical to applications. Recently, her group

has proposed a contamination-free method for transferring 2D materials to and from different substrates. Our ice-aided transfer/stamping method fundamentally solves the contamination issue that has perplexed the scientific community for over a decade. These previous relevant research works have been published in renowned journals such as Science, Nature Materials, Nature Nanotechnology, Nature communications, Science Advances, Chemical Reviews, JACS, etc., with Prof. Ly as the first/corresponding authors. She received the NSFC Excellent Young Scientists Award and was nominated as Fellow of International Association of Advanced Materials (IAAM) in 2022 and IAAM scientist medal in 2024.

[Session I] Talk 6: Yanfeng ZHANG

PHASE AND COMPOSITION CONTROLLED SYNTHESSES AND MAGNETIC PROPERTY EXPLORATIONS OF 2D METALLIC TRANSITION-METAL DICHALCOGENIDES

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Exploring new-type two-dimensional (2D) magnetic materials with high magnetic transition temperature and robust air stability has long been pursued for developing innovative spintronic devices.<sup>(1-3)</sup> Intercalation of native metal atoms into the van der Waals gaps of 2D layered transition metal dichalcogenides (TMDs) has been developed to form 2D non-layered magnetic TMDs, while only succeeded in limited systems (*e.g.*, Cr<sub>2</sub>S<sub>3</sub>, Cr<sub>5</sub>Te<sub>8</sub>). Herein, we report the stoichiometry-controlled syntheses of 2D chromium selenide (Cr<sub>x</sub>Se<sub>y</sub>) materials (rhombohedral Cr<sub>2</sub>Se<sub>3</sub> and novel monoclinic Cr<sub>3</sub>Se<sub>4</sub>), *via* a Cr-self-intercalation route by designing two typical chemical vapor deposition (CVD) strategies. The ultrathin Cr<sub>2</sub>Se<sub>3</sub> nanosheets exhibited metallic property, while Cr<sub>3</sub>Se<sub>4</sub> nanosheets present a novel transition from *p*-type semiconductor to metal with increasing the flake thickness. The ferromagnetic properties of 2D Cr<sub>2</sub>Se<sub>3</sub> and Cr<sub>3</sub>Se<sub>4</sub> were also uncovered at ~70 K and ~270 K, respectively. Moreover, composition-controllable syntheses of 2D non-layered iron selenide nanosheets (25% Fe-intercalated triclinic Fe<sub>5</sub>Se<sub>8</sub> and 50% Fe-intercalated monoclinic Fe<sub>3</sub>Se<sub>4</sub>) are firstly reported *via* a CVD strategy. The 2D Fe<sub>5</sub>Se<sub>8</sub> showed intrinsic room-temperature ferromagnetic property, due to the change of electron spin states based on density functional theory calculations. Overall, these work are expected to provide valuable references for the phase or composition-controllable synthesis and fundamental property exploration of metal self-intercalation induced novel TMDs compounds, thus propel their versatile applications and fundamental property explorations.

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Yanfeng ZHANG received her PhD from the Institute of Physics in the Chinese Academy of Sciences in 2005, China. Then, she worked as a JSPS fellow from 2006 to 2009 in Tohoku University, Japan. In 2010, she joined the Department of Materials Science and Engineering in the College of Engineering of Peking University, and now in the School of Materials Science and Engineering, and Center for Nanochemistry of Peking University, and served as a professor.

Her research interests relate to the controlled growth, accurate characterization and novel property exploration of two-dimensional layered materials such as graphene, h-BN-graphene heterostructures, and transition metal dichalcogenides (TMDCs) and their heterostructures. Prof. Zhang has published over 200 papers in *Science*, *Chem. Soc. Rev.*, *Nat. Commun.*, *Adv. Mater.*, etc. in her research career. All the papers are non-self-cited by over 15000 times. In 2012, she won the support of “National Natural Science Foundation for Excellent Young Scholar” from the National Natural Science Foundation of China (NSFC). She was also enrolled in the “Youth Project of the Yangtze River Scholar” in 2015. In 2019, she won the support of “National Natural Science Foundation for Distinguished Young Scholar” from NSFC.

**ELECTRON MICROSCOPY IMAGING OF ELECTRON BEAM-SENSITIVE CRYSTALLINE MATERIALS**

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This presentation will focus on our recent works pertaining to the high-resolution imaging of electron beam-sensitive materials using ultralow electron doses. The following technological advances will be discussed. First, the development of a suite of methods to address the challenges peculiar to low-dose TEM imaging, including rapid search for crystal zone axes, precise alignment of the image stack, and accurate determination of the defocus value, enables efficient imaging of electron beam-sensitive crystalline materials in the high-resolution TEM (HRTEM) mode [1-3]. Second, integrated differential phase contrast STEM (iDPC-STEM) has proven to be an effective method for acquiring directly interpretable atomic-resolution images under low-dose conditions [4]. Third, cryogenic focused ion beam (cryo-FIB) has demonstrated a unique power to prepare (S)TEM specimens for highly sensitive materials [5]. Finally, I will share my views on the great potential of four-dimensional STEM (4D-STEM) in imaging highly electron beam-sensitive materials and provide preliminary results to demonstrate its feasibility [6].

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Dr. Yu HAN obtained his Ph.D. from Jilin University in 2003 and served as a research scientist at A-Star in Singapore from 2003 to 2008. Between 2009 and 2023, he worked at King Abdullah University of Science and Technology in Saudi Arabia as a professor in the Department of Chemistry and Chemical Engineering. In September 2023, he joined South China University of Technology as the Director of the Center for Electron Microscopy. He has published over 400 academic papers, including in prestigious journals such as Nature, Science, Nature Nanotechnology, Nature Chemistry, and Nature Materials, with a total citation count exceeding 45,000 and an H-index of 106.

[Session II] Talk 8: Hiroshi KITAGAWA

PLATINUM GROUP METAL-BASED SOLID-SOLUTION ALLOY NANOCRYSTALS: BINARY TO HIGH-ENTROPY ALLOYS

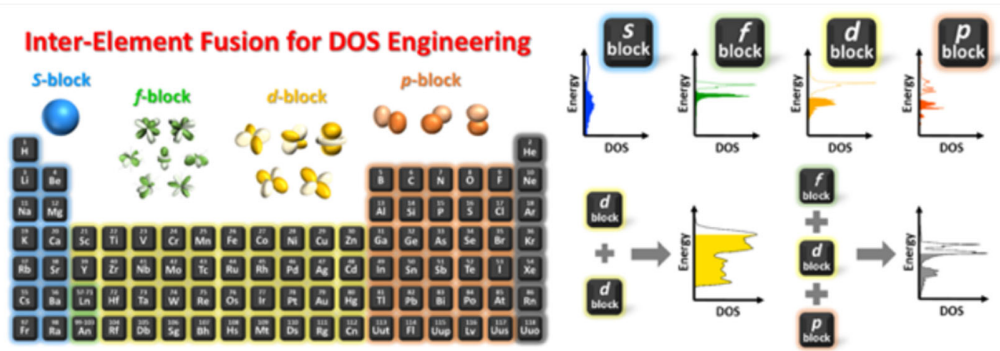
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Metal- Platinum group metal (PGM) nanoparticles (NPs) have been investigated in a variety of research fields such as catalysis and electronics. Among the types of alloys, solid-solution alloy NPs have the advantage of being capable of continuously changing their properties by tuning their composition. However, synthesizing PGM solid-solution alloy NPs with any combination and composition is not an easy task due to the metallurgical aspects. In this work, we have focused on PGM-based solid-solution alloy NPs, and particularly those with immiscible alloy systems<sup>1-17</sup>.

The physical and chemical properties of most solids are strongly correlated to their electronic structure, particularly the DOS at the  $EF$ . In 2015, our group proposed the “DOS engineering” concept for designing materials<sup>4</sup>, which calls for the control not only of the location of the d-band center, but also of a suitable DOS shape, such as the band width and the DOS shape of unoccupied and occupied states around  $EF$ . We propose that by means of “interelement fusion,” as shown in Figure 1 where the elemental periodic table is colored by the  $s$ ,  $p$ ,  $d$ , and  $f$  groups, it is possible to manipulate the shape of the DOS freely by choosing elements from the  $s$ ,  $p$ ,  $d$ , and  $f$  groups according to the properties desired.



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Hiroshi KITAGAWA was born in 1961 and finished his PhD at Kyoto University in 1991 and, after working as Assistant Professor at Institute for Molecular Science and Japan Advanced Institute of Science and Technology, he was appointed as an Associate Professor at University of Tsukuba in 2000. He became Professor at Kyushu University in 2003 and moved back to Kyoto University in 2009. He was engaged at Japan Science and Technology Agency (JST) as Director of “Science and Creation of Innovative Catalysts” and is now engaged at JST as Director of “Exploring Innovative Materials in Unknown Search Space”, and as Program Officer of Materials Science Panel, Fusion Oriented Research for Disruptive Science and Technology. He is also Vice Provost of Kyoto University for planning and strategy coordination. He has published more than 550 original research papers dealing with solid-state chemistry, coordination chemistry, nanoscience, low-dimensional electron systems, and molecule-based conductors.

**THE ROLE OF ATOMIC DEFECTS IN PHASE ENGINEERING OF 2D VAN DER WALLS STRUCTURES AND NANOPARTICLES**

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In this study, we explain how targeted energy input from an electron beam in a transmission electron microscope (TEM), combined with simultaneous heating in a MEMS holder, leads from the formation of atomic defects to new phases in four distinct low-dimensional materials. We conduct in-situ TEM experiments on: (1) few-layer transition metal phosphorus trichalcogenides (TMPTs), (2) graphene sandwich structures encapsulating lithium droplet, (3) graphene sandwich structures encapsulating a benzenehexathiol-based two-dimensional conjugated metal-organic framework, and (4) Pt nanocrystals on graphene.

Regarding (1), we report the controlled formation of MnS, MnSe, and NiSe phases at temperatures around 600°C. Our ab initio calculations predict distinct magnetic properties depending on orientation and thickness. For (2), we show that vacancies in graphene act as nucleation centres, enabling the growth of polycrystalline Li, three layers thick, during lithiation, while interstitial oxygen hinders the delithiation process via forming an lithium oxide. For (3), we demonstrate that while Cu<sub>3</sub>(BHT) exhibits high resistance to electron beams, heating in a MEMS holder induces a phase transition to a new crystalline CuS phase, occurring between 480°C and 620°C. In (4), we investigate the phase transformation of Pt nanoclusters from solid to liquid and the atomic mechanisms of solidification from the molten state. We discover that molten nanodroplets contain a small number of stationary Pt atoms, but when surrounded by these stationary Pt atoms—forming what we call a "corralled nanodroplet"—crystallization is effectively halted.

For our studies, we use the unique Cc/Cs corrected SALVE (Sub-Angstrom Low-Voltage Transmission Electron Microscopy) instrument, demonstrating its capability for in-situ TEM imaging and engineering new phases at the atomic scale.

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Ute KAISER received her Diploma and her Ph.D. in Crystallography from the Humboldt University Berlin, her Habilitation in Experimental Physics from the Friedrich-Schiller University, Jena, Germany, in 2002. Currently she is senior professor at Ulm University and was full professor at Ulm University in the Physics Department and Head of Ulm's Materials Science Electron Microscopy Centre from 2004-2023. Her research interests comprise the areas of TEM methods and instrumentation development, and applications such as in the fields of battery, semiconductor, and catalysts materials. From 2009 till 2018 she was the scientific director of the SALVE (Sub Angstroem Low-Voltage Electron Microscopy) project developing low-voltage transmission electron microscopy, including the chromatic and spherical aberration-corrected instrument, sample preparation methods, contrast calculation at lower accelerating voltage and its applications. By means of this unique TEM instrument, she dedicates her work

to unravel and functionalize the crystallographic and electronic properties of low-dimensional materials. Ute Kaiser has more than 400 peer-reviewed articles, and holds several honorary adjunct positions. She is currently the physical sciences editor for the journal .

[Session II] Talk 10: Jianwei John MIAO

**CRYSTAL NUCLEATION AND GROWTH IN HIGH-ENTROPY ALLOY NANOPARTICLES REVEALED BY ATOMIC ELECTRON TOMOGRAPHY**

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High-entropy alloys (HEAs) have emerged as a pinnacle of materials design, spanning both structural and functional fields. For example, they offer an exceptional balance between strength and ductility in metallurgy, while exhibiting near-continuum adsorbate binding energies in catalysis. However, despite significant advancements in synthesizing HEAs, characterizing their structural and chemical order, and pursuing their broad applications, fundamental insights into the crystal nucleation and growth of HEAs at the atomic scale—essential for understanding their synthesis-structure-property relationships—remain elusive. Here, we advance atomic electron tomography to determine the three-dimensional atomic structure and chemical composition of 8,094 HEA nuclei, captured at different stages of nucleation. We observe that early-stage nuclei exhibit a structural order that gradually decreases from the cores to the boundaries and is correlated with local chemical order. As the nuclei grow, their cores become more crystalline, and the structural order extends further along the radial direction. In the late stage of nucleation, most nuclei coalesce without misorientation, while a small fraction forms twin boundaries. Since these results differ from classical nucleation theory and the two-step nucleation model, we develop an equation called gradient nucleation pathways to better explain our experimental observations. These findings provide a fundamental understanding of crystal nucleation and growth in HEAs. Moreover, we expect that gradient nucleation pathways can be broadly applied to elucidate a wide range of nucleation processes.

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Dr. Jianwei (John) MIAO is a Professor of Physics & Astronomy at UCLA and a member of the California NanoSystems Institute. He earned his M.S. in Physics from the Chinese Academy of Sciences in 1994, followed by a Ph.D. in Physics, an M.S. in Computer Science, and an Advanced Graduate Certificate in Biomedical Engineering from the State University of New York at Stony Brook in 1999. After completing his Ph.D., he joined SLAC at Stanford University as a staff scientist. In 2004, he moved to UCLA as an Assistant Professor and was promoted to Full Professor in 2009. In 1999, Miao pioneered the first experiment extending crystallography to non-crystalline specimens, leading to the development of coherent diffractive imaging (CDI). CDI methods, including conventional CDI, Bragg CDI, holographic CDI, and modern ptychography, have revolutionized microscopy by integrating it with crystallography, replacing lenses with coherent scattering and computational algorithms. In 2012, he applied CDI algorithms to pioneer atomic electron tomography (AET), enabling 3D structure determination of crystal defects and disordered materials. In 2021, he advanced AET to solve a long-standing problem in the physical sciences: determining the 3D atomic structure of amorphous materials. MIAO is an Alfred P. Sloan Research Fellow, a Kavli Fellow, a Theodore von Kármán Fellow, a University of Strasbourg Institute for Advanced Study Fellow, a Fellow of the American Physical Society, a recipient of the Werner Meyer-Ilse Memorial Award, and the 2021 MRS Innovation in Materials Characterization Award.

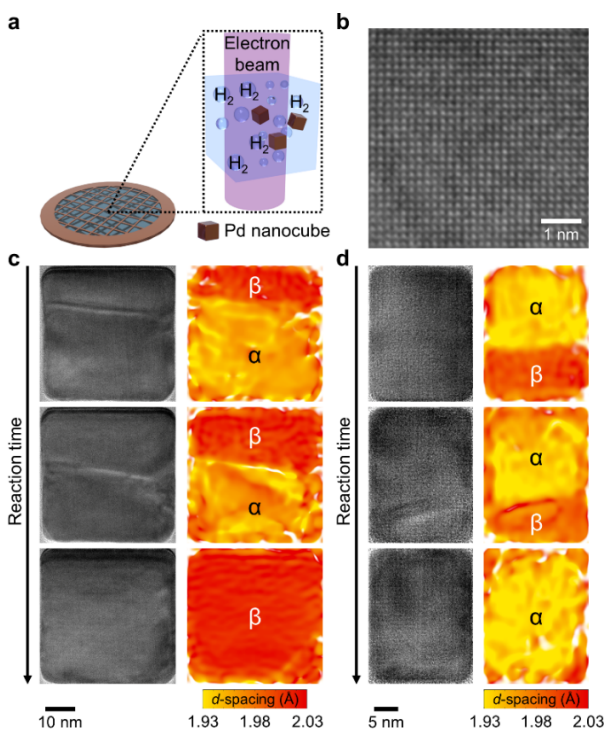
REVEALING KINETICALLY TUNED ATOMIC PATHWAYS FOR INTERFACIAL STRAIN RELAXATION

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Utilizing liquid phase transmission electron microscopy, we have achieved atomic-scale imaging of hydrogen-induced phase transformations of palladium nanocrystals with different transformation speeds. Our observation reveals that the fast phase transformation occurs with an expanded interface of mixed  $\alpha$ - and  $\beta$ -PdH<sub>x</sub> phases with lattice displacements to accommodate mismatch strain. In contrast, slow phase transformations lead to sharp interfaces with slipping misfit dislocations. Our kinetic Monte Carlo simulations show that fast phase transformation pushes the system far-from-equilibrium, generically roughening the interface; however, a smooth boundary minimizes strain near-equilibrium. Unveiling the atomic pathways of transformations from near-equilibrium to far-from-equilibrium, which was previously possible only computationally, this work holds significant implications for engineering microstructure of materials through modulating solid-solid transformations in a wide range of kinetics.



**Figure 1. *In situ* liquid phase TEM study of hydrogen absorption and desorption in Pd nanocubes.** **a**, Schematic illustration of the experimental setup. The electron beam radiolysis of water generates hydrogen gases in the liquid cell, and the hydrogen sorption behaviors in Pd nanocubes are observed in real-time with atomic resolution. **b**, An HRTEM image of Pd nanocube showing single-crystal structure. **c,d**, Sequential HRTEM images and corresponding *d*-spacing color maps of Pd nanocubes during hydrogen absorption (c) and desorption (d), leading to the  $\beta$ -PdH<sub>x</sub> and  $\alpha$ -PdH<sub>x</sub> phases, respectively.

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Prof. Haimei ZHENG is from Department of Materials Science and Engineering at University of California (UC), Berkeley. Her research interests are broadly in physical and chemical processes of materials, with a focus on dynamic phenomena at solid-liquid interfaces and nanoscale materials transformations. Her primary approach is by developing and applying in-situ liquid phase transmission electron microscopy (TEM). She was named a Materials Research Society (MRS) Fellow in 2021 and a Fellow of the Microscopy Society of America (MSA) in 2023.

Short Talk Session I

Short Talk 1: Hongfei CHENG

**CRYSTALLINITY MODULATION AND CATALYTIC PROPERTY STUDY OF PD-BASED NANOMATERIALS**

Hongfei CHENG  
Tongji University

Catalysts play an important role in chemical and energy fields, such as oil refinement, electrocatalytic water splitting, fuel cells. Therefore, developing high-performance catalysts has been the research focus in materials science, which is important for achieving carbon neutrality. Studies have shown that, due to the random atomic arrangement of amorphous phase, it has lower coordination number, higher defect density, and higher structural flexibility than crystal phase. Moreover, the composition of solid solutions is usually constrained by the crystal structure, thus a very limited range of composition is allowed in crystal solid solutions, whereas amorphous solid solutions do not have this limitation. These structural features play a key role in modulating the physicochemical properties of materials, such as electronic structures, surface energy, thus affecting their catalytic performance. Herein, we report several different methods for modulating the crystallinity of Pd-based nanomaterials, and further study their catalytic properties for energy applications, which include the following works. First, we develop a one-pot wet-chemical reduction method to prepare ultrathin Pd and PdCu nanosheets with amorphous-crystalline heterophase, whose crystallinity can be tuned by controlling reaction temperature, and we find that the crystallinity of nanosheets affect the catalytic activity and selectivity in hydrogenation reaction.<sup>[1,2]</sup> Second, we discover a thiol molecule that can induce crystalline fcc-Pd nanomaterials to transform into amorphous phase by ligand exchange at room temperature, and the obtained amorphous Pd nanoparticles exhibited much enhanced performance in electrocatalytic hydrogen evolution reaction.<sup>[3]</sup> Third, we find that hydrogen intercalation can induce amorphous PdP and PdNiP nanoparticles to transform into crystalline phase, and the resulted PdNiP-H nanoparticles exhibited better performance in direct formic acid fuel cells compared with commercial Pd/C.<sup>[4]</sup>

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**Short Talk 2: Ye CHEN**

**SYNTHESIS AND PHASE-DEPENDENT CATALYTIC BEHAVIORS OF UNCONVENTIONAL-PHASE NOBLE METAL NANOMATERIALS WITH FACET PRECISION**

Ye CHEN

The Chinese University of Hong Kong, Hong Kong, China

In this presentation, I will introduce our latest works about crystal phase controlled synthesis of noble metal nanomaterials and their proof-of-concept applications in catalysis, with a particular focus on precise control of unconventional-phase facets. Our recent works to obtain unconventional-phase Pt, Rh and Au facets via one-step or two-step methods will be introduced. Their unconventional crystal structure, stability, formation mechanism, and phase transformation behaviors will be discussed. Their enhanced catalytic properties in comparison to conventional-phase facet will be illustrated. Our works suggest that phase engineering of metal nanomaterials can be further studied at facet level. Based on our latest results, some perspectives about crystal phase controlled synthesis and phase-dependent applications will be shared.

Session III: Phase-Dependent Electrocatalysis and Photocatalysis

[Session III] Talk 12: Hua ZHANG

Phase Engineering of Nanomaterials (PEN)

Hua ZHANG

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[https://scholars.cityu.edu.hk/en/persons/hua-zhang\(8f4e048e-884d-4f19-b2b4-ca4d3d53c515\).html](https://scholars.cityu.edu.hk/en/persons/hua-zhang(8f4e048e-884d-4f19-b2b4-ca4d3d53c515).html)

Google Scholar: <https://scholar.google.com/citations?user=Cgo45S8AAAAJ&hl=en>

In this talk, I will summarize the recent research on phase engineering of nanomaterials (PEN) in my group, particularly focusing on the rational design and synthesis of novel nanomaterials with unconventional phases for various promising applications. For example, by using wet-chemical methods, for the first time, we have successfully prepared novel Au nanostructures (e.g., the hexagonal-close packed (*hcp*) 2H-Au nanosheets, 4H-Au nanoribbons, and crystal-phase heterostructured 4H/*fcc* and *fcc*/2H/*fcc* heterophase Au nanorods), epitaxially grown metal nanostructures on the aforementioned unconventional Au nanostructures and 2H-Pd nanoparticles, and amorphous/crystalline heterophase Pd, PdCu, Rh and Rh alloy nanosheets. By using gas-solid reactions, metastable 1T'-phase group VI transition metal dichalcogenides (TMDs), e.g., WS<sub>2</sub>, WSe<sub>2</sub>, MoS<sub>2</sub>, MoSe<sub>2</sub>, WS<sub>2</sub>xSe<sub>2(1-x)</sub> and MoS<sub>2</sub>xSe<sub>2(1-x)</sub>, have been prepared. Impressively, the 1T'-MoS<sub>2</sub>-supported single-atomically dispersed Pt (*s*-Pt) atoms with Pt loading up to 10 wt% exhibit superior performance in hydrogen evolution reaction. Importantly, 1T'-TMD monolayers can be stabilized on 4H-Au nanowires, which can be used for ultrasensitive SERS detection. Moreover, the salt-assisted 2H-to-1T' phase transformation of TMDs have been achieved, and the phase transformation of TMDs during our developed electrochemical Li-intercalation process has been observed. Impressively, the lithiation-induced amorphization of Pd<sub>3</sub>P<sub>2</sub>S<sub>8</sub> has been achieved. Currently, my group focuses on the investigation of phase-dependent physicochemical properties and applications in catalysis, (opto-)electronic devices, clean energy, chemical and biosensors, surface enhanced Raman scattering, photothermal therapy, etc., which we believe is quite unique and very important not only in fundamental studies, but also in future practical applications. Importantly, the concepts of phase engineering of nanomaterials (PEN), crystal-phase heterostructures, and heterophase nanomaterials are proposed.

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Dr. Hua ZHANG obtained his B.S. and M.S. degrees at Nanjing University in China in 1992 and 1995, respectively, and completed his Ph.D. with Prof. Zhongfan Liu at Peking University in China in July 1998. He joined Prof. Frans C. De Schryver's group at Katholieke Universiteit Leuven (KULeuven) in Belgium as a Research Associate in January 1999. Then he moved to Prof. Chad A. Mirkin's group at Northwestern University as a Postdoctoral Fellow in July 2001. He started to work at NanoInk Inc. (USA) as a Research Scientist/Chemist in August 2003. After that, he worked as a Senior Research Scientist at Institute of Bioengineering and Nanotechnology in Singapore from November 2005 to July 2006. Then he joined the School of Materials Science and Engineering in Nanyang Technological University (NTU) as an Assistant Professor. He was promoted to a tenured Associate Professor on March 1, 2011, and Full Professor on Sept. 1, 2013. In 2019, he joined the Department of Chemistry in City University of Hong Kong as a Chair Professor, and currently he is the Herman Hu Chair Professor of Nanomaterials and the Director of Hong Kong Institute for Clean Energy.

He has published **8** invited book chapters, over **100** patent applications (including **granted 1 China patent, 1 European patent, 3 Singapore patents, and 10 US patents**), and over **570** papers. Some of his papers have been published in *Nature*, *Science*, *Nat. Mater.*, *Nat. Chem.*, *Nat. Catal.*, *Nat. Rev. Mater.*, *Nat. Rev. Chem.*, *Nat. Commun.*, *Sci. Adv.*, *Nat. Protocols*, *Chem. Rev.*, *Chem. Soc. Rev.*, *Acc. Chem. Res.*, *Acc. Mater. Res.*, *J. Am. Chem. Soc.*, *Angew. Chem. Int. Ed.*, *Adv. Mater.*, etc. As at Oct. 2024, the total cited times are over **133,700** with H-index of **182** (*Web of Science*), and over **152,100** with H-index of **193** (*Google Scholar*). He has been invited to give more than **300** Plenary, Keynote or Invited Talks in international conferences, universities and institutes. He has organized several tens of international conferences and served as the Conference (Co-)Chair or Symposium Chair.

In **2020**, he was elected as a **Foreign Fellow** of the European Academy of Sciences (*EurASc*). In **2015**, he was elected as an **Academician** of the Asia Pacific Academy of Materials (*APAM*). In **2014**, he was elected as a **Fellow** of the Royal Society of Chemistry (*FRSC*). He was listed in the "*Highly Cited Researchers*" in *Materials Science* (Clarivate Analytics/Thomson Reuters, **2014-2023** (10 consecutive years)), in *Chemistry* (Clarivate Analytics/Thomson Reuters, **2015-2023** (9 consecutive years)), and in *Environment and Ecology* (Clarivate Analytics, **2022**). In **2015**, he was listed as **one of 19 "Hottest Researchers of Today"** in the world in the *World's Most Influential Scientific Minds 2015* (Thomson Reuters, **2015**). In **2014**, he was listed as **one of 17 "Hottest Researchers of Today"** and **No. 1** in *Materials and More* in the world in the *World's Most Influential Scientific Minds 2014* (Thomson Reuters, **2014**). Moreover, he also received the BOCHK Science and Technology Innovation Prize (**2024**, Hong Kong Alliance of Technology and Innovation), IUMRS-Frontier Materials Scientists Award (**2023**, IUMRS-ICFM), *EcoMat Mid-Career Research Award* (**2023**, Wiley-VCH), *Outstanding Research Award* (**2022**, City University of Hong Kong), *President's Award* (**2021**, City University of Hong Kong), *Young Investigator Award* (Young Giants of Nanoscience **2016**, Hong Kong), *Vice-Chancellor's International Scholar Award* (University of Wollongong, Australia, **2016**), *ACS Nano Lectureship Award* (**2015**), *World Cultural Council (WCC) Special Recognition Award* (**2013**), the *ONASSIS Foundation Lectureship* (Greece, **2013**), *Asian Rising Stars* (15<sup>th</sup> Asian Chemical Congress, **2013**), *SMALL Young Innovator Award* (Wiley-VCH, **2012**) and *Nanyang Award for Research Excellence* (**2011**).

Dr. ZHANG's research is highly interdisciplinary. His current research interests focus on phase engineering of nanomaterials (PEN) and controlled epitaxial growth of heterostructures, including the synthesis of ultrathin

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two-dimensional nanomaterials (*e.g.*, metal nanosheets, graphene, metal dichalcogenides, metal-organic frameworks, covalent organic frameworks, *etc.*), novel metallic and semiconducting nanomaterials, novel amorphous nanomaterials, and their hybrid composites for various applications, such as catalysis, clean energy, (opto-)electronic devices, chemical and biosensors, and water remediation.

[Session III] Talk 13: Shouheng SUN

**L1<sub>0</sub>-INTERMETALLICS: STRUCTURE STABILITY AND CATALYSIS ENHANCEMENT**

Shouheng SUN

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L1<sub>0</sub>-intermetallics is a class of transition metal-based alloy within which metal atoms are bonded via strong d-orbital interaction in a specific crystallographic direction. Compared to the common metallic alloys with solid solution structure, intermetallic alloys are generally more stable against chemical oxidation and etching, making them an ideal choice as catalysts in corrosive reaction systems.

This talk focuses on monodisperse intermetallic L1<sub>0</sub>-structured MPt nanoparticles (NPs), especially Pt-, Pd-, and Au-based L1<sub>0</sub>-NPs, as robust catalysts for electrochemical reduction and oxidation reactions.

Intermetallic core/shell L1<sub>0</sub>-FePt/Pt NPs with ~2 atomic layers of Pt shell were made by controlled annealing and acid etching of solid solution FePt NPs. The core/shell structure with compressed Pt shell is chemically stable against fast/deep Fe etching and is catalytically more active than the Pt counterpart for oxygen reduction reaction (ORR), showing superior mass activity and much improved durability under the fuel cell testing conditions at 80°C. When Fe is replaced by Co in the L1<sub>0</sub>-FePt/Pt structure, the Pt shell in the L1<sub>0</sub>-CoPt/Pt structure is compressed even more, and its ORR catalysis is further enhanced for ORR in the membrane electrode assembly at 80°C. When alloyed with Au, the AuPt shell in the L1<sub>0</sub>-MPt/AuPt structure (M = Fe or Co) is more active and stable for electro-oxidation of formic acid and alcohols with high CO tolerance. Our studies demonstrate a reliable way of structure-tuning NP catalysis from electrochemical reduction to oxidation reactions. This structure-catalysis tuning strategy can be further extended to many other composite systems, such as MAu/Au and MPd/Pd systems, opening a new path to tune and optimize NP catalysis for redox reactions that are key to green chemistry and sustainable energy.



Shouheng SUN received his BSc from Sichuan University (China), MSc from Nanjing University (China), and PhD from Brown University (USA). He joined the IBM T. J. Watson Research Center (Yorktown Heights, New York, USA) first as a postdoctoral fellow (1996-1998) and then as a research staff member (1998-2004). In 2005, he returned to Brown University as a tenured Associate Professor and was promoted to full Professor in 2007. He has been the Vernon K. Krieble Professor of Chemistry and Professor of Engineering since 2016. His main research interests are in chemical synthesis and self-assembly of nanoparticles for catalytic, magnetic and biomedical applications. He served as a co-Director of Brown's Institute of Molecular and Nanoscale Innovation (2008-2020) and an Associate Editor for the Royal Society of Chemistry Journals, *Nanoscale* and *Nanoscale Advances* (2012-2021). He has been a Fellow of the Royal Society of Chemistry since 2015.

[Session III] Talk 14: Wei-Xue Li

**SUPPORTED METAL CATALYSTS POWERED BY INTERPRETABLE MACHINE LEARNING**

Wei-Xue Li

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Oxide-supported transition metal catalysts are essential for numerous chemical reactions, determining the efficiencies and sustainability of many industrial processes, from petrochemical refining, chemical production to environmental protection. How metals interact with gaseous reactants and support underneath, *i.e.*, metal-reactant interactions and metal-support interactions, are two cornerstones of supported metal catalysts. Metal-reactant interactions determines activity and selectivity, where the nature of the active sites and their structure sensitivity are the keys to rational design of efficient catalysts but have been debated for almost one century in heterogeneous catalysis. While metal-support interaction is vital in stabilizing dispersed catalysts and impacting a variety of interfacial processes, including charge transfer, chemical composition, perimeter sites, particle morphology, and encapsulation. The significance of MSI makes its modulation one of the few strategies for enhancing catalytic performance, but developing a fundamental theory has been challenging because of the intricate interfaces.

To address these challenges, here, we harness the power of interpretable machine learning, domain knowledge, theoretical and experimental data to establish a general theory of metal-reactant and metal-support interaction grounded in topological under-coordinated number, metal-metal interaction and metal-oxygen interaction. It is physical and concise, providing a constructive strategy not only to understand the structure sensitivity but also to decipher the entangled geometric and electronic effects of metal catalysts, and transferable to metal-on-oxide and oxide-on-metal interfaces. The theory reveals that metallophilicity dominates support effects and suboxide encapsulation over metal nanoparticles. A principle of strong metallophilicity for encapsulation occurrence is thus proposed and substantiated by extensive experiments including 10 metals and 16 oxides, resolving the longstanding debates around strong metal-support interaction. The theory applies to other metal compound supports, paving the way to engineer the interfacial processes for advanced metal catalysts.

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Professor Wei-Xue LI, Chair Professor, University of Science and Technology of China (USTC), Executive Director, Department of Chemical Physics. He graduated from Wuhan University with a bachelor's degree in theoretical physics in 1992, graduated from the Institute of Mechanics of the Chinese Academy of Sciences with a doctor's degree in 1998, and engaged in postdoctoral research in Fritz Haber Institute in Germany and Aarhus University in Denmark from 1999 to 2004. Prof. Li worked at the Dalian Institute of Chemical Physics, Chinese Academy of Sciences from 2004 to 2015, and at the University of Science and Technology of China since 2015. Prof. Li's research interests are theoretical and computational catalysis, and more than 170 papers have been published, including **Science** (2), **Nature Catalysis** (2), **Nature Nanotechnology**, and Elsevier's "China Highly Cited Scholar". He has successively won honorary titles such as the Outstanding Youth of the National Natural Science Foundation of

China (2012), the China Catalysis Youth Award (2014), the National High-level Innovation Leader (2016), and the Outstanding Research President Award of the USTC (2021). He is currently presiding over the project "Fundamentals of Activity and Stability in Heterogeneous Catalysis" of the innovative research group of NSFC and is the associate editor of ACS Catalysis, a journal of the American Chemical Society.

[Session III] Talk 15: Lifeng CHI

FROM N-ALKANE TO CONJUGATED POLYENE AND THEIR AROMATIZATION VIA ON-SURFACE CHEMISTRY

Lifeng CHI

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On-surface chemistry is an emerging interdisciplinary discipline developed in recent years, which presents the great potential in breaking through limitations of traditional chemical synthesis and accurately preparing functional molecular nanostructures. After a series of explorations to address the challenging scientific problem of selective C-H bond activation and C-C coupling of saturated alkanes on Au(110) surface [1,2], we further realized the conversion of normal alkanes to conjugated polyenes on the surface of Cu(110) and interpreted the underline mechanisms[3-6]. More recently, we demonstrated the high selective dehydrogenative aromatization of n-alkane on different metal surfaces. Thereby new methods for the on-surface conversion from n-alkane to conjugated polyene and their aromatization are established.

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Lifeng CHI obtained her PhD in Max-Planck-Institute for Biophysical Chemistry (University of Goettingen) in 1989 and then went to University of Mainz and BASF working as a Postdoc. She became a Group Leader in Physics Institute of Muenster University from 1993 and granted a Lisa Meitner stipendium in 1997. She received National Outstanding Youth Science Foundation (Type B) of China in 1999 and became a professor in physics of Muenster University in 2004. In 2012, She was appointed as a chair professor in Soochow University. She was selected as a Foreign Academician of Academia Europaea, an Academician of Chinese Academy of Sciences and a Fellow of the World Academy of Sciences for the Advancement of science in developing countries (TWAS) respectively in 2020, 2021 and 2023.

She obtained the 2016 ACS Nano Lectureship Award and received Distinguished Women in Chemistry/Chemical Engineering Award of IUPAC in 2017. Currently, she is serving as the Associate Editor of ACS Nano and Chemical Research in Chinese Universities. Up to now, she has presided over 20 national-level research grants and published nearly 500 papers.

[Session III] Talk 16: Can LI

CHARGE SEPARATION IN PHOTOCATALYSIS FOR SOLAR HYDROGEN PRODUCTION FROM WATER SPLITTING



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The solar hydrogen can be produced via water splitting by photocatalysis, photoelectrocatalysis and/or electrolysis with renewable energy. While the photocatalysis water splitting efficiency is not yet high enough currently for large scale application. The great challenge of solar energy conversion via photocatalysis lies in its complicated processes including light absorption (harvesting), charge dynamics (separation and transfer), and catalytic reactions, particularly water oxidation. The lecture will focus on the research progress made in charge separation and transfer in photocatalyst particles for solar hydrogen production from water splitting.

The steady-state charge distribution on single photocatalyst particles has been mapped by microscopic techniques for phase junction and facets of photocatalyst particles, and furthermore the charge transfer dynamics in photocatalyst aggregations have been revealed by time-resolved spectroscopy, spatiotemporally evolving charge transfer processes in single photocatalyst particles has not been tracked, and their exact mechanism is unknown. We performed spatiotemporally resolved surface photovoltage measurements on cuprous oxide photocatalyst particles to map holistic charge transfer processes on the femtosecond to second timescale at the single-particle level. We find that photogenerated electrons are transferred to the catalytic surface quasi-ballistically through inter-facet hot electron transfer on a subpicosecond timescale, whereas photogenerated holes are transferred to a spatially separated surface and stabilized through selective trapping on a microsecond timescale. We demonstrate that these ultrafast-hot-electron-transfer and anisotropic-trapping regimes, which challenge the classical perception of a drift-diffusion model, contribute to the efficient charge separation in photocatalysis and improve photocatalytic performance.

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Can Li, a chair professor and director of the Fundamental Research Center for Artificial Photosynthesis at the Dalian Institute of Chemical Physics (DICP), Chinese Academy of Sciences (CAS). He received his Ph.D. degree (in 1988) in Physical Chemistry from DICP CAS with a joint program at Tokyo Institute of Technology, Japan. He did post-doctoral work at Northwestern University, USA. He was elected as a member of the Chinese Academy of Sciences in 2003, a member of the Academy of Science for Developing Countries (TWAS) in 2005, a foreign member of Academia European in 2008, and a Fellow of the Royal Society of Chemistry in 2008. His research interests span *in-situ/operando* spectroscopic studies on catalysts and catalytic reactions. During last two decades, his research has been focused on photocatalytic, photoelectrocatalytic and electrolysis water splitting and CO<sub>2</sub> reduction utilizing renewable energy for solar fuel production.

He was the president of the International Association of Catalysis Societies (2008-2012). Currently, he is the president of the Catalysis Society of China, Dean of Materials and Chemical Science School of University of Science and Technology of China (USTC). Awards received include International Catalysis Awards, Japan Photochemistry Prize, Hong Kong “Qiu-Shi” Prize, and National Catalysis Award of China, *etc.*

Session IV: Phase-Dependent Wet-Chemical Synthesis

[Session IV] Talk 17: Younan XIA

**PHASE-CONTROLLED SYNTHESIS OF NOBLE-METAL NANOCRYSTALS: TEMPLATING EFFECT *VERSUS* REACTION KINETICS**

Younan XIA

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The properties of noble-metal nanocrystals are traditionally tuned by tailoring parameters such as size, shape, and internal structure. Exploring the polymorphism of nanocrystals, specifically controlling their crystal structures or phases, represents a nascent research area with many mechanistic details yet to be elucidated, reminiscent of the early days of shape-controlled synthesis. In recent years, seed-mediated growth has become as a simple and versatile method for achieving phase-controlled synthesis. Under optimal conditions, the deposited shell can replicate both the crystal and surface structures of the preformed seed, leading to the formation of a metastable phase. Despite the successful demonstrations of many examples, the explicit role(s) played by reaction kinetics in affecting the packing of atoms in the bulk is yet to be resolved. Our recent effort aims to discern which factor—the reduction kinetics or the templating effect from the seed—exerts a greater impact on the crystal phase of the deposited overlayers. With Ru as a model system, we demonstrated a correlation between the phase and the initial reduction rate and revealed the explicit role played by reduction kinetics in the phase-controlled growth on preformed seeds. By leveraging polyols with distinct reducing powers and Ru nanocrystals of varying phases as templates, a series of Ru nanocrystals with tunable sizes of 3–7 nm and different patterns of crystal phases were synthesized. Our findings suggest that the reduction kinetics played a more dominant role than the templating effect from the seed in dictating the crystal phase of the deposited Ru, despite their intertwined effects on successful epitaxial growth. This work highlights the intricate balance between templating effect and reaction kinetics in generating noble-metal nanocrystals with desired phases for catalysis, energy conversion, and related applications.

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XIA is the Brock Family Chair and Georgia Research Alliance (GRA) Eminent Scholar at the Georgia Institute of Technology. He received his B.S. degree in chemical physics from the University of Science and Technology of China in 1987, M.S. degree in chemistry from University of Pennsylvania (with Alan G. MacDiarmid) in 1993, and Ph.D. degree in physical chemistry from Harvard University (with George M. Whitesides) in 1996. His group invented many nanomaterials with well-controlled properties for use in applications related to plasmonics, electronics, display, catalysis, energy conversion, controlled release, nanomedicine, and regenerative medicine. For example, the silver nanowires invented by his group has found use in commercial production of flexible, transparent, and conductive coatings for applications such as touchscreen, flexible electronics, and photovoltaics. His technology on the fabrication of aligned nanofibers has been commercialized for multiple clinical products related to regenerative medicine, including those for the management of surgical and trauma wounds. Xia has co-authored more than 880 publications in peer-reviewed journals, together with a total citation of about 200,000 and an h-index of 218. He has been named a Top 10 Chemist and Materials Scientist based on the number of citation per publication. He has received a number of awards, including ACS National Award for Creative Invention (2023), MRS Medal (2017), ACS National Award in the Chemistry of Materials (2013), NIH Director's Pioneer Award (2006), and NSF CAREER (2000). More information can be found at <http://www.nanocages.com>.

[Session IV] Talk 18: Nanfeng ZHENG

TOWARDS PRECISE CONTROL OF CHEMICAL REACTIONS ON METAL

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Solid surface is the place where many chemical reactions take place, directly influencing the chemical properties of solids. Surface modification has thus become a vital method for precisely controlling the chemical reactions on metal surfaces. Two prevalent strategies for modifying the surfaces of heterogeneous metal catalysts involve using organic ligands or inorganic composites. These modifications often lead to the formation of interfacial coordination interactions between metal atoms and the modifiers. The interactions make impacts on the chemical interaction between reactants/intermediates/products and metal sites so that different interface effects are observed. Understanding these interface effects at the molecular level is essential for precise control of chemical reactions on metal. However, research in surface and interface coordination chemistry is still limited and faces challenges due to the lack of advanced characterization methods for surface and interface coordination structures. This presentation will focus on our efforts to understand how the chemical properties (e.g., catalysis, corrosion protection) of metal nanomaterials are manipulated at the molecular level through the surface and interface modification with small inorganic and organic coordinative molecules. The understanding has been successfully applied to enhance the catalytic behavior of metal nanomaterials, particularly in the green production of high-end fine chemicals.



Nanfeng ZHENG received his B.S. from Xiamen University in 1998. In 2005, he obtained Ph.D. degree from University of California-Riverside. During 2005-2007, he worked as a research associate at University of California-Santa Barbara. In 2007, he moved to Xiamen University as a full professor. He has received several awards, including the Distinguished Young Investigator Award from NNSF-China (2009), the Chinese National Young Scientist Award (2016), the National Natural Science Award of China (Second Prize, 2018), and the Xplorer Prize (2019). In 2023, he was elected as an Academician of the Chinese Academy of Sciences, and selected as a New Cornerstone Investigator. His research focuses on the surface and interface chemistry of functional materials, targeting applications in energy, catalysis, and biology. He has published >320 articles with over 38000 citations and H-index of 104. His team has developed over 10 different metal catalysts, with a total annual production of 10 tons, for the eco-friendly production of fine chemicals. As the current director of iKKEM, he leads the innovation laboratory in its mission to conduct pioneering research and facilitate the transfer of technology, with a focus on advancing new energy solutions for societal benefit.

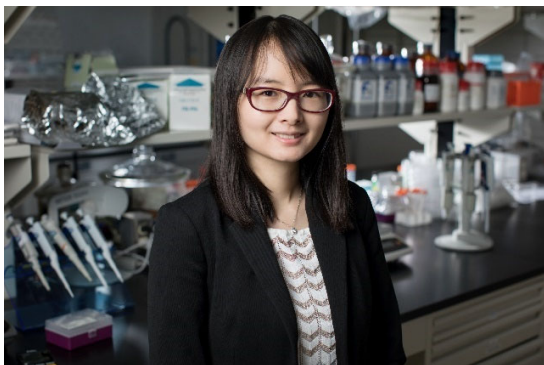
[Session IV] Talk 19: Qian CHEN

**ELECTRON VIDEOGRAPHY OF COLLOIDAL NANOPARTICLES**

Qian CHEN

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I will present our group's recent progress on establishing and utilizing "electron videography" to image, understand, and manipulate soft materials systems, in space and time at a nanometer resolution. This involves systems that underpin the fundamentals of structure–functional relationship for a wide range of phenomena and applications. In this talk, we will discuss in detail two types of such systems. The first focuses on metallic nanoparticles assembling into various complex lattices such as Maxwell lattice, a chiral pinwheel lattice, a colloidal moiré pattern, and nanoparticle swarms as promising optical and mechanical metamaterials. The second is on the structural fluctuations and fingering dynamics of membrane protein lipid assemblies. We will show how we build electron videography upon liquid-phase transmission electron microscopy, electron tomography, and four-dimensional scanning transmission electron microscopy, while coupling them with machine learning and molecular dynamics simulations. This coupling enables us to study the phase transition of dynamic, squishy, multifunctional soft and biological systems in liquid and at operation at the otherwise inaccessible spatiotemporal resolution.



Prof. Qian CHEN is currently a professor and Racheff Scholar in the Department of Materials Science and Engineering at the University of Illinois at Urbana-Champaign. She obtained her PhD degree from the same department with Prof. Steve Granick (2012) and completed her postdoctoral research with Prof. Paul Alivisatos at the University of California, Berkeley, under a Miller Fellowship. She became an assistant professor in 2015, promoted to associate professor in 2021, and then to full professor in 2024. She has received awards for the research in her group, such as the Forbes 30 under 30 Science List (2016), the AFOSR YIP (2017), the NSF CAREER award (2018), the Sloan Research Fellow in Chemistry (2018), the ACS Unilever Award (2018), the Hanwha-TotalEnergies IUPAC Young Scientist Award (2022), the Soft Matter Lectureship (2023), the Provost's Award for Excellence in Graduate Student Mentoring (2024), and the MRS Outstanding Early-Career Investigator Award (2024). Her group's research focuses on imaging, understanding, and engineering soft, biological, and energy materials at the nanoscale.

[Session IV] Talk 20: Yu HUANG

**UNLOCKING THE FUTURE OF CLEAN ENERGY: PREDICTING AND DESIGNING DURABLE CATALYSTS  
FOR HYDROGEN FUEL CELLS**

Yu HUANG

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Hydrogen as a clean and versatile energy carrier has the potential to decarbonize various sectors, including transportation, industry, and energy generation. It plays a crucial role in reducing greenhouse gas emissions and advancing the transition toward a more sustainable and environmentally friendly energy future. Electrocatalysis plays a central role in hydrogen energy technologies. Despite significant progress, many electrocatalytic systems, such as hydrogen fuel cells, continue to face challenges related to insufficient catalytic efficiency, poor stability, and the high cost of precious metal catalysts. Rapidly advancing beyond trial-and-error methods is imperative to address the imminent energy and climate crisis. This presentation will delve into the development of experimentally attainable descriptors capable of predicting the catalytic activity and stability of catalysts, which facilitates the accelerated discovery of more efficient catalysts. Furthermore, we will explore practical catalyst structure design, tailored to enhance both catalyst activity and stability in full-cell operation, thereby maintaining the overall performance of the device.



Dr. Yu HUANG is the Traugott and Dorothea Frederking Endowed Chair in Engineering and Professor of the Department of Materials Science and Engineering at University of California Los Angeles. She received her B.S. in Chemistry from University of Science and Technology of China (USTC), and her Ph.D in physical chemistry from Harvard University. She was a Lawrence Postdoctoral Fellow and held a joint postdoctoral position with Lawrence Livermore National Lab (LLNL) and Massachusetts Institute of Technology (MIT). Her research focuses on mechanistic understanding of nanoscale phenomena and on exploiting the unique properties of nanoscale materials for various applications.

Prof. HUANG is Highly Cited Researcher, the elected Fellow of Materials Research Society (MRS), Fellow of Royal Society of Chemistry (RSC). Recognitions she received include the ENI Award in Energy Transition, International Society of Electrochemistry (ISE) Prize for Experimental Electrochemistry, the International Precious Metal Institute (IPMI) Carol Tyler Award, Kavli Fellow, Sloan Fellow, the Presidential Early Career Award in Science and Engineering (PECASE), the National Institute of Health (NIH) Director's New Innovator Award, the Defense Advanced Research Projects Agency (DARPA) Young Faculty Award, the World's Top 100 Young Innovators award, the International Union of Pure and Applied Chemistry (IUPAC) Young Chemist Award, and the Nano 50 Award etc.

[Session IV] Talk 21: Rongchao JIN

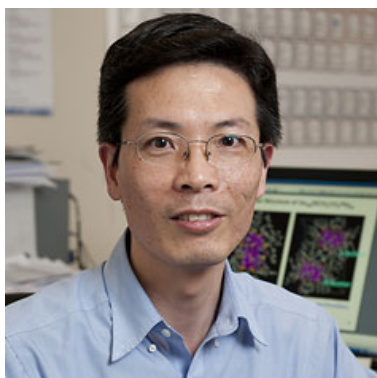
PHASE ENGINEERING OF ATOMICALLY PRECISE GOLD NANOCCLUSERS

Rongchao JIN

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Recent research in nanoscience has advanced toward controlling nanoparticles with atomic precision. In this talk I will present progress in atomically precise gold nanoclusters with a focus on their phase engineering. These perfect gold nanoclusters possess well-defined formulas of  $Au_n(SR)_m$ , where SR = thiolate ligand,  $n$  and  $m$  refer to the precise number of gold atoms and surface ligands, respectively. With synthetic breakthroughs, significant progress has been achieved in both size and shape control with atomic precision in the range of tens to hundreds of gold atoms per core. While bulk gold is almost exclusively face-centered cubic (fcc), its nanoscale form can adopt a variety of phases such as body-centered cubic (bcc) and hexagonal close-packed (hcp) structures as revealed by X-ray crystallography analysis on single crystals assembly from atomically precise nanoclusters. A myriad of new properties of  $Au_n(SR)_m$  nanoclusters have been discovered through phase engineering, including the quantum-state manipulation at the single-electron level, tailoring the optical and catalytic properties at the single-atom level, and many others. The attainment of atomically precise nanoclusters with phase engineering has offered exciting opportunities in both fundamental studies and practical applications in optics, catalysis, and medicine.



Rongchao JIN received his Ph.D. in Chemistry from Northwestern University in 2003. Then, he conducted postdoctoral research at the University of Chicago (2003-2006). He joined the chemistry faculty of Carnegie Mellon University in 2006, and was promoted to Associate Professor in 2012 and Full Professor in 2015. His current research focuses on atomically precise metal nanoclusters.



[Session IV] Talk 22: Xun HONG

SYNTHESIS AND CATALYTIC PROPERTIES OF AMORPHOUS NANOSHEETS

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The catalytic performance of noble metal nanomaterials is closely related to their size, crystal facets, and atomic coordination environment. Compared with crystalline structures, atomic arrangements in amorphous structures do not exhibit periodicity and translational symmetry. The lack of long-range ordered structure results in local atomic structures of amorphous nanomaterials that are different from corresponding crystalline materials. Due to the structural advantages of amorphous materials, such as a wide range of coordination environments and electronic structure modulation, and many coordination unsaturated sites, they have great potential for enhancing the intrinsic activity of catalysts. We have achieved the synthesis of amorphous nanosheets through salt-assisted organic degradation methods, including dozens of amorphous nanosheets such as Ru, Rh, Ir, and transition metal oxides. Amorphous Ir nanosheets exhibit excellent catalytic performance in acid oxygen evolution reactions. Based on the synthesis of amorphous nanosheets, we have also controlled the short/medium-range atomic structures of amorphous oxide nanosheets. In addition, we have achieved a universal method for constructing amorphous-crystalline phase interfaces in nanosheet planes by controlling the atomic migration rate during the nucleation and growth of nanomaterials. We use the synthesized noble metal ultrathin amorphous nanomaterials as a model system and rely on in-situ high-resolution transmission electron microscopy imaging and spectroscopic techniques to conduct in-depth atomic-scale research on key fundamental issues in the synthesis of noble metal amorphous ultrathin nanosheets, such as nucleation, growth, and phase transitions.

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Xun HONG is a professor at the Department of Applied Chemistry, University of Science and Technology of China. He received his PhD degree from USTC in 2010. He started working as a postdoctor at Tsinghua University and Nanyang Technological University in 2010 and 2012, respectively. In 2014, he joined USTC as a Principal Investigator. His research program aims at the synthesis and characterization of amorphous nanomaterials and supported single atom nanomaterials for electrocatalysis application.

Session V: Phase-Based Heterostructures for Electronics and Catalysis

[Session V] Talk 23: Young Hee LEE

CONTEMPORARY CHALLENGES IN VAN DER WAALS LAYERED SEMICONDUCTORS

Young Hee LEE

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Since the advent of one-dimensional carbon nanotubes (CNTs) in 1991 and two-dimensional graphene in 2004, followed by transition metal dichalcogenides (TMDs), there has been an explosion of research exploring their unique fundamental science and technological applications. Motivated by the limitations of CNTs and graphene in certain applications, other 2D layered materials such as TMDs, hexagonal boron nitride (hBN), and black phosphorus (BP) have been extensively studied, opening new horizons in physics, electronics, and optoelectronics. These materials also offer exciting possibilities in emerging fields like valleytronics, spintronics, twistrionics, and orbitronics. The key physics behind include strong Coulomb interactions, reduced charge screening, large exciton binding energies, and significant spin-orbit coupling, which present valuable opportunities for both fundamental research and practical applications. In this presentation, I will discuss recent and ongoing challenges in the field of vdW semiconductors and devices including Ohmic contact, mobility/on-current, ferromagnetic semiconductors at room temperature, hot-carrier solar cell, and Bose-Einstein condensation in electronics etc.



Young Hee LEE has been a full professor of the Physics Department at SKKU, since 2001. He received Ph. D. from Kent State University in Ohio (1986) in physics. Prior to joining SKKU in 2001, Prof. Lee was a full professor in the Physics Department at Chonbuk National University since 1986. He was a visiting scholar at Ames Laboratory, Iowa State University in 1989, IBM, Zurich in 1993, and Michigan State University in 1996. He was a Director of Center for Integrated Nanostructure Physics, Institute for Basic Science (IBS) at SKKU in 2012-2023. He has been a fellow of Korean Academy of Science and Technology since 2007 and Academician, Chinese Academy of Sciences since 2021. Currently, he is a HCR distinguished professor at SKKU. He serves for an Associate Editor of ACS Nano. He was awarded the first SKKU fellow in 2004 at SKKU, Science award from Korean Physical Society in 2005, Lee Hsun Research Award, IMR, Chinese Academy of Sciences, China in 2007, and Einstein Award IMR, Chinese Academy of Sciences, China in 2017. He was also nominated as a National Scholar by Ministry of Education in 2006. He recently got Sudang prize in 2015, Kyung Am prize in 2019, and Song-Bong prize in 2020. He was highly cited researcher (HCR) for 2018-2024.

[Session V] Talk 24: Manish CHHOWALLA

**METALLIC TWO-DIMENSIONAL TRANSITION METAL DICHALCOGENIDES**

Manish CHHOWALLA

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I will start with a brief description of the different phases of 2D transition metal dichalcogenides. Then I will report on the realization of high-performance lithium-sulfur batteries using metallic 1T phase of two-dimensional molybdenum disulfide as binder-free conducting cathodes for hosting sulfur. The metallic MoS<sub>2</sub>-based ampere-hour-scale pouch cells can deliver gravimetric energy density of >500 Wh kg<sup>-1</sup>. These metrics compare exceptionally favourably with current state-of-the-art in Li-S batteries. Our results provide unique insights into new designs for Li-S cathodes based on electrocatalytically active and conducting two-dimensional (2D) materials.



Manish CHHOWALLA, FEng, is the Goldsmiths' Professor of Materials Science at the University of Cambridge. His research interests are in the fundamental studies of atomically thin two-dimensional transition metal dichalcogenides (TMDs). In particular, his group studies the optical and electronic properties of different phases of 2D TMDs. He has demonstrated that it is possible to induce phase transformations in atomically thin materials and utilize phases with disparate properties for field effect transistors, catalysis, and energy storage.

[Session V] Talk 25: Hyeon Suk SHIN

PHASE ENGINEERING OF WS<sub>2</sub> AND MOS<sub>2</sub> MONOLAYER QUANTUM DOTS BY RHENIUM DOPING

Hyeon Suk SHIN

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Transition metal dichalcogenides (TMDs) occur in the thermodynamically stable trigonal prismatic (2H) or the metastable octahedral (1T) phase. Phase engineering of TMDs has proven to be a powerful tool for applications in energy storage devices as well as in electrocatalysis. However, the mechanism of the phase transition in TMDs and the synthesis of phase-controlled TMDs remain challenging. Here we report the synthesis of Re-doped WS<sub>2</sub> monolayer quantum dots (MQDs) using simple colloidal chemical process. We find that the incorporation of small amount of electron-rich Re atoms in WS<sub>2</sub> changes the metal–metal distance in the 2H phase initially, which introduces strain in the structure (strained 2H (S2H) phase). Increasing the concentration of Re atoms sequentially transforms the S2H phase to the 1T and 1T' phases to release the strain. In addition, we performed controlled experiments by doping Re in MoS<sub>2</sub> to distinguish between Re and Mo atoms in scanning transmission electron microscopy images, and quantified the concentration range of Re atoms in each phase of MoS<sub>2</sub> indicating that the phase engineering of WS<sub>2</sub> or MoS<sub>2</sub> is possible by doping different amounts of Re atoms. We demonstrate that the 1T' WS<sub>2</sub> MQDs with 49 at. % Re shows superior catalytic performance (low Tafel slopes of 44 mV/dec, low overpotentials of 158 mV at a current density of 10 mA/cm<sup>2</sup>, and long-term durability up to 5000 cycles) for the hydrogen evolution reaction. Our findings provide understanding and control of phase transitions in TMDs, which will allow efficient manufacture and translation of phase engineered TMDs.



Hyeon Suk SHIN is the director of IBS Center for 2D Quantum Heterostructures at SKKU and a professor at Department of Energy Science and Department of Chemistry, SKKU. Before joining IBS center at SKKU, he was a UNIST endowed chair professor at Department of Chemistry, Ulsan National Institute of Science and Technology (UNIST), Korea. He received his PhD from Department of Chemistry at POSTECH in 2002. After working as a postdoctoral fellow at University of Cambridge, UK and subsequently as a research Professor at POSTECH, he joined UNIST in 2008 and recently moved to SKKU to become the director of the IBS center at SKKU in 2024. He received 'Scientist of the Month' award (Ministry of Science and ICT) in 2023, Grand Academic Award (UNIST) in 2023, 'Top 100 National R&D Outstanding Achievements' award (Ministry of

Science and ICT) in 2021, Sigma-Aldrich Excellent Chemist Award (Korean Chemical Society) in 2021, Basic Researcher of the Year award (Ministry of Science and ICT, Republic of Korea) in 2020, Creative Knowledge Award (Minster Award by Ministry of Science, ICT, and Future Planning) in 2015, outstanding researcher award (Materials Chemistry Division, KCS) in 2015, the Faculty of the Year award of UNIST in 2014, and the Minister award of Ministry of Knowledge Economy, Korea in 2012. His current research focuses on 2D materials, their amorphous structures, and their applications for energy conversion and storage and quantum information technology.

**SOLUTION PROCESSED NANOSHEETS FOR ELECTRONIC DEVICES: TOWARDS HOMO- AND HETERO-STACKS WITH CONTROLLED INTERFACES**

Jonathan N COLEMAN

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Solution-processable two-dimensional (2D) materials offer significant promise for a wide range of printed electronics applications, including transistors, capacitors, diodes, and circuits. However, realizing devices with state-of-the-art performance necessitates advances in nanosheet processing and printing techniques. Key to this progress is enhancing the electrical properties of nanosheet networks and heterostructures and translating these improvements into superior device performance. While high intrinsic nanosheet properties, such as carrier mobility, are important, the primary challenge lies in controlling the interfaces between adjacent nanosheets. For instance, in the case of 2H-MoS<sub>2</sub> nanosheets within a printed transistor channel, the inter-nanosheet junction resistance directly affects network mobility. Achieving high-performance devices requires the development of nanosheets with high aspect ratios and sufficient flexibility to form conformal junctions with neighbouring sheets, along with scalable deposition methods to maintain these conformal junctions over large areas. Despite these principles, considerable work remains to maximize the aspect ratio of nanosheets, produce clean junctions free of processing residues, and achieve low junction resistance. Additionally, understanding the charge transfer mechanisms at these junctions, and how they are influenced by factors such as nanosheet area and thickness, is critical.

Moreover, real-world printed electronic devices incorporate multiple materials, such as semiconducting nanosheets for active channels, conductive nanosheets for electrodes, and insulating nanosheets for dielectrics, each creating different inter-layer interfaces. Controlling the quality of metal-semiconductor interfaces to enhance charge injection, and optimizing insulator-semiconductor interfaces to minimize leakage, maximize capacitance, and ensure uniform threshold voltages, are crucial for device performance. Here, phase control may be crucial. For example, we might expect printed interfaces of 2H- MoS<sub>2</sub>/1T- MoS<sub>2</sub> nanosheets to be an ideal model system for such work. These challenges necessitate access to appropriate nanosheet types, precise control over nanosheet deposition and extensive characterization of the resulting interfaces and their surrounding regions.

In this presentation, I will discuss these critical factors and outline our recent progress in advancing the understanding and development of high-performance printed electronic devices using 2D materials.

## Nature Conference on Phase Engineering of Nanomaterials 2024 | Nov 20-22, 2024



Jonathan COLEMAN is the Erasmus Smith's Professor of Natural and Experimental Philosophy (1724) in the School of Physics, and a Principal Investigator in the AMBER Research centre at Trinity College Dublin. He graduated with First Class Honours and a Gold Medal in Physics in 1995 and completed a PhD in Physics in TCD in 1999, working in the research group of Werner Blau. He became a junior lecturer in 2001, rising to the Chair of Chemical Physics in 2011. He was appointed to his current position in 2022.

Prof COLEMAN's area of interest is in solution processing of nano-materials, predominately carbon nanotubes, nanowires and 2D nanosheets such as graphene. He is most well-known for developing Liquid Phase Exfoliation, a versatile and widely used method for preparing 2D materials. These solution processing methods allow the formation of dispersions, suspensions and solutions of nanostructures and facilitate the production of coatings, thin films and composites. Coleman works on applying these materials and

methods in a number of areas including electro-mechanical sensors, printed electronics and energy storage materials.

Prof COLEMAN has been involved in a number of industry-academic collaborative projects with companies including Hewlett-Packard, Intel, SAB Miller, Nokia-Bell Labs and Thomas Swan.

He has published >350 papers in journals including Nature and Science and has been cited >100,000 times. He was recently listed by Thomson Reuters among the world's top 100 materials scientists and has collaborated with many companies including Hewlett-Packard, Intel, SAB Miller, Nokia-Bell Labs and Thomas Swan.

More info at [Jonathan COLEMAN \(physicist\) - Wikipedia](#)

[Session V] Talk 27: Xiangfeng DUAN

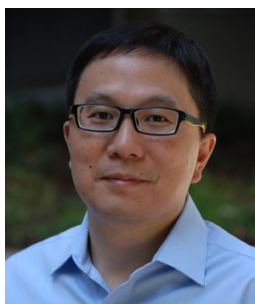
**VAN DER WAALS SUPERLATTICES: THE BO(U)NDLESS FRONTIER**

Xiangfeng DUAN

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The rise of two-dimensional atomic crystals (2DACs) and van der Waals heterostructures (VDWHs) has inspired a bonding-free approach to constructing heterostructures beyond traditional epitaxial methods. This talk begins with an overview of early explorations into van der Waals (VDW) interactions for integrating disparate materials with pristine electronic interfaces. I will then focus on our recent advancements in synthesizing and exploring a diverse family of VDW superlattices (VDWSLs) composed of alternating layers of 2DACs and self-assembled molecular interlayers with customizable chemical compositions and structural motifs. I will highlight how these molecular interlayers can tailor the electronic and optical properties of 2DACs, with a particular emphasis on chiral molecular intercalation superlattices that exhibit robust chiral-induced spin selectivity and intriguing chiral superconductivity. With versatile molecular design and modular assembly strategies, 2D-molecular VDWSLs offer boundless opportunities to tailor electronic, optical, and quantum properties, creating a rich platform for emerging technologies.



Dr. Xiangfeng DUAN received his B.S. Degree from University of Science and Technology of China in 1997, and Ph.D. degree from Harvard University in 2002. From 2002-2008, he was a Founding Scientist responsible for advanced technology development at *Nanosys Inc.*, a nanotechnology startup founded based partly on his doctoral research. Dr. DUAN joined UCLA with a Howard Reiss Career Development Chair in 2008, and was promoted to Associate Professor in 2012 and Full Professor in 2013. His research interest includes nanoscale materials, devices and their applications in future electronics, energy and health technologies. Dr. DUANs has received many awards for his pioneering research in nanoscale science and technology, including MIT Technology Review Top-100 Innovator Award, NIH Director's New Innovator Award, NSF Career Award, Alpha Chi Sigma Glen T. Seaborg Award, US Presidential Early Career Award for Scientists and Engineers (PECASE), ONR Young Investigator Award, DOE Early Career Scientist Award, Human Frontier Science Program Young Investigator Award, Dupont Young Professor, the Beilby Medal and Prize, International Society of Electrochemistry Zhao-Wu Tian Prize for Energy Electrochemistry, Materials Research Society Middle Career Researcher Award, IEEE Nanotechnology Council Distinguished Lectureship, the IEEE Pioneer Award in Nanotechnology and most recently Royal Society of Chemistry Materials Chemistry Horizon Prize (Stephanie L. Kwolek Prize) and Faraday Horizon Prize . He is currently a Fellow of Royal Society of Chemistry, American Association for the Advancement of Science and National Academy of Inventors.

Short Talk Session II

Short Talk 3: Bolong HUANG

**ADVANCED ATOMIC CATALYSTS DESIGN FOR ENERGY SYSTEMS**

Bolong HUANG

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Currently, atomic catalysts (ACs) as the frontier research topics have attracted tremendous attention due to their ultra-high electroactivity and broad applications in different energy systems. However, a large number of possible combinations between metals and support materials, the complexity of catalytic materials, as well as the complicated reaction mechanisms are still the main difficulties for designing novel ACs. To supply theoretical guidance for designing novel electrocatalysts, we have carried out comprehensive theoretical studies of ACs supported on graphdiyne (GDY) through density functional theory (DFT) calculations and machine learning (ML) techniques. First, we have proposed the “Redox Barrier Model” to quantify the capability of electron exchange and transfer. For the hydrogen evolution (HER) process, we have extended the conventional indicator of proton binding energy to more diverse criteria, where the screened electrocatalysts for HER are also verified ML. To design dual atomic catalysts (DACs), the formation stability and electronic modulations for all the combinations between transition metals (TMs) and lanthanide (Ln) metals are compared. Due to the electronic self-balance effects by f-d orbital coupling, the combinations of the Ln metals and TMs achieve optimized stability and electroactivity of GDY-DACs. For the applications of GDY-ACs in the CO<sub>2</sub> reduction reaction (CO<sub>2</sub>RR), a comprehensive reaction pathway mapping of C<sub>1</sub> and C<sub>2</sub> products is achieved for the first time, where the integrated large-small cycle mechanism and double-dependence correlations are identified. Moreover, the first principles machine learning (FPML) approach is proposed to predict the reaction trends for different products and C-C couplings for novel C<sub>3</sub> products. Therefore, these theoretical explorations have supplied important insights and effective approaches for the design of novel ACs, opening a new avenue to enable broad applications of ACs towards different energy systems.



Short Talk 4: Xiao ZHOU

REALIZATION OF STABLE AND MULTI-LEVEL STATES IN PHASE CHANGE HETEROSTRUCTURE BY NOVEL CRYSTALLINE-TO-CRYSTALLINE TRANSITION

Xiao ZHOU<sup>a</sup>, Ruirui LIU<sup>b</sup>, Jiwei ZHAI<sup>c</sup>, Zhitang SONG<sup>d</sup>, Sannian SONG<sup>d</sup>

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Phase-change random-access memory (PCRAM) stands out as a promising candidate for non-volatile memory. Effective phase regulation is essential for realizing Multi-Level Cell (MLC) technology and multi-level storage states, despite typical challenges such as increased resistance drift and undesirable operation endurance. Here, we introduce a phase-change heterostructure (PCH) featuring alternately stacked phase-change and confinement nanolayers to achieve precise phase composition control via novel crystalline-to-crystalline transition. This structure supports MLC with five distinct storage states and maintains four stable resistance levels. Our device demonstrates exceptional operation characteristics, sustaining up to  $10^5$  cycles with ultralow power consumption (0.43 pJ) and ultralow resistance drift. These results underscore the superior performance of our PCRAM design and its substantial potential for PCRAM.

Short Talk 5: Huabin ZHANG

STORIES ABOUT SINGLE ATOM CATALYSIS

Huabin ZHANG

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Increasing demand for sustainable energy has accelerated research on various renewable technologies. Developing catalytic energy conversion technologies for replacing the traditional energy source is highly expected to resolve the fossil fuel exhaustion and related environmental problems. Exploring stable and high-efficiency catalysts is of vital importance for the promotion of these technologies. Single-atom catalysts (SACs), containing single metal atoms anchored on supports, represent the utmost utilization of metallic catalysts and thus maximize the usage efficiency of metal atom.<sup>1</sup> However, with the decreasing of particle size, the surface free energy increases obviously, and tends to aggregate into clusters or particles. Selection of an appropriate support is necessary to interact with isolated atoms strongly, and thus prevents the movement and aggregation of isolated atoms, creating stable, finely dispersed active sites. Furthermore, with uniform single-atom dispersion and well-defined configuration, SACs afford great space for optimizing high selectivity and activity.

Our research interest focuses on the development of single-atom catalysts with the particular configuration for sustainable energy conversion, including photocatalysis, electrocatalysis, and thermal catalysis.<sup>2</sup> His research also extends to the operando investigation for monitoring the structural evolution of the reactive centers, as well as the mutual interaction between the reactive center and reactant in the catalytic process. The widespread adoption of SACs in diverse catalytic reactions will be comprehensively introduced.<sup>3, 4</sup> By presenting these advances and addressing some future challenges with potential solutions related to the integral development of catalysis over SACs, we expect to shed some light on the forthcoming research of SACs for catalytic energy conversion.

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**Short Talk 6: Guobin WEN**

**MASS TRANSFER ENHANCED ELECTROCATALYTIC CO<sub>2</sub> CONVERSION**

Guobin WEN

Hunan University

The improvement of conversion efficiency for electrocatalysis is one of the important topics in the development of new quality productive forces. Focusing on the challenges of multi-level mechanism and regulation for mass transport and reaction activity, the applicant developed the coupled enhancements of electrocatalytic reaction and mass transport to improve the conversion efficiency of CO<sub>2</sub> electrolysis, and realized a series of achievements: 1) Developed an "exsolution-transport" electrolysis reactor to enhance bulk mass transport by controlling pressure of flow field, boosting the conversion yield over 10 times (Nat. Energy, 2022, 7, 978); 2) Constructed orderly micro/nano mass transport channels for the electrode to quantify and regulate the reaction microenvironment, forming the concept of coupled enhancements for mass transport and reactions. (Angew. Chem. 2020. 59, 31, 12860; J. Am. Chem. Soc. 2021. 143, 18, 6855) 3) Designed stereoscopic lamellar structure to enhance mass and charge transfer and achieve efficient expression of catalytic activity. (Adv. Mater. 2023, 2310822; Nat. Commun. 2022, 13, 2486)

Dr. Wen has published 16 papers as the first/corresponding author, including Nat. Energy, Angew. Chem., JACS, Nat. Commun., Adv. Mater., etc., containing 5 ESI highly cited papers.

Poster Presentation

Poster 1: Zhenyu SHI

**SINGLE-ATOMICALLY DISPERSED PT SUPPORTED ON 1T'-MoS<sub>2</sub> FOR HIGHLY EFFICIENT ELECTROCATALYTIC HYDROGEN EVOLUTION**

Zhenyu SHI, Hua ZHANG

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Crystal phase is crucial in determining the properties and functions of the 2D transition-metal dichalcogenides (TMDs), which commonly serve as supports for metal catalysts for various catalytic reactions. Although diverse TMD-supported catalysts have been reported, the used TMD templates are normally in the conventional 2H phase or mixed phases, how the TMD crystal phase affects the growth of the secondary material is poorly understood. For instance, when MoS<sub>2</sub>-supported Pt nanoparticles (PtNPs) were used as electrocatalysts for hydrogen evolution reaction (HER), only ~65% of the PtNPs were epitaxially grown on the MoS<sub>2</sub> nanosheet (NS) template which was composed of metallic/semimetallic 1T/1T' phase but with thermodynamically stable and poorly conducting 2H phase mixed in. In the meantime, the poor conductivity of the remaining 2H phase in these MoS<sub>2</sub>-based electrocatalysts severely limits their overall performances. Therefore, constructing noble metal/MoS<sub>2</sub> hybrids based on high purity 1T/1T'-MoS<sub>2</sub> is essential for understanding the phase-dependent growth of noble metals and preparing efficient electrocatalysts.

In this work, we report the preparation of 1T'-MoS<sub>2</sub> and 2H-MoS<sub>2</sub> NSs with high phase purity, which are then used as supports for noble metal Pt. We found that the 2H-MoS<sub>2</sub> templates facilitate the epitaxial growth of PtNPs, while the 1T'-MoS<sub>2</sub> nanosheets support single-atomically dispersed Pt (s-Pt) under similar experimental conditions. Being used as an electrocatalyst for the HER in acidic media, the obtained s-Pt/1T'-MoS<sub>2</sub> possesses a mass activity of 85±23 A mg<sub>Pt</sub><sup>-1</sup> at the overpotential of -50 mV and a mass-normalized exchange current density of 127 A mg<sub>Pt</sub><sup>-1</sup> as revealed by high mass-transport floating electrode technique. Density functional theory (DFT) calculations indicate that the s-Pt adsorbed on the top site of Mo exhibits a hydrogen adsorption free energy close to zero, which could contribute to the efficient H<sub>2</sub> evolution of s-Pt/1T'-MoS<sub>2</sub>. Importantly, the s-Pt/1T'-MoS<sub>2</sub> exhibits high stability during HER in both H-type cell and prototype proton exchange membrane electrolyser. Our work demonstrates that 1T'-TMDs can be ideal supports for catalysts used for various important reactions.

Poster 2: Zijian LI

**1T'-TRANSITION METAL DICHALCOGENIDE MONOLAYERS STABILIZED ON 4H-AU FOR ULTRASENSITIVE SERS  
DETECTION**

Zijian LI, Hua ZHANG

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Unconventional 1T'-phase transition metal dichalcogenides (TMDs) have attracted tremendous research interest due to their unique phase-dependent physicochemical properties and applications. To date, various synthetic strategies, such as gas-solid reaction, chemical vapor deposition, lithium intercalation and molecular beam epitaxy have been developed to prepare 1T'-TMDs. However, the aforementioned synthetic approaches still suffer from harsh synthetic conditions or complicated synthetic protocols, it is important to develop a mild and rapid method to prepare 1T'-TMDs with high phase purity.

Au substrates/templates are widely used as ideal substrates/templates for the controllable growth of high-quality TMD monolayers (MLs), which, however, normally possess a pure 2H phase, or mixed phase of 1T' and 2H. In addition, due to its metastable nature, the semi-metallic 1T' phase prepared via the aforementioned methods could gradually transform into the thermodynamically stable semiconducting 2H phase, severely hindering the study of intrinsic physicochemical properties and phase-dependent applications of 1T'-TMDs.

In this work, we report that the unconventional 4H-Au nanowires (NWs), when used as templates, can induce the quasi-epitaxial growth of high phase-purity and stable 1T'-TMD MLs, including WS<sub>2</sub>, WSe<sub>2</sub>, MoS<sub>2</sub> and MoSe<sub>2</sub>, via a facile and rapid wet-chemical method. Systematic characterization and calculation results reveal that the formation and stabilization of high phase-purity 1T'-TMD MLs on the 4H-Au NWs could be ascribed to their strong interaction, charge doping from the oleylamine in solution, and the unique 4H phase of Au template. The as-synthesized 4H-Au@1T'-TMD core-shell NWs can be used for ultrasensitive surface-enhanced Raman scattering (SERS) detection. For instance, the 4H-Au@1T'-WS<sub>2</sub> NWs have achieved attomole-level SERS detections of Rhodamine 6G and a variety of SARS-CoV-2 spike proteins. This work provides new insights into the preparation of high phase-purity and stable 1T'-TMD MLs on metal substrates/templates, showing great potential in various promising applications.

Poster 3: Mohsen TAMTAJI

REACTION MECHANISM OF CARBON MONOXIDE ELECTROREDUCTION TO PROPYLENE AND CYCLOPROPANE (C<sub>3+</sub>)  
OVER TRIPLE ATOM CLUSTERS

Mohsen TAMTAJI<sup>1</sup>, Soonho KWON<sup>2</sup>, Charles B. MUSGRAVE III<sup>2</sup>, William A. Goddard III<sup>2\*</sup>, GuanHua CHEN<sup>1,3\*</sup>

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The carbon monoxide reduction reaction (CORR) towards C<sub>2+</sub> and C<sub>3+</sub> products such as propylene and cyclopropane can not only reduce anthropogenic emissions of CO and CO<sub>2</sub>, but also produce value-added organic chemicals for polymer and pharmaceutical industries. Here we introduce the concept of triple atom catalysts (TACs) which have three intrinsically strained and active metal centers for reducing CO to C<sub>3+</sub> products. We applied grand canonical potential kinetics (GCP-K) to screen twelve transition metals (M) supported by nitrogen-doped graphene denoted as M<sub>3</sub>N<sub>7</sub>, where M stands for Mn, Fe, Co, Ni, Cu, Ru, Rh, Pd, Ag, Ir, Pt, and Au. We sought catalysts with favorable CO binding, hydrogen binding, and C-C dimerization energetics, identifying Fe<sub>3</sub>N<sub>7</sub> and Ir<sub>3</sub>N<sub>7</sub> as the best candidates. We then studied the entire reaction mechanism from CO to C<sub>3</sub>H<sub>6</sub> and C<sub>2</sub>H<sub>4</sub> as a function of applied potential via, respectively, 12-electron and 8-electron transfer pathways on Fe<sub>3</sub>N<sub>7</sub> and Ir<sub>3</sub>N<sub>7</sub>. Density Functional Theory (DFT) predicts an overpotential of 0.17 V<sub>RHE</sub> for Fe<sub>3</sub>N<sub>7</sub> towards propylene and an overpotential of 0.42 V<sub>RHE</sub> towards cyclopropane at 298.15 K and pH=7. Also, DFT predicts an overpotential of 0.15 V<sub>RHE</sub> for Ir<sub>3</sub>N<sub>7</sub> towards ethylene. This paper provides fundamental insights into the design of advanced catalysts for C<sub>2+</sub> and C<sub>3+</sub> synthesis at room temperature.

Poster 4: Ahsanulhaq QURASHI

RATIONAL SYNTHESIS OF CATALYTIC MATERIALS FOR CLEAN ENERGY GENERATION APPLICATIONS

Ahsanulhaq QURASHI

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To advance the progress of clean energy, various promising new materials-based devices and systems have been systematically investigated in the past few years. In this context, atomically precise noble metal nanoclusters (NMNCs) are highly desirable to unravel the size and structure-activity relationships in catalysis, their synthesis in a controlled way at the atomic level is challenging [1,2]. Herein, we present the structure and gram scale synthesis of a highly symmetric 2-phenylethanethiol (PETH) and triphenylphosphine (TPP)-protected 32-atom AgCu alloy nanocluster (NC)  $[\text{Ag}_8\text{Cu}_{24}\text{H}_6(\text{PET})_{16}\text{Cl}_8(\text{TPP})_8][\text{BF}_4]_2$  with a cuboid shape, denoted as Ag<sub>8</sub>Cu<sub>24</sub>. Also The solvent induced polymorphism in  $[\text{Cu}_{15}(\text{PET})_{13}(\text{TPP})_6][\text{BF}_4]_2$  (Cu<sub>15</sub>) (TPP = triphenylphosphine, PET = 2-phenylethanethiol), and double-helical assembly of  $[\text{Cu}_{18}\text{H}(\text{PET})_{14}(\text{TPP})_6\text{Cl}_3]$  (Cu<sub>18</sub>) nanocluster (NC) from the reaction intermediate will be discussed. Also in this talk, we will discuss various potential electrode materials for hydrogen and oxygen production through water splitting, CO<sub>2</sub> conversion process and other clean energy production and storage applications [3]. Finally, an overview of challenges, frontiers and opportunities of materials for energy conversion and storage systems will be conversed.

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**Poster 5: Pinxian XI**

**MICROSTRUCTURE-ORIENTED MANUFACTURING OF RARE EARTH INORGANIC MATERIALS**

Pinxian XI

Lanzhou University, Lanzhou City, Gansu Province, China

The advancement of industrial alkaline water electrolysis (AWE) technology is primarily hindered by the limited adsorption coverage of anodic  $\text{OH}^-$  under high current density conditions, leading to changes in surface microenvironment pH value and a decrease in oxygen-containing active species. To address these scientific challenges, we have developed a controlled synthesis method utilizing rare earth ions for the directional construction of rare earth-modified  $\text{NiS}_2$  catalysts. The interface formation process between rare earth particles has been elucidated through in-situ infrared and in-situ fluorescence spectra during the synthesis process. By employing multiple in situ spectroscopy techniques including isotope-labeled experiments and time-resolved absorption spectroscopy, we have established the relationship among  $\text{OH}^-$  coverage, active site density, and catalytic activity based on a series of rare earth-modified  $\text{NiS}_2$  materials. Furthermore, the stability of operating conditions has been verified for over 100 hours using a kW-level AWE device. This research provides novel insights into rare earth modification as a potential solution to enhance anodic  $\text{OH}^-$  coverage.



**Poster 6: Moulay Ahmed Said AZIZI SAMIR**

**NANOCELLULOSE AS INSPIRING SUPPORT FOR INNOVATIVE FUNCTIONAL NANOHYBRIDS**

Moulay Ahmed Said AZIZI SAMIR  
LGP2, INP Grenoble, France

Innovative materials are highly needed to answer the challenging properties and multifunctionalities demand emerging from different sectors. In the same time ecofriendly and low impact materials and process must be developed to answer the emerging global awareness related to environmental protection. Designing materials at the Nano scale is a promising strategy to achieve these goals.

Trees are an inspiring example of material Nano-design with bioengineered processes. Nanocellulose are a building-block of cellulose fibers, they are critical component in the cell wall structure. So, they are vital for the role trees are playing in the earth ecosystem via photosynthesis. In addition to plants, cellulosic nanofibers could be extracted from marine species like tunicate and biosynthesized by some bacteria strains. These nanofibers have larger specific surface area, more reactivity when compared to cellulose fibers and could be building-blocks for innovative materials. Cellulose nanofibers present high mechanical properties with 150 GPa estimated axial elastic modulus. Nanocellulose could be a perfect model of nanostructured biomaterials nano-designed to ensure very specific functionalities.

Nanohybrids are a class of materials combining organic and inorganic components at the nanoscale. The inorganic nanophase could ensure new functionalities when controlled composition, size and structure could be achieved.

Our work demonstrates feasibility of making new nanohybrids using different nanocellulosic morphologies. Bacterial nanocellulose and Copper were used as biphasic model to design new hybrids. Structure and morphologies of the prepared hybrids were explored by SEM, AFM and XRD.

Results demonstrate promising new materials with possible tailored final properties and high potential applications in fields such as energy and catalysis.

Poster 7: Sheng CHEN

Acid-stable ebonex-phase  $\text{Ti}_4\text{O}_7$  for continuous-flow nitrogen electrofixation

Sheng CHEN

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Acidic nitrogen electrofixation offers the benefits of abundant protons sources and improved solubility of  $\text{N}_2$  that can facilitate the reaction kinetics at three-phase interfaces. However, excessive protons would simultaneously boost competitive hydrogen evolution that consume electrons otherwise for nitrogen electrofixation, leading to low selectivity to ammonia. In this paper, we report an acid-stable ebonex ( $\text{Ti}_4\text{O}_7$ ) characteristic of excellent catalytic performances in 0.1 M HCl electrolyte (pH=1). As comparison to its rutile-phase ( $\text{TiO}_2$ ) counterpart, the ebonex-phase catalyst demonstrates an optimal Faradic efficiency of 23.57% and large ammonia yield rate of  $45.52 \mu\text{g h}^{-1}\text{cm}^{-2}$ . Further mechanism study has been conducted by using density function theory (DFT) calculations and X-ray absorption near-edge structure (XANES), which indicate the structural advantages of ebonex such as intrinsic electrical conductivity and low oxidation valence of Ti and Jahn-Teller-type structural distortion. Consequently, the ebonex catalyst can suppress hydrogen evolution, leading to a favorable associative-alternating nitrogen electrofixation pathway with the rate-limiting step of  $\text{N}_2^* \rightarrow \text{NNH}^*$

Professor Sheng Chen has devoted to the design, preparation and application of low-dimensional nanomaterials for carbon-neutral energy catalysis. He has served as the academic editor, editorial board member and young editorial board member for such journals as Exploration, Catalyst, Carbon Energy, Journal of Energy Chemistry, Carbon Neutralization, etc. He is also the Member of the Expert Committee of Chinese Energy Society. Within the past years, he has studied and worked at Nanjing University of Science and Technology (phD), Monash University (exchange student), University of Adelaide (Postdoctoral), University of New South Wales (Research fellow) in Australia and Max Planck Institute of Colloids and Interfaces in Germany (Alexander von Humboldt Fellowship). He has published more than 100 papers in world-leading journals like Nature Communications, Angew Chem Int Ed, Advanced Materials, ACS Nano, Energy Environmental Science, etc. His research papers have received more than 12,000 citations. Further, he has been awarded as world's top 2% most-cited scientists, ESI Highly Cited Researcher (Clarivate), China's Highly Cited Scientists (Elsevier), and international association for advanced materials (IAAM) scientist award. He has filed/applied more than 20 invention patents and developed new materials/techniques that have been widely industrialized".

Poster 8: Ming ZHAO

**PHASE-REGULATABLE RU-BASED NANOCAGES TOWARD HIGHLY EFFICIENT ALKALINE HYDROGEN EVOLUTION**

Ming ZHAO

National University of Singapore

Engineering the crystal phase of nanocatalysts represents a promising strategy to modulate the catalyst–adsorbate interactions for enhanced catalysis. However, conventional methods for phase regulation suffer from unsatisfactory time- and cost-effectiveness in large-scale production and lack precise control over the catalyst composition at the atomic level, which is detrimental, especially for reactions involving multiple intermediates. Herein, we report a first-of-its-kind protocol for simultaneously regulating the crystal phase and composition (single-atom Pt doping) of Ru ultrathin nanocages (<2 nm), achieving efficient hydrogen evolution reaction (HER) in alkaline electrolytes. In situ characterizations and theoretical calculations reveal that Ru atoms in a metastable face-centered cubic (fcc) phase and Pt single atoms collectively optimize the adsorption of intermediates for accelerated HER kinetics. Consequently, the Pt-doped fcc Ru nanocages exhibit impressive alkaline HER performance with a near-zero overpotential of 8.5 mV at 10 mA cm<sup>-2</sup> and an extremely low Tafel slope of 21 mV dec<sup>-1</sup>. Moreover, the practicality of the obtained catalyst is demonstrated by constructing an anion exchange membrane water electrolyzer and a continuous-flow reactor for scalable catalyst preparation.

Poster 9: Yixuan ZHAO

**AUTOMATIC PROCESSING AND TRANSFER OF TWO-DIMENSIONAL MATERIALS WITH ROBOTICS**

Yixuan ZHAO<sup>1</sup>, Li LIN<sup>2,3\*</sup>, Zhongfan LIU<sup>1,3\*</sup>

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The mature and well-developed chemical vapor deposition (CVD) growth technologies have enabled two-dimensional (2D) materials and their heterostructures to take the centre stage in developing material platforms for next-generation electronics and advanced photonic devices for the semiconductor industry, quantum technologies, etc. However, the gap between 2D material production and end-user applications is the lack of a scalable technique to transfer the high-quality CVD-grown materials from their growth substrates to target substrates.

Herein, by engineering the interfacial adhesion and strain, we have achieved an automatic processing and the transfer of 2D materials with robotics. The deep insights into common challenges in delamination and lamination processes of 2D materials were discussed and addressed by introducing an ultrathin layer of Al coating and an Al oxidation step, which facilitate the fine tuning and precise control of interfacial adhesion and strain. The developed transfer technique and automated system are industrially compatible for batch production, which are demonstrated by the enhanced production capability, highly reliable transfer quality, and high uniformity and repeatability of the transferred 2D materials.

Demonstrated by life-cycle assessment (LCA), the automated robotic system delivers a green and sustainable transfer route with advantages in all environmental impact categories. This automatic processing technique bridges the gap between 2D material production industry and the industry of advanced electronics and photonics, and has the potential to be extended to other material and nanotechnology system, thus, could boost the rapid development of the whole industry of 2D material manufacture and application industries.

Poster 10: Junhao LIAO

**DIELECTRIC-LAYER-ASSISTED TRANSFER FOR TWO-DIMENSIONAL MATERIAL DEVICES WITH ULTRAHIGH CARRIER MOBILITY AND LONG-TERM STABILITY**

Junhao LIAO<sup>1,3</sup>, Yanfeng ZHANG<sup>1,2,3\*</sup>, Li LIN<sup>1,2,3\*</sup>, Zhongfan LIU<sup>1,3\*</sup>

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By confining the electrons in the two-dimensional (2D) channel, 2D materials have become promising for next-generation electronics. Despite recent breakthroughs in synthesizing single-crystal 2D channel material wafers, critical challenges still exist in the preparation of single-crystal dielectric wafers and reliable methods to integrate dielectric on 2D semiconductors with ultraclean interfaces, sufficiently large gate capacitance, and low leakage current. Here we achieved the epitaxial growth of transferable, ultrathin, single-crystal  $\text{Sb}_2\text{O}_3$  dielectric wafers on graphene-covered  $\text{Cu}(111)$  surface, which exhibited a fine gate controllability with equivalent oxide thickness (EOT) of 0.60 nm. The conformal growth of  $\text{Sb}_2\text{O}_3$  enabled the crack and wrinkle-free transfer of graphene onto application-specific substrates and highly improved graphene device performance across 4-inch wafers with a maximum carrier mobility of  $29,000 \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$  and long-term stability. By minimizing the interfacial traps and defects, the clean interface and single-crystal nature of  $\text{Sb}_2\text{O}_3$  allow for an on/off ratio of  $10^8$  and minimum subthreshold swing (SS) of  $64 \text{ mV dec}^{-1}$  in  $\text{MoS}_2$  devices. This study offers a reliable method for growing single-crystal dielectric wafers with outstanding gate capacitance and fabricating wafer-scale 2D material devices with fine device yield and satisfactory performance, which would propel advancements in electronic applications of 2D materials.

Poster 11: Jian LIU

BIOINSPIRED INTERFACE ENGINEERING OF CATALYTIC MATERIALS FOR HYDROGEN-RELATED REACTIONS

Jian LIU

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Enzymes are highly efficient natural catalysts. Inspired by the structure and function of enzymes especially metalloenzymes in nature, we have developed a series of bioinspired catalytic systems featuring well-defined catalytic site and modulated microenvironments for NADH regeneration, catalytic hydrogenation, hydrogen production from H<sub>2</sub>O splitting and CO<sub>2</sub> reduction, focusing on the proton coupled electron transfer process and gas-liquid-solid interface issues.

1) For achieving the high-rate alkaline water splitting, we have developed several superwetttable electrodes featuring superhydrophilicity and superaerophobicity for accelerating the bubble detachment and electrolyte wetting. 2) For addressing cofactor NADH regeneration involving the charge and mass transportation processes, we have developed a series of photocatalytic NADH regeneration systems. Recently, we developed a new electro-enzyme coupling pathway that uses formate produced by CO<sub>2</sub> electroreduction to mediate NADH regeneration and then drive enzyme-catalyzed reactions, achieving continuous synthesis of high-value chemicals. 3) Inspired by the hydrophobic "pocket" of metalloenzymes, several hydrophobic catalytic materials featuring well-defined atomic site and hydrophobic microenvironment were developed for sustainable chemical synthesis in green H<sub>2</sub>O.

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Poster 12: Peng HAN

**BORON-INSERTION-INDUCED PHASE REGULATION OF RH NANOCRYSTALS TOWARDS ENHANCED ELECTROCATALYTIC NITRIC OXIDE REDUCTION TO AMMONIA**

Peng HAN, Ye CHEN

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Electrocatalytic nitric oxide (NO) reduction reaction (NORR) toward ammonia (NH<sub>3</sub>) synthesis is recognized as a sustainable strategy to balance the global nitrogen cycle and alleviate environmental challenges. Unfortunately, due to the sluggish kinetics and lack of highly efficient electrocatalysts, it is still far from practical application. Optimizing the electronic structure of the active sites can greatly improve the performance of electrocatalysts. Herein, Boron (B) inserted Rh nanocrystals with the regulated phases including *amorphous* Rh<sub>4</sub>B nanoparticles (NPs) and hexagonal close-packed (*hcp*) RhB NPs were synthesized through a facile wet-chemical method by tuning the B insertion temperature. A high Faradaic efficiency (92.1%) and yield rate ( $629.5 \pm 11.0 \mu\text{mol h}^{-1} \text{cm}^{-2}$ ) of ammonia are realized over *hcp* RhB NPs which are far superior to those of *fcc* Rh NCs and *amorphous* Rh<sub>4</sub>B NPs. Through the combination of density functional theory calculations and in-situ characterizations, the superior electrocatalytic activity on the *hcp* RhB NPs can be attributed to the upshift of d-band center and enhanced adsorption/activation profile with NO molecules as well as greatly reducing energy barriers of rate-determining step during NORR. Moreover, an assembled proof-of-concept Zn–NO battery using *hcp* RhB NPs as the cathode outputs a power density of  $4.33 \text{ mW cm}^{-2}$ , realizing the simultaneous NO removal, NH<sub>3</sub> green synthesis, and electricity output. Our work not only provides a new strategy for the phase regulation of noble-metal-based nanostructures to enhance their catalytic activity and stability, but also offers an attractive catalyst for electrocatalytic NORR for sustainable NH<sub>3</sub> synthesis.

Poster 13: Gang WANG

SHAPE-CONTROLLED SYNTHESIS OF UNCONVENTIONAL-PHASE AU NANOMATERIALS FOR HIGHLY EFFICIENT CO<sub>2</sub> REDUCTION REACTION

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Colloidal gold (Au) nanomaterials with fine controlled size and shape possess unique physicochemical properties and great potential in various applications. However, most of the reported Au nanomaterials typically crystallize in the thermodynamically stable face-centered cubic (3C) phase, and there are still great challenges in synthesizing hexagonal close-packed (2H type) Au nanomaterials with controlled size and shape. Here, we report the synthesis of free-standing ultrasmall 2H Au nanomaterials with different shapes *via* wet-chemical methods. Moreover, the 2H Au nanomaterials exhibit superior electrocatalytic performance toward CO<sub>2</sub> reduction reaction than 3C Au nanoplates, possessing high Faradaic efficiency in a wide applied potential window. Our work provides an effective strategy to design and synthesize Au nanomaterials with unconventional crystal structure and demonstrates the potential of phase engineering in boosting catalytic performances of noble metal nanomaterials.



Poster 14: Long ZHENG

**SYNTHESIS OF HEXAGONAL-CLOSE PACKED RHODIUM NANOPLATES AND CRYSTAL STRUCTURE-DEPENDENT CATALYTIC BEHAVIORS OF RH IN ELECTROCATALYSIS**

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Phase engineering plays a crucial role in tuning the physicochemical properties of noble metal nanomaterials. However, the synthesis of high-purity unconventional-phase noble metal nanomaterials is highly challenging via current wet-chemical methods. Therefore, it is necessary to develop a new paradigm to prepare metastable phases based on rational design. Herein, we obtain unconventional hexagonal-close packed (2H) Rh nanoplates (NPLs) via a novel wet-chemical method. Impressively, the fabricated Rh NPLs have pure 2H lattice with well-defined facets and good thermostability, which provides an ideal model to study the phase-dependent catalytic performance of Rh. Specifically, compared to the conventional face-centered cubic (3C) Rh nanocubes, the 2H Rh NPLs achieve higher ammonia (NH<sub>3</sub>) Faradaic efficiency and NH<sub>3</sub> yield rate with lower overpotentials for nitrate reduction reaction (NO<sub>3</sub>RR). Density functional theory calculations reveal that the unconventional 2H surfaces have lower activation energies for elemental steps, providing excellent NO<sub>3</sub>RR performance for 2H Rh NPLs. This work opens new avenues for the highly controlled synthesis of unconventional-phase noble metal nanomaterials and provides important directions for designing high-performance catalysts for NO<sub>3</sub>RR.

Poster 15: Hwa Seob CHOI

3D AND 2D ALL-ORGANIC PEROVSKITES

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All-organic perovskites represent the latest version of perovskite families, characterized by both cations and anions being composed of organic components. These materials offer notable advantages such as structural tunability and solution-processability. Recently, 3D all-organic perovskites with ferroelectric properties have demonstrated high polarization values ( $22 \mu\text{C}/\text{cm}^2$ ), comparable to inorganic  $\text{BaTiO}_3$ . However, they are limited by a lower coercive field compared to their inorganic counterparts. Our study reveals that the coercive field of ferroelectric all-organic perovskites can be tailored by adjusting the strength of hydrogen bonding.

Meanwhile, the synthesis and utilization of all-organic perovskites in 2D form remain largely unexplored because the design principle has not been developed. We present the successful synthesis of a metal-free 2D layered perovskite, denoted as the Choi-Loh van der Waals phase (CL-v phase), with the chemical formula  $\text{A}_2\text{B}_2\text{X}_4$ , where A represents a larger-sized cation compared to B and X denotes an anion. The CL-v phase exhibits a van der Waals gap enabled by interlayer hydrogen bonding and can be exfoliated or grown as molecularly thin 2D organic crystals. The dielectric constants of the CL-v phase range from 4.8 to 5.5 and we demonstrate their potential as gate dielectrics for thin-film transistors.

Poster 16: Tianshuo ZHAO

**CHEMICALLY DRIVEN SINTERING OF COLLOIDAL CU NANOCRYSTALS FOR MULTISCALE ELECTRONIC AND OPTICAL DEVICES**

Tianshuo ZHAO<sup>1,2</sup>, Jun XU<sup>2</sup>, Anne-Marie ZACCARIN<sup>2</sup>, Xingyu DU<sup>2</sup>, Shengsong YANG<sup>3</sup>, Yifan NING<sup>3</sup>, Qiwen XIAO<sup>4</sup>, Shobhita KRAMADHATI<sup>2</sup>, Yun Chang CHOI<sup>3</sup>, Christopher B. MURRAY<sup>3,4</sup>, Roy H. Olsson III<sup>2</sup>, Cherie R. KAGAN<sup>2,3,4</sup>

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Emerging applications of Internet of Things (IoT) technologies in smart health, home, and city, in agriculture and environmental monitoring, and in transportation and manufacturing require materials and devices with engineered physical properties that can be manufactured by low-cost and scalable methods, support flexible forms, and are biocompatible and biodegradable. Here, we report the fabrication and device integration of low-cost and biocompatible/biodegradable colloidal Cu nanocrystal (NC) films through room temperature, solution-based deposition, and sintering, achieved via chemical exchange of NC surface ligands. Treatment of organic-ligand capped Cu NC films with solutions of shorter, environmentally benign, and noncorrosive inorganic reagents, namely,  $\text{SCN}^-$  and  $\text{Cl}^-$ , effectively removes the organic ligands, drives NC grain growth, and limits film oxidation. We investigate the mechanism of this chemically driven sintering by systemically varying the Cu NC size, ligand reagent, and ligand treatment time and follow the evolution of their structure and electrical and optical properties.  $\text{Cl}^-$ -treated, 4.5 nm diameter Cu NC films yield the lowest DC resistivity, only 3.2 times that of bulk Cu, and metal-like dielectric functions at optical frequencies. We exploit the high conductivity of these chemically sintered Cu NC films and, in combination with photo- and nanoimprint-lithography, pattern multiscale structures to achieve high-Q radio frequency (RF) capacitive sensors and near-infrared (NIR) resonant optical metasurfaces.

Poster 17: Wendong WANG

**STRUCTURAL PHASE TRANSITIONS AND ATOMIC DEFECT TRACKING IN TRANSITION METAL dihalides**

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Scanning transmission electron microscopy (STEM) is a powerful tool for characterizing the atomic structure of materials. However, its application to highly air sensitive 2D materials such as 2D transition metal halides has been limited due to challenges in sample fabrication. In this study, we developed a novel inorganic stamping based method, using Silicon Nitride membranes to fabricate pristine suspended 2D material samples suitable for STEM analysis. This technique enables hermetic encapsulation of extremely air-sensitive 2D materials by protecting them with graphene layers on both sides. The simple, fast and polymer free technique causes no mechanical damage to the sample, preventing degradation due to minor imperfections in the seal. Using this method, we structurally characterized transition metal dihalides ( $\text{FeI}_2$ ,  $\text{CoI}_2$ ,  $\text{NiI}_2$ ) across various thicknesses, from bulk to monolayer structures for the first time. We observed a thickness dependent stacking transition in  $\text{FeI}_2$ , where the preferred arrangement changed from bulk 1T stacking to bilayer 3R stacking. Additionally, in monolayer  $\text{FeI}_2$ , we characterised and analysed the movement of individual halide vacancies. This work demonstrates thickness-dependent structural phase transitions in atomically thin transition metal dihalides and highlights the ability to track atomic-scale defects in monolayers. Our findings will allow use of STEM (and complementary techniques which require suspended samples) to investigate the atomic structure of highly air-sensitive thin 2D materials.

**Poster 18: Jingrun RAN**

**ATOMIC-REGULATION ON PHOTOCATALYST FOR ENERGY-RELATED REACTION**

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The global energy crisis and environmental issue impel the aggressive exploration for a clean and renewable energy resource to replace fossil fuel. Hence, conversion of renewable solar energy into clean fuel and valuable chemical is of great significance. The core challenge of this advanced technology lies in the exploration of low-cost and environmentally benign photocatalysts with remarkable activity and robustness. Hence, the rational design and synthesis of photocatalysts at the atomic level to achieve efficient and robust solar-to-chemical conversion is highly promising. Furthermore, both advanced characterizations (e.g., aberration-corrected atomic-resolution transmission electron microscopy, synchrotron-based X Ray absorption spectroscopy and various in situ element/space/time-resolved characterization) and theoretical computation are adopted to investigate the atomic-level structure/composition-performance relationship and mechanism in photocatalyst. Finally, a universal rule to develop high-performance photocatalysts for efficient solar-to-chemicals energy conversion is concluded.

Poster 19: Qian YANG

**CONNECTING THE TWISTING OF ULTRATHIN FCC AU NANOWIRES TO THE FORMATION OF 4H PHASE**

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The unconventional phases of Au nanomaterials have attracted considerable attention due to their improved plasmonic and catalytic performances relative to the face-centred cubic (*fcc*) phase. Unfortunately, the existing synthesis methods are closely related. Similar pathways and narrow parameter windows make it difficult for deconvoluting the formation mechanisms. As a result, the formation mechanisms of unconventional Au phases remain poorly understood.

To overcome these challenges, we developed a novel and general phase transformation approach to synthesize 4H metal nanowires. Using ultrathin *fcc* Au nanowires as templates, the deposition of Au on them induced a phase transformation from *fcc* to 4H phase, resulting in the formation of heterophase Au nanowires with 4H segments. To the best of our knowledge, this is the first example of *fcc* to 4H transformation for Au nanomaterials under mild ambient conditions. Furthermore, 4H Ag or Pd structures could also be synthesized when these metals were deposited on the same templates-ultrathin *fcc* Au nanowires, demonstrating the broad applicability of this method.

More importantly, by adjusting the kinetics of metal reduction, we can control the transformation modes: slow reduction rates result in the twisting of the ultrathin *fcc* Au nanowires into double helices, while rapid reduction rates lead to the formation of 4H phase. This dual-pathway transformation underscores the influence of reduction kinetics. It suggests that the formation of 4H phase might result from states where the nanowires are slightly or partially twisted during metal deposition.

This work sheds light on the complex mechanisms behind the formation of 4H phases and opens promising avenues for developing various new unconventional phase structures, holding the potential to revolutionize material design across nanotechnology.

Poster 20: Jie WANG

**PHASE ENGINEERING OF NOBLE METAL NANOCATALYSTS AND THEIR PHASE-DEPENDENT PROPERTIES IN ELECTROCATALYSIS**

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Noble metal nanomaterials are favorable electrocatalysts because of their high activity, robust stability, and excellent selectivity in various electrocatalytic reactions. Benefiting from the notable progress in the modulation of size, shape, facet, dimension, composition and architecture of noble metal nanomaterials, their properties can be rationally tuned for specific catalytic applications. Besides, the crystal phase of noble metal nanomaterials has been evidenced as another critical structural feature in modulating their electrocatalytic properties. Therefore, phase engineering of nanomaterials (PEN), as an important strategy, is indispensable for developing highly efficient electrocatalysts.

Herein, we present a series of work about phase engineering of noble metal-based nanomaterials as well as their catalytic applications in the energy field, including: 1. 2H-Au Nanosheet-Templated Growth of PdFe for Electrocatalytic Methanol Oxidation: PdFe alloy can be epitaxially deposited on Au nanosheets with unconventional 2H phase (2H-Au NSs) and inherit the 2H phase, generating Au@PdFe NSs. Furthermore, 2H-Au should be gradually transformed into the thermodynamically stable phase--face-centered cubic (fcc) by tuning the Pd/Fe atomic ratio and thus the 2H/fcc phase ratio in Au@PdFe NSs can be controlled correspondingly, which directly proportional to their methanol electrocatalytic oxidation (MOR) activity<sup>[1]</sup>. 2. Epitaxial Growth of Unconventional 4H-Pd Based Alloy Nanostructures on 4H-Au Nanoribbons towards Highly Efficient Electrocatalytic Methanol Oxidation: using Au nanoribbons with 4H phase (4H-Au NRBs) as templates, a series of Pd-based alloy with 4H phase can be synthesized by epitaxial co-deposition of Pd and M (M = Fe, Ir and Ru) atoms on 4H-Au NRBs, forming 4H-Au@PdM NRBs, among which, the 4H-Au@PdFe NRBs exhibited superior MOR activity<sup>[2]</sup>. 3. Crystal Phase-Controlled Growth of PtCu and PtCo Alloys on 4H Au Nanoribbons for Electrocatalytic Ethanol Oxidation Reaction: PtCu alloys with 4H and fcc phase can be created when the thicknesses of PtCu shell deposited on 4H-Au NRBs are thin and thick, respectively, and PtCu alloys with the 4H phase exhibit better performance than the fcc counterparts in the electrocatalytic ethanol oxidation reaction under alkaline conditions<sup>[3]</sup>.

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[2] **J. Wang**, G. Liu, Q. Yun, X. Zhou, X. Liu, et al. Epitaxial Growth of Unconventional 4H-Pd Based Alloy Nanostructures on 4H-Au Nanoribbons towards Highly Efficient Electrocatalytic Methanol Oxidation. *Acta Phys. -Chim. Sin.*, **2023**, 39, 2305034.

[3] **J. Wang**, J. Zhang, G. Liu, C. Ling, et al. Crystal phase-controlled growth of PtCu and PtCo alloys on 4H Au nanoribbons for electrocatalytic ethanol oxidation reaction. *Nano Res.* **2020**, 13, 1970.