Oct.31 – Nov.2, 2025 Beijing, China

# 第五届北京科技大学-日本东北大学双边学术交流会

# The 5th USTB-TU Symposium

北京科技大学
University of Science and Technology Beijing

TOHOKU UNIVERSITY

# The 5th USTB-TU Symposium

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北京科技大学
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The 5th USTB-TU Symposium

# OVERVIEW

## Hosted by

University of Science and Technology Beijing (USTB)

## Date

2025. 10. 31 – 2025. 11. 02

## Venue

Chongyang Lizheng Hall
Swan Lakeview Hotel
Huairou District
Beijing, China

# Schedule : Oct. 31st

| Venue: Chongyang Lizheng Hall | |
|---|---|
| 8:45-9:00 | Registration |
| 9:00-9:20 | Opening ceremony |
| 9:20-9:30 | Group photo |
| 9:30-10:30 | Keynote speech |
| 10:30-10:50 | Tea break |
| 10:50-11:30 | Keynote speech |
| 11:30-13:30 | Lunch |
| 13:30-15:30 | Keynote speech |
| 15:30-15:50 | Tea break |
| 15:50-17:50 | Oral presentation |
| 18:00-19:30 | Dinner |

# Schedule : Nov. 1st

| Venue: Chongyang Lizheng Hall | |
|---|---|
| 9:00-10:30 | Oral presentation |
| 10:30-10:50 | Tea break |
| 10:50-11:35 | Oral presentation |
| 11:40-12:30 | Lunch |
| 13:00-17:00 | Lab tour |

# Map of vicinity

The 5th USTB-TU Symposium

# CONFERENCE SCHEDULE

## Oct.30th

| | |
|---|---|
| 11:45-20:35 | TU participants' arrival at Beijing Capital International Airport<br>Check in at Swan Lakeview Hotel |
| 14:00-22:00 | Discussion on Collaboration between USTB and TU, focus on Materials Synthesis, Characterization and Functional Development |

## Oct.31st

| | |
|---|---|
| 8:45-9:00 | Registration |
| **Venue** | Chongyang Lizheng Hall |
| 9:00-9:05 | Opening remarks by Prof. Shuqiang JIAO from USTB |
| 9:05-9:10 | Speech by Prof. Kiyoshi KANIE from TU |
| 9:10-9:15 | Speech by Dr. Yimingjiang Maimaiti from Huairou District Commission of Science and Technology |
| 9:15-9:20 | Speech by Prof. Qingliang LIAO from USTB |
| 9:20-9:30 | Group photo (at the Hotel front gate) |

**Chair: Prof. Wenbin Cao**

| | |
|---|---|
| 9:30-9:50 | Keynote by Tohoku-1<br>Kiyoshi KANIE, Professor, IMRAM, TU<br>**A Nanoparticle mist Deposition Method: Preparation of High performance ITO Flexible Thin Films under Atmospheric Conditions** |
| 9:50-10:10 | Keynote by USTB-1<br>Xiaolu PANG, Professor, USTB<br>**High-density twin boundaries in transition metal nitride ceramic coatings with boron doping** |
| 10:10-10:30 | Keynote by USTB-2<br>Jikun CHEN, Professor, USTB<br>**Role of $^{1}H$ composition to superconductivity in infinite-layer nickelates from measurements of nuclear interactions** |
| 10:30-10:50 | Tea break |

**Chair: Prof. Kiyoshi KANIE**

| | |
|---|---|
| 10:50-11:10 | Keynote by Tohoku-2<br>Takaaki TOMAI, Professor, IMRAM, TU<br>**Japanese Process Science Project Toward Design and Control of Nanomaterials** |
| 11:10-11:30 | Keynote by USTB-3<br>Yong ZHANG, Professor, USTB<br>**Discoveries in the high-entropy and entropic materials** |
| 11:30-13:00 | Lunch |

**Chair: Prof. Jikun CHEN**

13:30-13:50 Keynote by Tohoku-3

Yuichi NEGISHI, Professor, IMRAM, TU

**Creation of High-Performance Energy and Environmental Catalysts by Controlling the Aggregation of Metal Atoms**

13:50-14:10 Keynote by USTB-4

Mingxue TANG, Professor, USTB

**Local structure and dynamics from NMR**

14:10-14:30 Keynote by USTB-5

Naisheng JIANG, Professor, USTB

**Probing the Structure and Dynamics of Polymeric Materials via X-ray and Neutron Scattering Techniques**

**Chair: Prof. Yuichi NEGISHI**

14:30-14:50 Keynote by Tohoku-4

Shu YIN, Professor, IMRAM, TU

**Hydrothermal Synthesis of Vanadium Compounds and their Functionality Development**

14:50-15:10 Keynote by USTB-6

Qi WANG, Professor, USTB

**Controllable synthesis of multi-morphology nitrides fillers and their application in thermally conductive composites**

15:10-15:30 Keynote by USTB-7

Kangkang MENG, Professor, USTB

**Non-Orthogonal Spin Current in PtMnGa**

15:30-15:50 Tea break

**Chair: Assistant Prof. Megumi SUYAMA**

15:50-16:05 Oral presentation by Tohoku-1

Takuya HASEGAWA, Associate Professor, IMRAM, TU

**Anti-thermal Quenching Photoluminescence in Yb/Er/Tm Multi-doping in YSZ host**

16:05-16:20 Oral presentation by USTB-1

Yunwei GUI, Associate Professor, USTB

**Data-driven assisted metallurgical defect control and the mechanism of strengthening and toughening for additively manufactured metal parts**

16:20-16:35 Oral presentation by USTB-2

Bin LI, Associate Professor, USTB

**Preparation and Performance of Alumina Fibers Based on Sol Structure Regulation**

16:35-16:50 Oral presentation by USTB-3

Xiaoou YI, Associate Professor, USTB

**Damage microstructure, hardening and deuterium retention in neutron irradiated tungsten and tungsten-rhenium alloy**

**Chair: Prof. Yunwei GUI**

16:50-17:05 Oral presentation by Tohoku-2

Megumi SUYAMA, Assistant Professor, IMRAM, TU

**Phosphine-Ligand Effects on the Crystallization-Induced Emission of $AuCu_{14}$ Clusters**

17:05-17:20 Oral presentation by USTB-4

Yujuan ZHANG, Associate Professor, USTB

**Research on Surface Modification of MXene and Its Adsorption Mechanism for Nuclide Ions**

17:20-17:35 Oral presentation by Tohoku-3

Yibei XUE, Assistant Professor, IMRAM, TU

**Element Doping Strategies for Energy-Saving $VO_2$ Smart Windows**

17:35-17:50 Oral presentation by USTB-6

Lihong LI, Associate Professor, USTB

**Topological synthesis of anisotropic micro/nano materials and device preparation**

18:00-19:30 Dinner

**Nov.1st**

**Venue** Chongyang Lizheng Hall

**Chair: Qiuyu JIN**

9:00-9:15 Oral presentation by Tohoku-4

Taisei HANGAI, Doctoral candidate, IMRAM, TU

**Reduction-Driven Luminescence Quenching in $Eu^{3+}$-Doped $Bi_2MoO_6$ for $H_2S$ Gas Detection**

9:15-9:30 Oral presentation by USTB-5

Yongqing CHEN, Doctoral candidate, USTB

**Transformation mechanisms in hexagonal close-packed crystals and implications for the design of advanced lightweight structure materials**

| | |
|---|---|
| 9:30-9:45 | Oral presentation by USTB-6<br>Jin ZHOU, Doctoral candidate, USTB<br>**Statistical in situ scanning electron microscopy investigation on the failure of oxide scales** |
| **Chair: Yongqing CHEN** | |
| 9:45-10:00 | Oral presentation by Tohoku-5<br>Qiuyu JIN, Doctoral candidate, IMRAM, TU<br>**Layered Black Phosphorus Microspheres via Solvothermal Self-Assembly for Sensitive Ammonia Detection** |
| 10:00-10:15 | Oral presentation by USTB-7<br>Ni LU, Doctoral candidate, USTB<br>**Theoretical Investigation of Microstructure-Driven Enhancement in the CrCoNi Medium-Entropy Alloy** |
| 10:15-10:30 | Oral presentation by USTB-8<br>Jie TU, Doctoral candidate, USTB<br>**Chemical strain for ferroelectric photovoltaic properties in double-perovskites films** |
| 10:30-10:50 | Tea break |
| **Chair: Jin ZHOU** | |
| 10:50-11:05 | Oral presentation by Tohoku-6<br>Ryusei TAKAYANAGI, MSc student, IMRAM, TU<br>**Effect of hydrothermal reaction field on $CO_2$ reduction performance of nanoporous gold catalyst** |
| 11:05-11:20 | Oral presentation by USTB-9<br>Zejun LI, MSc student, USTB<br>**Effect of Mn addition on the corrosion behavior of FeCrNiMnxSi alloys in simulated seawater environment** |
| 11:20-11:35 | Oral presentation by USTB-10<br>Hui LIU, MSc student, USTB<br>**High-temperature dislocation substructures in heavy-ion irradiated long-range-ordered $(Fe, Ni)_3V$ alloy** |
| 11:40-12:30 | Lunch |
| 13:00-17:00 | Lab tour |
| **Nov.2nd** | |
| | TU participants' departure from Beijing Capital International Airport |

The 5th USTB-TU Symposium

# ABSTRACT
# Keynote

Keynote TU- 1

# A Nanoparticle mist Deposition Method: Preparation of High performance ITO Flexible Thin Films under Atmospheric Conditions

Indium tin oxide (ITO) thin films with low resistivity and high transparency in the visible light region have been prepared on flexible plastic films by a deposition method using water mist containing ITO nanoparticles (NPs) under atmospheric conditions. The ITO NP-mist was generated by ultrasonic irradiation of a water dispersion. Our developed protrusion-rich ITO NPs were applied as the ITO NPs. The ITO NPs show high dispersion stability in water without the use of any dispersant. Comparison investigations revealed that utilization of the ITO NPs played a critical role in fabricating high-performance ITO thin films on flexible films, and the resistivity reached 9.0 x 10-3 Ω·cm. The system could be expected to provide promising advances in the development of a mild and sustainable fabrication procedure for ITO thin films under mild atmospheric conditions without the use of expensive vacuum production systems or harmful and environmentally undesirable chemicals.

## Short CV of Prof. Kiyoshi KANIE

Kiyoshi Kanie is a Professor in International Center for Synchrotron Radiation Innovation Smart at Tohoku University in Sendai (Concurrent post: Institute of Multidisciplinary Research for Advanced Materials). He received his PhD from Kyoto University in 2000. He held research associate positions at The University of Tokyo and Tohoku University before being appointed an Associate Professor at Tohoku University in 2008 and a Full Professor in 2019. His research interests encompass the design and synthesis of functional materials, liquid phase synthesis of functional inorganic nanoparticles with controlled size and shape and the development of organic-inorganic hybrid materials with dynamic functions. He was the recipient of the Science Award of the division of colloid and surface chemistry of the Chemical Society of Japan in 2010 and received the Japan Institute of Metals and Materials meritorious award in 2014.

# Japanese Process Science Project Toward Design and Control of Nanomaterials

In order to realize fine control and design of nanomaterials and promote thier social implementation, “Process Science” project to build a platform for nanomaterials engineering had been conducted from 2019 in Tohoku University.

In this project, based on thermodynamics and chemical engineering, dispersion/aggregation prediction, construction of prediction equations for nanofluids’ transport properties (diffusivity, viscosity, thermal conductivity), and design of unit operations (classification, separation, mixing) for nanomaterials have been realizing. Furthermore, knowledge has been accumulated on the prediction and design of structure formation of nanomaterials.

To address the thermodynamics for nanoparticles, we treated nanoparticles as pseudo-molecules, enabling the extension of classical thermodynamics. Using decanoic-acid-modified $CeO_2$ nanoparticles, pressure–volume– temperature (PVT) relationships were modeled with the conventional Equation of State, and dispersibility was predicted via the Hansen Solubility Parameter approach. Moreover, a new viscosity correlation model was proposed, accurately predicting nanofluid rheology across concentrations. Furthermore, drying pattern formation was classified using Peclet and Marangoni numbers, linking flow dynamics to film morphology.

This integrated framework connects thermodynamics, transport, and unit operations, transforming nanoparticle processing from empirical practice into predictive process engineering.

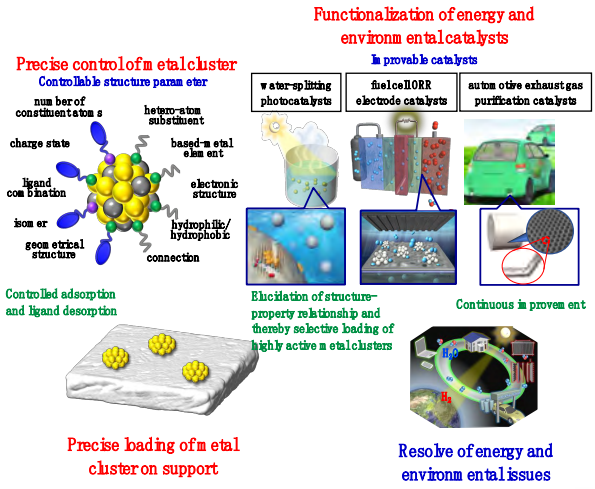
## Short CV of Prof. Takaaki TOMAI

Prof. Takaaki TOMAI graduated from The University of Tokyo in 2008, and received his Doctor of Science from the same institution in 2008. He was appointed as Professor in Tohoku University in 2023. His current research focuses on hierarchical structural control of nanomaterials and development of novel chemical process toward carbon neutral chemical industry. He has published more than 100 papers, with over 3,000 citations, and has an h-index of 30.

## Keynote TU- 3

# Creation of High-Performance Energy and Environmental Catalysts by Controlling the Aggregation of Metal Atoms

In order to build a sustainable society, it is indispensable to create new innovative materials that can solve the problems of the current society. Strict control of the structure of materials at the nanoscale is expected to lead to the creation of such materials. We have established techniques for the precise synthesis of metal clusters and their use to control the metal clusters on the supports with atomic precision. By using the obtained materials, the correlation between the number of atoms/chemical composition of the supported metal clusters in each material and the material function has been clarified with atomic precision, and through such research, clear design guidelines have been successfully obtained for the further enhancement of water splitting photocatalysis and fuel cells electrocatalysts in the future. These our research is unique in that it consistently achieves the atomic-level control of the metal clusters throughout the entire research, from synthesis to control on the support. This presentation summarizes our recent works concerning these topics.




## Short CV of Prof. Yuichi NEGISHI

Prof. Yuichi Negishi is a Professor in the Institute of Multidisciplinary Research for Advanced Materials, Tohoku University, Japan. With expertise in physical chemistry, cluster chemistry, and nanomaterial chemistry, he has published over 280 research papers. Prof. Negishi has received several awards, including The Chemical Society of Japan Award for Young Chemists and the Japan Society for Molecular Science Award for Young Scientists. He was also awarded the Yagami Prize, the Distinguished Award for Novel Materials and Their Synthesis, the International Investigator Awards of the Japan Society for Molecular Science, and The Chemical Society of Japan Award for Creative Work.

# Hydrothermal Synthesis of Vanadium Compounds and their Functionality Development

Vanadium dioxide exhibits an abrupt change in infrared transmittance due to its metal-insulator transition near 68°C. This property is applied in smart windows, where element doping adjusts the transition temperature to near ambient, indicating its potential for energy-saving film. Layered vanadium oxyphosphate forms large-sized plate-like particles via hydrothermal synthesis, displaying pearlescence from the the interlayer structure and color variation through valence control. As a novel single-component pearl pigment, it shows promise in cosmetics, automotive coatings, and decorative plastics. Vanadium dioxide nanostructures may also detect gases via adsorption-desorption resistance changes. Monoclinic vanadium dioxide exhibits temperature-dependent response inversion to similar gases. Using this phenomenon with elemental doping, we achieved excellent selective detection of VOC through a unique gas response behavior. Vanadium-based materials play crucial roles across energy conservation, decorative materials, and gas sensing through nanostructure design.

## Short CV of Prof. Shu YIN

Prof. Shu YIN received his Ph.D. in Applied Chemistry from Tohoku University in 1999, where he is now a Professor at the Institute of Multidisciplinary Research for Advanced Materials (IMRAM) and the Advanced Institute for Materials Research (WPI-AIMR). He has received several prestigious awards, including the CerSJ Award for Academic Achievements in Ceramic Science and Technology, The Ceramic Society of Japan (2015), Academic Award of the Japan Society of Inorganic Materials (2015), and Academic Award of the Japan Association of Inorganic Phosphorus Chemistry (2025). His research focuses on environmental functional catalysts, morphology-controlled nanomaterials, optical functional materials, and green chemical synthesis. He has published over 600 papers (Google Scholar: 20,000+ citations, h-index 78,) and has led numerous national research projects. He also serves in leadership roles for international academic societies and conferences, and as an editorial board member of several journals.

## Keynote USTB- 1

# High-density twin boundaries in transition metal nitride ceramic coatings with boron doping

The formation mechanism of twin boundaries in transition metal nitrides has remained largely unexplored owing to their high stacking fault energy that hinders twin boundary formation. Herein, we fabricated TiB0.11N1.16 coatings with high-density twin boundaries, including coherent twin boundaries and incoherent twin boundaries. The experimental results revealed that [111] orientation provides an orientation advantage and indirectly promoting the formation of twin boundaries. Theoretical analyses indicated that boron segregation leads to the formation and stabilization of incoherent twin boundaries via two aspects: i) it reduces incoherent twin boundary energy and ii) forms large internal stress, which stabilizes the reduced incoherent twin boundary energy and prevents detwinning. Owing to the stress field change caused by the nonuniform distribution of boron, some twinned columns transform into the matrix orientation driven by system energy minimization, thus forming coherent twin boundaries. Moreover, the hardness and toughness of the TiB0.11N1.16 coatings were superior to those of twin-free ceramic coatings.

## Short CV of Prof. Xiaolu PANG

Prof. XiaoLu Pang received a Ph.D. in materials science and engineering from University of Science and Technology Beijing (USTB) in 2008. After that, he became a research assistant, associate professor, and then a full-time professor at the USTB. Now, he is the director of national science center for materials service safety. His research interests include the study of protective coatings on metal material surfaces, especially in the preparation of high-strength and tough nanotwinned ceramic coatings. He improved the theory for protecting the metal substrate from damage caused by brittle ceramic coatings cracking, improved the fatigue resistance of coated metal materials. He has published nearly 190 SCI papers, including Acta Mater, Corros Sci and other journals, with over 6800 citations.

Keynote USTB- 2

# Role of $^{1}H$ composition to superconductivity in infinite-layer nickelates from measurements of nuclear interactions

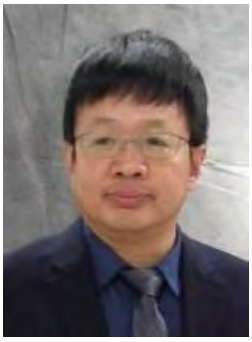
Superconductivity is the property of certain materials to conduct electricity without electrical resistance when cooled below a critical temperature, which is typically very low. Cuprates are a specific class of layered materials containing copper-oxide planes with critical temperatures significantly above the boiling point of liquid nitrogen, making them suitable for various applications, including magnetic resonance imaging, particle accelerators, power transmission, and quantum computing. Despite extensive experimental and theoretical studies conducted over the past 40 years, the mechanism behind high-temperature superconductivity in cuprates remains elusive. However, the recent discovery of superconducting nickelates, which exhibit strong similarities to cuprates in terms of structure and electronic and magnetic correlations, has opened new avenues for exploration. It was previously believed that hydrogen incorporation is critical for nickelates to become superconducting, but this notion has been challenged by recent studies. The central debate arises due to the quantification of hydrogen using conventional spectroscopic techniques, which can be easily influenced by electron-involved mechanisms, raising concerns about their reliability. This work shows how a measurement technique based on nuclear interactions at the MeV energy scale can effectively mitigate these undesirable processes, thereby confirming the irrelevance of hydrogen content to the superconductivity in finite-layer nickelates.

## Short CV of Prof. Jikun CHEN

Prof. Jikun CHEN received the bachelor education in Tsinghua University, and master education in Shanghai Institute of Ceramics, Chinese Academy of Science, and obtained the PhD degree from ETH Zurich (Switzerland). Afterwards, he worked in Harvard University (USA), the university of Tokyo (Japan), and the Kyoto University (Japan) as either postdoc or senior visiting scholar. He worked in the university of Science and Technology of Beijing since 2015 on electronic phase transition materials and devices.

## Keynote USTB- 3

# Discoveries in the high-entropy and entropic materials



High entropy and entropic matters and materials which was defined according to the number and contents of the constitute components, furthermore the entropy of the materials, in another word, order and disorder or chaos. Theoretically, the higher entropy of the materials, the more stable in an isolated system. However, the materials are used in the open system, the temperature, the pressure, and diffusion can not be avoided to occur. When the components mixed, the similar one can be replaced each other, random solid solution will be form, e.g. atomic size difference, or components volume difference is very small; while for the dissimilar components, the enthalpy effect will be the dominant. The plastic deformation mechanism and flow units from the cryogenic to the higher temperature will be discussed. For the human being, we can study the local matters, nanostructure, microstructure, macrostrutcure, etc., by using the data we collected and observed, we hope to guess the mysteries of the world. Several typical high entropy alloys will also be discussed.

## Short CV of Prof.Yong ZHANG

Prof. Yong Zhang received his Ph.D. in Materials Science from the University of Science and Technology Beijing (USTB) in 1998. After two years of postdoctoral work at the Institute of Physics (IOP), Chinese Academy of Science (CAS), he then worked as a research fellow at the National University of Singapore (NUS) from 2000 to 2004 as part of the Singapore-Massachusetts Institute of Technology (MIT) Alliance (SMA). He was recruited to the USTB as a professor, working at the State Key Laboratory (SKL) for Advanced Metals and Materials. In 2005, Dr. Zhang received an award from the Ministry of Education of China under the New Century Excellent Talents (NCET) in Universities program. His main research interest is the development of new materials in bulk, film, fiber, and particle forms using the high-entropy and materials-genome-initiative (MGI) strategies.

# Local structure and dynamics from NMR

Solid-state nuclear magnetic resonance (NMR) is very sensitive to the local environment at atomic and molecular scale, together with dynamic information from temperature dependent NMR spectral linewidth and relaxation analysis. The NMR shift is closely correlated to the electron configuration (magnitude and direction of the local induced magnetic field) surrounding the studied nuclear, and it can provide the chemical bond and direction information for better understanding the molecular crystalline nature and ion migration pathway (Fig. 1). This talk will show the application of solid-state NMR for the crystalline and amorphous materials. In addition, the *in-situ* NMR under potential and pressure will be briefly introduced to demonstrate its capabilities.

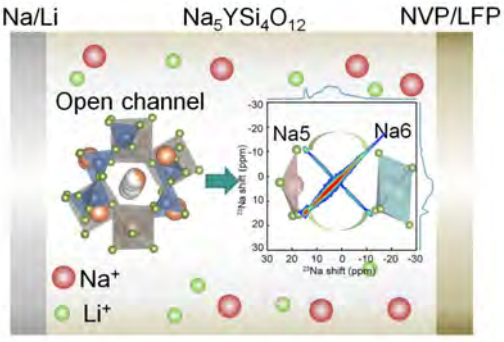



Fig. 1. Exchange NMR for sodium pathway in $Na_5YSi_4O_{12}$ electrolyte.

## Short CV of Prof. Mingxue TANG

Dr. Tang obtained his PhD degree in Physical Chemistry at University of Paderborn (Germany), followed with years Post-doc training in France. Currently, his research interests mainly focus on developing novel NMR/EPR techniques for characterization of optoelectronic materials. Additionally, designing non-destructive tools, in operando NMR/EPR, to determine the mechanisms of the obtained materials under operation (such as electrochemical cycling and photo stimulation).

Keynote USTB- 5

# Probing the Structure and Dynamics of Polymeric Materials via X-ray and Neutron Scattering Techniques

Long-chain macromolecules or polymers, as typical soft matter systems, often exhibit pronounced nonlinear responses and nonequilibrium behaviors. Their structural evolution under varying environments or within different systems is typically complex and difficult to predict. Compared with conventional microscopy techniques, synchrotron X-ray and neutron scattering techniques can enable in situ or operando, nondestructive characterization of polymer structures and dynamics in complex systems across wide ranges of length and time scales. These techniques can not only reveal the structural evolution of polymers from molecular conformation and chain orientation to microstructural morphology, but can also elucidate dynamical processes ranging from segmental relaxations to interdiffusion, thereby offering powerful tools for understanding and controlling the multiscale structures and dynamics of macromolecules within complex multiphase systems.

## Short CV of Prof. Naisheng JIANG

Naisheng Jiang is currently a professor in the School of Materials Science and Engineering at the University of Science and Technology Beijing. He received his Bachelor's degree in Polymer Materials and Engineering from Sichuan University in 2009, and his Ph.D. in Materials Science and Engineering from Stony Brook University in 2014. He then worked successively as a postdoctoral researcher at Case Western Reserve University and Louisiana State University before joining the faculty of the University of Science and Technology Beijing in 2019. His research focuses on investigating the structure and dynamics of polymeric systems using X-ray and neutron scattering techniques.

Keynote USTB- 6

# Controllable synthesis of multi-morphology nitrides fillers and their application in thermally conductive composites

With the rapid miniaturization and integration of electronic devices, heat dissipation has become a critical bottleneck restricting the advancement of the electronics industry. The development of high-performance thermally conductive composites is therefore essential to address this challenge. Nitrides such as aluminum nitride (AlN) and silicon nitride (Si3N4), featuring high thermal conductivity and excellent electrical insulation, are considered ideal thermally conductive fillers. Morphological control—particularly in the form of spherical and one-dimensional (1D) structures—can meet the multiscale construction requirements of thermal conduction pathways, which is crucial for effective thermal management. However, due to the absence of a melting point and the anisotropic surface energy of nitrides, morphology regulation remains challenging. Conventionally synthesized nitrides tend to develop angular structures, severely limiting their performance in thermal conduction applications.

In this study, we achieved controlled and unconventional growth of nitrides by regulating reaction kinetics, enabling the synthesis of spherical and 1D AlN and Si3N4 fillers. Guided by the concept of thermally conductive unit alignment, these nitrides were directionally assembled within polymer matrices to construct ordered thermal networks, resulting in composites with significantly enhanced thermal conductivity. Moreover, a three-dimensional continuous AlN porous scaffold was directly fabricated via an in situ reaction strategy, further improving the overall heat transfer performance of the composites. Through precise morphology control and multiscale structural design, a series of high-performance thermally conductive composites were successfully developed, offering new insights and design strategies for next-generation thermal management materials.

## Short CV of Prof. Qi WANG

Qi Wang received her Bachelor's degree from the University of Science and Technology Beijing (USTB) in 2010 and her Ph.D. degree from Tsinghua University in 2015. She is currently a Professor at the School of Materials Science and Engineering, USTB. Her research focuses on the controllable synthesis of nitride ceramics and their applications in thermal management materials. She has published 48 SCI-indexed papers as the first or corresponding author and has been selected for the Young Elite Scientists Sponsorship Program of the China Association for Science and Technology (CAST) and the Beijing Nova Program.

## Keynote USTB- 7

# Non-Orthogonal Spin Current in PtMnGa

An important goal of spintronics research is to discover efficient methods of spin current generation. Generally, the symmetry conditions restrict spin polarizations to be orthogonal to both the charge and spin flows in nonmagnetic metals. However, in addition to the standard orthogonal component, the interplay of spin-orbit coupling and particular structural symmetry permits the generation of spin current with different orientations. Here, we report the observation of nonorthogonal spin current in PtMnGa thin film, where the composition gradient for both Pt and Mn elements along the film normal direction results in mirror symmetry breaking about the film plane. Through second harmonic Hall (SHH) resistance, spin-torque ferromagnetic resonance (ST-FMR) and spin-orbit torques induced magnetization switching measurements on the PtMnGa/ferromagnets films, the robust spin current with x-($s_x$), y-($s_y$) and z-($s_z$) polarizations generated in the PtMnGa was confirmed and supported by density functional theory calculations. The spin Hall angles for the $s_{i(i=x,y,z)}$ have been calculated based on SHH and ST-FMR methods respectively, which are consistent with each other. A zero-field partial magnetization switching has been realized in the perpendicularly magnetized PtMnGa/Co/Pt multilayers due to the presence of $s_x$ and $s_z$ spin current. Our results demonstrate that the PtMnGa could be an ideal material for spin current source, providing a key strategy for finding new device functionalities.

## Short CV of Prof. Kangkang MENG

Professor Kangkang Meng has over ten years of interdisciplinary research experience in magnetic materials & spintronic devices and medical-engineering intelligent algorithms. Over the past five years, he has published 20+ first/corresponding author papers in journals including Advanced Functional Materials, Physical Review Applied and Physical Review B. In magnetic materials, he designed the combined high-resolution magnetic force microscopy-electrical transport system operating under multi-field (ultra-low temperature/strong magnetic field) environments, overcoming limitations of traditional single-field characterization. In spintronics, during his 2022-2023 visit to the University of Tokyo, he collaborated with Professor Eiji Saitoh to propose a quantum correction model for spin transport. In medical-engineering integration, he led the development of a deep learning-based real-time segmentation algorithm for orthopedic surgical robots (patented) and collaborated with Toronto General Hospital and Lenovo AI Lab on an automated abdominal multi-organ CT/MRI segmentation system. Related achievements were published in The Lancet Digital Health.

The 5th USTB-TU Symposium

# ABSTRACT
# Oral Presentation

## Oral presentation TU-1

# Anti-thermal Quenching Photoluminescence in Yb/Er/Tm Multi-doping in YSZ host

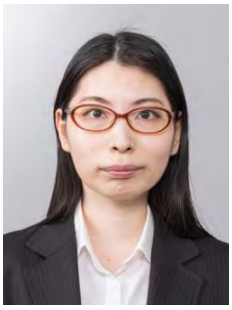
This research presents the design of an innovative dual-mode ratiometric temperature sensing platform employing $Zr_{0.85}Y_{0.15}O_{1.925}$:$Yb^{3+}$ phosphors co-activated with $Er^{3+}$ and $Tm^{3+}$ ions, which harnesses both near-infrared (NIR) up-conversion and down-shifting luminescence mechanisms. NIR excitation offers distinct benefits for bio-imaging purposes owing to its enhanced ability to penetrate biological tissues, rendering it highly suitable for remote temperature detection. By means of controlled incorporation of Yb, Er, and Tm ions into yttria-stabilized zirconia (YSZ) host matrices, this work validates the effectiveness of luminescence intensity ratios (LIR) as a reliable method for accurate thermal measurements.

When subjected to 980 nm laser irradiation, the prepared YSZ:Yb-Er/Tm phosphors displayed characteristic emission bands spanning both visible and NIR wavelength ranges. Notably prominent were the intense up-conversion photoluminescence (UCPL) centered at 800 nm arising from $Tm^{3+}$ transitions and the down-shifting photoluminescence (DSPL) occurring in the 1400-1700 nm region associated with $Er^{3+}$ ions. Investigations of temperature-dependent optical behavior revealed distinct contrasts: whereas UCPL exhibited standard thermal quenching phenomena, DSPL demonstrated extraordinary anti-thermal quenching (anti-TQ) properties, characterized by enhanced emission intensity upon temperature elevation. This novel dual-mode strategy delivered outstanding performance characteristics, featuring thermal sensitivity values surpassing 3% $K^{-1}$ at 283 K and temperature resolution below 0.1 K, thereby confirming its substantial promise for sophisticated biomedical thermal sensing implementations.

## Short CV of Assoc. Prof. Takuya HASEGAWA

Dr. Takuya Hasegawa received his Ph.D. in engineering from Niigata University in 2016. Subsequently, he began his academic career as an assistant professor at Kochi University. Later, he moved to the IMRAM at Tohoku University, where he continued as an assistant professor. He was promoted to senior lecturer in 2022, and then associate professor in 2025. His research interests include phosphor materials, photo-functional inorganic materials, particle morphology control, and structural analysis, among others.

# Phosphine-Ligand Effects on the Crystallization-Induced Emission of $AuCu_{14}$ Clusters



Ligand-protected metal clusters exhibit a variety of physical properties derived from their electronic and geometric structures that differ from those of bulk metals and nanoparticles by controlling structural factors such as size of metal core (number of constituent atoms), composition, shape and ligands. Therefore, they have attracted much attention to be the building blocks of functional nanomaterials. In order to use ligand-protected metal clusters as building blocks for functional materials, it is important to control their physical properties in the assembly. Here, we have synthesized emissive $AuCu_{14}(SPh^tBu)_{12}(PR_3)_6$ clusters with three different phosphine ligands (R = Ph, $C_4H_3S$, *p*-Tol) and investigated the photoluminescence (PL) properties in the crystalline states. Notably, the emission wavelengths in the crystalline state depended on the phosphine ligands ($\lambda_{em}$ = 659, 639, 614 nm for R = Ph, $C_4H_3S$, *p*-Tol, respectively), while those in solution were identical for all the three clusters (836 nm). This crystallization-induced changes in the emission wavelengths can be attributed to the ligand interactions between adjacent clusters in the crystal, which suppress the structural relaxation in the excited state. The differences in the phosphine ligands also significantly affected the PL quantum yields (QYs) of the crystalline clusters. In particular, their PLQYs were measured to be 56.3%, 31.7%, 21.4% for R = Ph, $C_4H_3S$, *p*-Tol, respectively, while those in the solution were comparable for the three clusters (ca. 35%). This difference can be explained by the degree of enhancement of the non-radiative relaxation process dominates the PLQY in the crystalline state compared to that of the radiative process. The findings of this study reveal the importance of designing interactions between surface ligands in controlling the physical properties of cluster in the solid state.

## Short CV of Asst. Prof. Megumi SUYAMA

Dr. Megumi Suyama is an assistant professor of Institute of Multidisciplinary Research for Advanced Materials (IMRAM), Tohoku University. She received her PhD degree from the University of Tokyo under the supervision of Prof. Tatsuya Tsukuda. Her main research target is ligand-protected metal clusters, especially coinage metal clusters. She recently interests in controlled assembly of ligand-protected metal clusters and its applications.

## Oral presentation TU-3

# Element Doping Strategies for Energy-Saving $VO_2$ Smart Windows

Vanadium dioxide ($VO_2$) exhibits temperature-responsive modulation of near-infrared (NIR) transmittance due to its unique metal-insulator transition (MIT), making it an excellent candidate for energy-efficient smart windows. However, high MIT temperatures and undesirable optical properties limit $VO_2$ applications. In virtue of atomic and electric structure modulation, element doping provides a flexible approach to tuning MIT.

In our work, W was incorporated into the $VO_2$ lattice via hydrothermal synthesis. By controlling the W concentration, the MIT temperature was successfully tuned within a wide range of −34.8 to 66.0 °C, spanning approximately 100 °C. Although the goal of achieving a room-temperature MIT was realized, the NIR transmittance modulation capability of $VO_2$ was impaired. To address this issue, we proposed a cation/anion co-doping strategy by sequentially incorporating W and N via a two-step process for the first time. An exceptional synergistic effect is achieved, realizing a reduced phase transition temperature along with simultaneous enhancements in both luminous transmittance ($T_{lum}$) and solar-energy modulation ability ($\Delta T_{sol}$). The superior performance of W/N co-doped $VO_2$ stems from the synergistic roles of W (metallic phase stabilization) and N (defect regulation), and is boosted by the special advantage of the two-step doping, W-facilitated N incorporation. This offers valuable design insights for overcoming the multiple performance trade-offs of $VO_2$ smart windows.

## Short CV of Asst. Prof. Yibei XUE

Dr. Yibei XUE received her Ph.D. from Tohoku University in 2024 under the guidance of Prof. Shu YIN. After that, she became an assistant professor in Prof. S. YIN's team, affiliated with the Institute of Multidisciplinary Research for Advanced Materials (IMRAM). Her research focuses on smart materials. Her research interests include synthesis, modification, and development of novel applications for smart material. These applications include smart windows, gas sensors, and photocatalysis, etc.

Oral presentation TU-4

# Reduction-Driven Luminescence Quenching in $Eu^{3+}$-Doped $Bi_2MoO_6$ for $H_2S$ Gas Detection

Luminescence-based gas sensor, which monitor the modulation of luminescence by target gases, have gained increasing interest. Luminescence-based gas sensors provide an intuitive method for visually detecting the presence of gases. In this study, we focused on $Eu^{3+}$-doped $Bi_2MoO_6$ (BMO:Eu) nanophosphors for luminescent-based detection of hydrogen sulfide ($H_2S$). BMO:Eu nanophosphors were successfully synthesized using hydrothermal reaction methods and exhibited typical red luminescence due to the $Eu^{3+}$ ions. The red luminescence intensity decreased by 42 % upon exposure to 500 ppm $H_2S$, and the decrease rate showed a dependence on $H_2S$ concentration (10–500 ppm), indicating that BMO:Eu is capable of quantitatively detecting $H_2S$. XRD analysis showed an increase in lattice volume following $H_2S$ exposure, while diffuse reflectance spectra revealed a reduction in reflectance in the visible region, suggesting the reduction of $Bi^{3+}$ or $Mo^{6+}$. XPS analysis further confirmed the presence of peaks attributed to $Bi^{2+}$ and $Mo^{5+}$, establishing that the luminescence quenching of BMO:Eu was due to the reduction of $Bi^{3+}$ and $Mo^{6+}$. Moreover, in-situ lifetime measurements under $H_2S$ exposure indicated a reduced lifetime of 0.62 ms compared to 0.76 ms before exposure. This reduction in lifetime indicates that the formation of quenching centers played a critical role in diminishing the overall luminescence.

## Short CV of Taisei HANGAI

Taisei HANGAI is currently pursuing his doctoral degree (D3) under the supervision of Prof. Shu Yin in Institute of Multidisciplinary Research for Advanced Materials, Tohoku University.

## Oral presentation TU-5

# Layered Black Phosphorus Microspheres via Solvothermal Self-Assembly for Sensitive Ammonia Detection

Black phosphorus (BP), a two-dimensional semiconductor with a tunable direct bandgap and high carrier mobility, shows great potential for room-temperature gas sensing. In our work, BP was synthesized via a solvothermal method using red phosphorus and ethylenediamine at 160 °C for 48 h. The resulting product exhibited a self-assembled spherical morphology composed of ultrathin nanosheets, as confirmed by SEM observation. This hierarchical structure provides a large surface area and abundant active sites, facilitating efficient gas adsorption and diffusion. When tested as a gas sensor, the BP showed a clear, reversible, and concentration-dependent response toward $NH_3$ in the range of 2.5–24.7 ppm at room temperature, consistent with its p-type semiconducting behavior. In contrast, the response toward volatile organic compounds (VOCs) such as toluene and ethanol was irregular and unstable, indicating weak and non-specific adsorption on the BP surface. Stability tests further revealed that the $NH_3$ response remained largely reproducible after multiple cycles, though slight degradation occurred over time due to surface oxidation. Overall, the solvothermal synthesis provides a safe, low-cost, and scalable route to obtain crystalline BP with excellent NH3 sensitivity and acceptable stability, making it a promising material for low-power environmental gas sensors.

## Short CV of Qiuyu JIN

Qiuyu JIN received his B.E. from the College of Materials and Energy, Lanzhou University, where he conducted research on photocatalysis. He obtained his M.S. degree from Tohoku University, Japan, and is currently pursuing his Ph.D. (D1) under the supervision of Prof. Shu Yin. Since his master's study, his research has focused on gas sensing materials and devices. He is a fellow of the International Joint Graduate Program in Integrated Chemistry (GP-Chem) at Tohoku University.

Oral presentation TU-6

# Effect of hydrothermal reaction field on $CO_2$ reduction performance of nanoporous gold catalysts

**[Introduction]** Electrochemical $CO_2$ reduction reaction ($CO_2RR$) has attracted attention as an important technology for achieving a carbon neutral society since it can recycle $CO_2$ by renewable electricity. However, the slow reaction rate of $CO_2RR$ remains one of the major challenges for practical applications. Here, we attempted to improve the reaction rate by two strategies: employing a porous structure with a large surface area and using a hydrothermal reaction field1 that promotes mass diffusion of reaction substrates. This study investigated how the $CO_2RR$ activity was affected by a porosity of the electrodes and a hydrothermal reaction field.

**[Experiment]** The $CO_2RR$ activity was evaluated on planar Au (Au), nanoporous Au (NpAu) or macroporous Au (MpAu) electrodes. NpAu was prepared by alloying/dealloying process, and MpAu was obtained by heat treatment of NpAu.

**[Result and discussion]** The increase in current density during constant voltage electrolysis caused by introducing a porous structure was more pronounced at high temperature electrolysis conditions. This is due to the improved mass diffusion inside the nanoporous structure and reduced solution resistance, allowing the inside of the nanoporous structure to contribute electrochemical reaction. The temperature dependence of partial current densities for $CO_2RR$ products revealed that, despite its high specific surface area, NpAu exhibited an extremely low partial current density for CO production at 100 °C compared to other catalysts such as Au and MpAu. These results suggest that the enhanced mass diffusion at high temperatures promoted electrode reaction inside the nanoporous structure, which in turn created an extremely basic environment that suppressed the current density for CO production.

## Short CV of Ryusei TAKAYANAGI

Master's student (2nd year), Department of Chemical Engineering,
Graduate School of Engineering, Tohoku University

## Oral presentation USTB-1

# Data-driven assisted metallurgical defect control and the mechanism of strengthening and toughening for additively manufactured metal parts

To address the key challenge of precisely controlling the forming quality and mechanical properties during the preparation of alloys by electron beam selective melting additive manufacturing, a new framework for optimizing the forming process was designed and developed based on machine learning technology. The key influence mechanisms of forming parameters on metallurgical defects and mechanical properties were studied. The results show that based on the machine learning model, the internal metallurgical defects of electron beam selective melting formed parts can be successfully predicted by detecting and classifying surface morphology information. One of the key points of this method is that the numerical simulation calculation of the molten pool model helps to reveal the correlation mechanism between process parameters, surface morphology and internal defects, highlighting the importance of surface information of the formed parts. Another key point is that the machine learning model is based on the above correlation mechanism, which makes it physically meaningful to predict metallurgical defects by predicting surface morphology using the machine learning model. This method has shown high efficiency and accuracy in the electron beam selective melting forming of carbon steel, titanium alloy, etc., and the alloy performance is far superior to that reported in the literature.

## Short CV of Assoc. Prof. Yunwei GUI

Assoc. Prof. Yunwei GUI received a Ph.D. in engineering from Tohoku University in 2022. Subsequently, he served as an assistant professor at the Institute for Materials Research (IMR) at Tohoku University before advancing to the position of associate professor at the School of Materials Science and Engineering, University of Science and Technology Beijing. His research focuses on the development of high-performance metallic materials and additive manufacturing technologies leveraging machine learning, among other areas. He has authored over 30 papers as the first or corresponding author in Additive Manufacturing and various academic journals, and has led several scientific research projects, including those funded by the National Natural Science Foundation of China.

# Preparation and Performance of Alumina Fibers Based on Sol Structure Regulation

Alumina fiber is a material with excellent performance, and it is widely used in fields such as aerospace, machinery manufacturing, high-temperature filtration, energy chemical industry and electronic information. Through first-principles calculations and molecular dynamics simulations, it is found that $Al_{13}$ can effectively anchor polymer long chains via its abundant surface hydroxyl groups. This enables $Al_{13}$ to act as dynamic entanglement points for polymer long chains, promoting the formation of a dendritic network structure in the sol that is favorable for spinning. Based on the strong adsorption between PVP and $Al_{13}$, the spinning fluid can maintain the integrity of the network structure through the dynamic reorganization of $Al_{13}$-PVP hydrogen bonds during the stretching process. This endows the sol with excellent spinning performance. Guided by this mechanism, an aluminum sol with high $Al_{13}$ content was prepared via forced hydrolysis technology, and after modification with PVP and concentration, a sol with high spinning performance was obtained. Using the structurally optimized sol with high spinning performance, combined with precise control of the sintering process, continuous alumina fibers with low structural defects and small diameters were successfully prepared. The sol-gel method realizes the uniform mixing of components at the molecular scale, allowing nano-sized t-$ZrO_2$ to be uniformly distributed in the $Al_2O_3$ fiber matrix. This not only achieves phase transition toughening, but also effectively inhibits the high-temperature coarsening of alumina grains, significantly improving the high-temperature stability and mechanical properties of the fibers.

## Short CV of Assoc. Prof. Bin LI

Li Bin obtained his doctoral degree from University of Science and Technology Beijing in 2016. He was a visiting scholar at Tohoku University in 2021 and has been teaching at the School of Materials Science and Engineering at University of Science and Technology Beijing since 2019. Since working, he have been engaged in research on ceramic materials, refractory materials, and other aspects. Currently, as the first author/corresponding author in *J. Adv. Ceram., Inorg. Chem. Commun*. and other journals have published over 20 papers and granted 7 patents.

## Oral presentation USTB-3

# Damage microstructure, hardening and deuterium retention in neutron irradiated tungsten and tungsten-rhenium alloy

Tungsten is a key candidate armour material for plasma-facing components in ITER and has been planned for use in DEMO. During service, simultaneous high flux thermal loading, plasma-wall interaction and neutron damage accumulation may lead to severe embrittlement and possible loss of structural integrity in the material. A reliable prediction of tungsten performance requires the establishment of a quantitative evolution map of neutron damage microstructure, as well as an accurate correlation model connecting defect statistics and material property degradation. In this work, a summary of recent progress on neutron irradiations in pure tungsten (CVD-W, W-rod) and tungsten-rhenium alloy is presented. The specimens were subjected to neutron irradiation in the Belgian BR2 reactor, across a temperature and fluence range of "< 210°C−800°C" and "$4\times10^{22}-1\times10^{25}$n/m2 ($E_n$> 1 MeV)", respectively, to mimic the damage effects of fusion neutrons. By combination of defect microscopy, micro/nano-hardness evaluation, linear plasma exposure and thermal desorption spectroscopy analysis, a damage microstructure map is unveiled, and the irradiation hardening and deuterium retention behaviours are investigated.

## Short CV of Assoc. Prof. Xiaoou YI

Dr. Xiaoou Yi is an Associate Professor in the School of Materials Science and Engineering at the University of Science and Technology Beijing (USTB). She received her PhD (DPhil) from the University of Oxford in 2014 and served as a Culham Junior Research Fellow at Oxford's Department of Materials for three years. Dr. Yi's expertise lies in the electron microscopy characterization of irradiation defects in metallic systems induced by high-energy particle irradiation. She has authored over 70 publications that have garnered more than 2,200 citations. Additionally, Dr. Yi serves as an editorial board member for the Elsevier journal *Nuclear Materials and Energy*.

Oral presentation USTB-4

# Research on Surface Modification of MXene and Its Adsorption Mechanism for Nuclide Ions

The nuclear disaster that occurred at the Fukushima nuclear power plant in 2011 culminated in a massive discharge of radioactive substances into the environment, posing a long-term threat to both human health and eco-system. Strontium-90 ($^{90}Sr$) and Cs are regarded as one of the most hazardous fission products of nuclear reactors, characterized by high solubility and mobility, considerable fission product yields, and relatively long half-life. Given the dangerous nature, the effective treatment of radioactive Sr ions in wastewater to prevent their discharge into the environment is an urgent matter that demands our serious attention. Among various purification techniques including chemical precipitation, ion exchange, solvent extraction and membrane treatment, solid phase adsorption has been widely studied due to its simple operation, low cost, high removal efficiency and less secondary pollution.

MXenes, a novel intriguing family of two-dimensional transition metal carbides/nitrides first discovered in 2011, have shown promising application potentials in various areas, due to their unique structures rendering rich active surface sites, high hydrophilicity, high electronic conductivity and excellent mechanical properties. To propel the application of MXene materials as heavy metal ions adsorbents in the field of wastewater purification treatment, issues of oxidative degradation and low adsorption capacity and selectivity for adsorbates are to be addressed.

In order to address the challenges posed by the structural stability and adsorption performance of MXene as an adsorbent, our group has conducted research in recent years on surface modification of MXene by covalent modification of S and N atoms, as well as methods for embedding CB5 molecules into the interlayer space of MXene.

## Short CV of Assoc. Prof. Yujuan ZHANG

Yujuan Zhang is an Associate Professor specializing in the research and prediction of material structures and properties using first-principles calculations, molecular dynamics, phase-field methods, and machine learning techniques. Her current research focuses on the following areas: (1) Separation of nuclides using novel two-dimensional graphene-like MXene materials and derived inorganic nanomaterials; (2) Investigation of the irradiation evolution, corrosion behavior, and defect mechanisms of advanced actinide carbonitride nuclear fuels;(3) Theoretical study on the structural design, physicochemical properties, and defect evolution mechanisms of tungsten alloys as first-wall materials for nuclear fusion.

## Oral presentation USTB-5

# Topological Synthesis of Anisotropic Micro/nano Materials and Device Preparation

With the rapid rise of future industries such as artificial intelligence, the use of renewable energy or low-power devices has attracted widespread attention. However, the origin of this lies in the preparation and modification of functional materials. Topological chemical synthesis is a method of chemical synthesis based on the invariance of morphology or structure, which enables the specific enhancement of the properties of micro nano materials. We use graph theory to perform topological chemical synthesis, maintain the similarity of the lattice of intermediate products during transformation, and achieve several controllable two-dimensional atomic level thick chalcogenides functional materials. Based on optimized structures, performance enhancement is achieved. Two dimensional atomic level thick transition metal chalcogenides nanosheets rich in sulfur vacancy defects with enhanced performance in electrochemical hydrogen and oxygen evolution reactions have been achieved. Two dimensional transistors with high carrier mobility and switching ratio have been printed and constructed, as well as several high-performance, low-energy, multifunctional flexible sensor devices.

## Short CV of Assoc. Prof. Lihong LI

Li Lihong, Associate Professor and Doctoral Supervisor at Beijing University of Science and Technology. Postdoctoral fellow at Tsinghua University in 2013, visiting scholar at UCLA from 2017 to 2018. Mainly researching the preparation of low dimensional materials and devices, published 30 papers as first author or corresponding author in *Matter, Adv. Mater., Mater. Today, Nano Micro Lett., Adv. Sci*, etc; She has published over 50 SCI papers, with more than 3100 citations and an average citation frequency of 52.09 per paper, with an H-index of 31. She was selected for the China Science and Technology Think Tank Talent Program, Nano Research Youth Editorial Board, and participated in peer reviews for journals such as *Mater. Today, Adv. Func. Mater, Nano Energy*, etc.

# Transformation mechanisms in hexagonal close-packed crystals and implications for the design of advanced lightweight structure materials

Twinning is an essential deformation mode of crystals which is attracting growing attention due to its potential in simultaneously improve the strength and ductility of metals. It is generally believed that twinning is mediated by shear and atomic shuffles on an invariant twinning plane. Here, by using in situ high resolution transmission electron microscopy (TEM), we report on an extension twinning mode in rhenium nanocrystals along the <10-1-4> direction on the {20-21} plane, which can be mediated by the formation of interfacial defects that fall between the parent prismatic plane and the twin pyramidal plane which are a pair of corresponding planes of the {20-21} twinning mode. The incoherent twin boundary can partly evolve into the coherent twinning plane during detwinning. The findings provide direct evidences to the {20-21} twin in hexagonal close-packed metals and corroborate the conjecture that twinning nucleation is essentially a transformation that conforms to and establishes the lattice correspondence which can be mediated by interfacial processes other than homogeneous shear on the twinning plane.

In addition, by using in situ TEM, we uncover direct evidence on the nucleation and growth of FCC-Ti right in front of the crack tip in the α-Ti matrix. Atomic resolution images further reveal that the transformation can be mediated by either partial dislocations on basal planes or shear and atomic shuffle on the FCC{110}|HCP{10-10} interfaces.

## Short CV of Yongqing CHEN

Yongqing Chen, PhD candidate at University of Science and Technology Beijing. Research focuses on twinning mechanism in hexagonal close-packed using in situ transmission electron microscopy.

Oral presentation USTB-7

# Statistical in situ scanning electron microscopy investigation on the failure of oxide scales

Oxide scales play pivotal role in obstructing surface chemical and electrochemical reactions, hence hindering chemo-mechanical effects such as liquid metal embrittlement of steels. Therefore, the critical conditions and failure mechanism of the oxide film are of major interest in the safe service of steels. Though in situ microscopic methods may directly visualize the failure mechanism, they are often challenged on the lack of statistically reliable evaluation of the critical conditions. Here, by combining in situ scanning electron microscopy with tapered specimen tensile test in a single experiment, we uniquely achieve mechanistic study with statistically reliable quantification on the critical strains for each step of the dynamic process of film rupture. This is demonstrated with the oxide films formed on a ferrite-martensite steel in liquid lead-bismuth eutectic alloy at elevated temperatures, with in situ results fall right into the predictions of the statistical analysis. Explicitly, the integrated experimental methodology may facilitate the materials genome engineering of steels with superior service performance.

## Short CV of Jin ZHOU

Jin Zhou, PhD candidate at University of Science and Technology Beijing. Focused on characterizing the performance and degradation of ferrite-martensite steel in liquid lead-bismuth eutectic alloy.

Oral presentation USTB-8

# Theoretical Investigation of Microstructure-Driven Enhancement in the CrCoNi Medium-Entropy Alloy

CrCoNi medium entropy alloy (MEA) exhibits high strength and ductility, yet the microstructural origins of its performance remain incompletely resolved. This work quantified strengthening from a deformation-induced 9R phase and the effect of hydrogen on vacancy defects using first-principles meta-GGA calculations with special quasi-random structure (SQS) models. A 9R model consistent with experimental orientation relationships was constructed and evaluated against the FCC matrix. The 9R phase showed ~12% higher bulk modulus (B) and ~7% higher Poisson's ratio than FCC. Substitutional Mo, Ta, and W were assessed. Mo and W promoted 9R formation and improved 9R/FCC interfacial properties, as indicated by higher work of adhesion and fracture-toughness surrogates due to dopant-induced orbital hybridization.

Hydrogen–defect interactions were analyzed. Hydrogen lowered the formation energy of H-capturing vacancies by ~0.36 eV and reduced the unstable stacking-fault energy by 0.01–0.02 $J \cdot m^{-2}$. Large clusters were destabilized and tended to decompose into smaller point defects. Elastic calculations for vacancy-containing models showed no marked reduction in B. For large clusters, the B/G ratio dropped by 6.3-17.1%, indicating reduced ductility.

This work clarified the strengthening role of the 9R phase and the hydrogen-defect pathway. It provided a guidance for microstructure control in hydrogen-rich service.

## Short CV of Ni LU

Ni Lu received the B.E. degree in Material Physics from China University of Geosciences Beijing, Beijing, China, in 2021. Ni Lu received the M.S. degree in Physics from University of Science and Technology Beijing, Beijing, China, in 2024. She is currently working toward the D.S. degree in Physics at the University of Science and Technology Beijing, Beijing, China. Her research interests include DFT, MD, force field, superalloy, high entropy alloy, hydrogen damage, fatigue.

## Oral presentation USTB-9

# Chemical strain for ferroelectric photovoltaic properties in double-perovskite films

Double-perovskite thin films are widely studied in multiferroic and multifunctional fields due to their modifiability. The chemical strain strategy shows great potential in optimizing the electronic and physical properties of functional oxide films. However, challenges exist in the complex preparation of double-perovskite thin films and the uncontrollable application of chemical strain. Specifically, issues such as phase transitions and compositional segregation caused by extensive atomic substitution often occur during the preparation process, and chemical strain can only be applied through uncontrollable methods (e.g. structural adjustment). We solve these problems using controllable magnetron sputtering processes: temperature adjustment is employed to control the composition of double-perovskite thin films, while varying the flowing oxygen pressure enables the application of controllable chemical strain. This approach achieves the optimization of ferroelectric-related properties, including ferroelectric enhancement, photoelectric enhancement, and multi-level open-circuit voltage improvement for optical storage. Notably, regulating chemical strain via substrate strain enhances the remanent polarization of $BiSmFe_2O_6$ double-perovskite thin films by 6-7 times (approximately 4.8 $\mu C/cm^2$) , which is the highest value among type-II multiferroic materials at that time. Non-equivalent substitution increases the short-circuit current of $(Bi_{1-x}Ba_x)_2FeMnO_6$ thin films from 3.61 $\mu C/cm2$ to 135.67 $\mu C/cm^2$, a value that ranks highest for ferroelectric thin films with a thickness of hundreds of nanometers. Further, adjusting the chemical strain (ranging from 0 to -0.32 GPa) in $BiSmFe_2O_6$-δ thin films achieves a tunable narrow bandgap and a giant multi-level switchable ferroelectric photoelectric voltage of approximately 1.56 V, with more than 7 types of open-circuit voltages. This performance makes the film applicable to ferroelectric non-volatile optical memory. We envision the chemical strain strategy as a model for exploring double-perovskite derivatives with abundant coupled states, which will bring intriguing multifunctionalities to electronic and spintronic devices.

## Short CV of Jie TU

Jie Tu, is a doctoral student at University of Science and Technology Beijing, focusing on structural design of ferroelectric functional information bismuth-based double-perovskite thin films and device research. He has over 20 SCI papers, with first/co-first author works in *Sci. Adv., Nat. Commun., Adv. Mater., and J. Am. Chem. Soc*., plus 1 authorized and 3 pending patents.

Oral presentation USTB-10

# Effect of Mn addition on the corrosion behavior of FeCrNiMnxSi alloys in simulated seawater environment

This study investigates the effect of Mn content (x=0, 10, 20, 30 wt%) on the corrosion behavior of $Fe_{57-x}Cr_{19}Ni_{22}Mn_xSi_2$ medium entropy alloys (MEAs) in 3.5 wt% NaCl solution, simulating a seawater environment. Microstructural characterization via XRD and EBSD reveals single FCC structures in alloys with x≤20, while the 30Mn MEA exhibits secondary BCC and Mn-Ni-Si phases. Electrochemical tests (cyclic potentiodynamic polarization, EIS) show that increasing Mn reduces open circuit potential (OCP), breakdown potential Eb, and protection potential Ep, indicating degraded corrosion resistance. XPS analysis demonstrates that higher Mn content decreases the oxide/hydroxide ratio in passive films, particularly reducing Cr-oxide/Cr-hydroxide ratios, which weakens film stability. For the 30Mn MEA, microgalvanic corrosion occurs due to multi-phase interfaces (FCC matrix, BCC, and Mn-Ni-Si phases), confirmed by SKPFM and SEM, leading to severe localized attack at grain boundaries. Mott-Schottky analysis reveals that passive films exhibit duplex semiconducting behavior, with increased defect density NA and ND as Mn content rises, further compromising film protectiveness. In summary, Mn addition deteriorates corrosion resistance by destabilizing passive films and inducing microstructural heterogeneity, with excessive Mn (≥30 wt%) triggering multi-phase-driven galvanic corrosion. These findings provide insights into alloy design for marine applications by highlighting the critical role of Mn content in balancing microstructural stability and corrosion protection.

## Short CV of Zejun LI

Zejun Li is a master's student at the University of Science and Technology Beijing. During her master's studies, she has made contributions to multi-principal-element alloys (MEAs), with 2 first-author papers published in Corrosion Science and Surface Technology—the work focuses on corrosion behavior and mechanical properties, two core topics in the MEA field. She has also participated in three research projects, including one supported by the National Natural Science Foundation of China (NSFC).

Oral presentation USTB-11

# High-temperature dislocation substructures in heavy-ion irradiated long-range-ordered $(Fe, Ni)_3V$ alloy

$(Fe, Ni)_3V$ is a promising material system for structural components in advanced nuclear energy systems, owing to its excellent room-temperature toughness and ductility, robust high-temperature mechanical properties, inherent resistance to radiation defect accumulation from its long-range ordered structure, and wide compositional tunability. In this work, we present a systematic investigation on $(Fe, Ni)_3V$ alloys, irradiated with 6/6.4 MeV Fe-ions (DuET and IBML facility), across a temperature and dose range of "500−600 °C" and "1-10 dpa", respectively, to mimic the displacement damage effects of fast neutrons. By combinations of defect microscopy, computer-based automated image processing, as well as nano hardness testing, the statistical characters of irradiation defects and microstructure evolution are unveiled, and a quantitative correlation between irradiation defect statistics and irradiation-induced swelling/hardening is established. The current research shall bring new insights upon the fundamental studies of high-temperature structural materials for nuclear applications, provide experimental validation and theoretical basis from a perspective of "long-range-ordered structures".

## Short CV of Hui LIU

Hui Liu is a third-year master's student at the University of Science and Technology Beijing (USTB), supervised by Assoc. Prof. Xiaoou Yi. His research investigates the effects of high-energy particle irradiation on $(Fe, Ni)_3V$ long-range ordered alloys, focusing on their order-disorder transition, dislocation behavior, and mechanical response. The goal of this work is to elucidate the irradiation damage mechanisms in these advanced materials and to assess their potential as critical structural components for Generation IV nuclear systems.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