



# THE 22<sup>nd</sup> INTERNATIONAL CONFERENCE ON TERNARY AND MULTINARY COMPOUNDS (ICTMC-22)

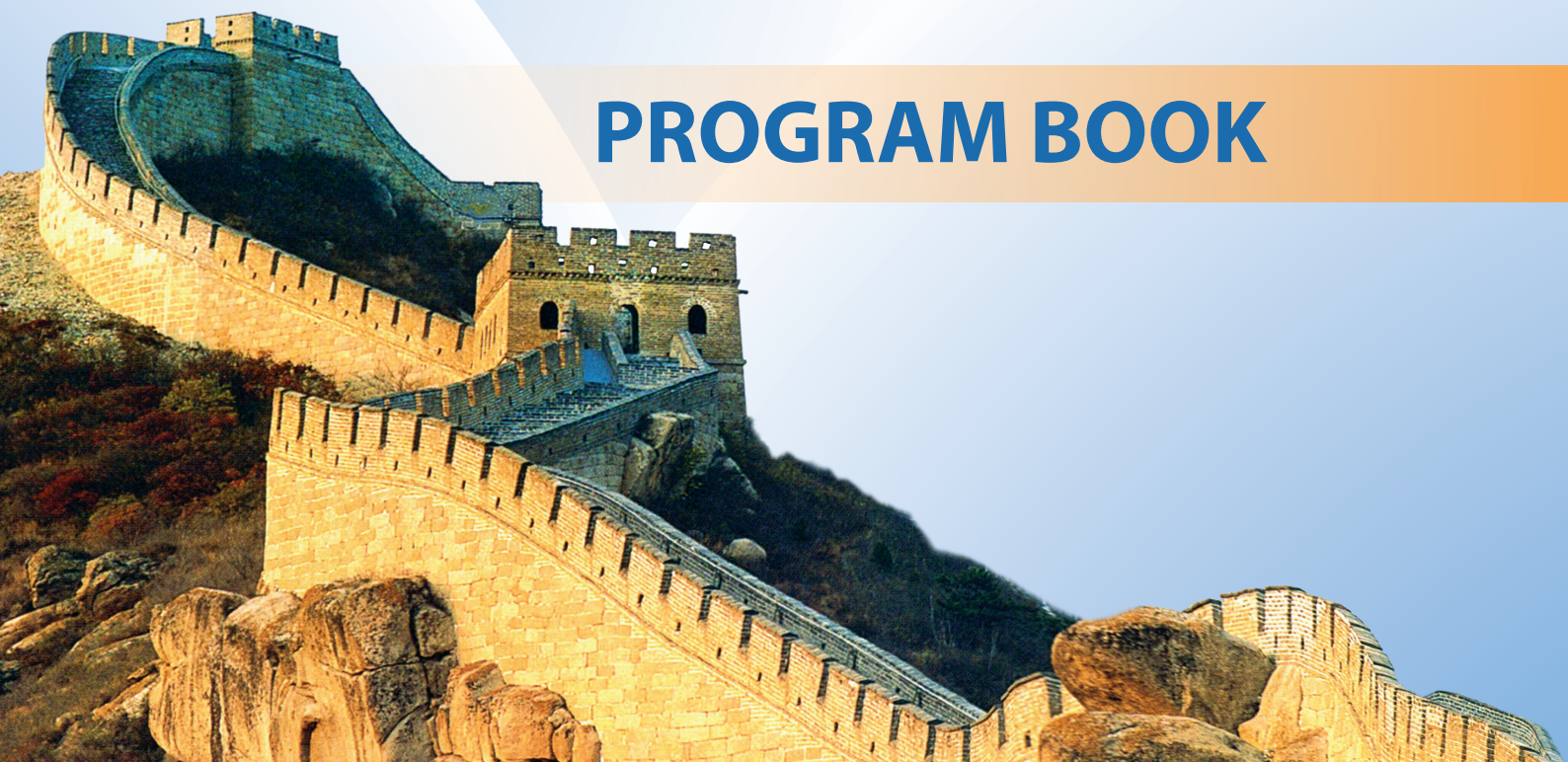
September 9 -13, 2024 • Beijing, China

Eastern Institute of Technology, Ningbo, China

Institute of Semiconductors, Chinese Academy of Sciences

Key Laboratory of Computational Physical Sciences (Fudan University), Ministry of Education

## PROGRAM BOOK



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## WELCOME MESSAGE

On behalf of the Conference Chairs, it is our great pleasure to announce that the 22<sup>nd</sup> International Conference on Ternary and Multinary Compounds (ICTMC-22) will take place from September 9-13, 2024, at the Beijing Chunhui International Conference Center in Beijing, China.

Since its inception in 1973, ICTMC has been a premier forum for discussing advancements in ternary and multinary compounds. This biennial event continues to offer a comprehensive exploration of the physics, chemistry, growth, characterization, theory, and applications of these compounds. ICTMC-22 will encompass both fundamental scientific research and practical technological applications.

We are excited to extend a warm invitation to you to join us at ICTMC-22. Your presence will not only contribute to the rich scientific discussions but also facilitate meaningful networking and collaborative opportunities with esteemed academics, researchers, industry professionals, and students.

We look forward to your participation and to a conference filled with insightful exchanges and new discoveries.



Prof. Su-Huai Wei, Xin-Gao Gong, Jun-Wei Luo  
Chairs, Organizing Committee of ICTMC-22

## ORGANIZING COMMITTEE

### International Advisory Committee

- David Cahen, Weizmann Institute of Science, Israel
- Xin-Gao Gong, Fudan University, China
- J. F. Guillemoles, French National Centre for Scientific Research, France
- Shu-Shen Li, Institute of Semiconductors, CAS, China
- Hai-Qing Lin, Zhejiang University, China
- Junwei Luo, Institute of Semiconductors, CAS, China
- Nazim Mamedov, Azerbaijan National Academy of Sciences, Azerbaijan
- Angus Rockett, Colorado School of Mines, USA
- Roland Scheer, Martin Luther University Halle-Wittenberg, Germany
- Susan Schorr, Helmholtz-Zentrum Berlin, Germany
- William Shafarman, University of Delaware, USA
- Susanne Siebentritt, University of Luxembourg, Luxembourg
- Takahiro Wada, RyuKoku University, Japan
- Kazuki Wakita, Chiba Institute of Technology, Japan
- Su-Huai Wei, Eastern Institute of Technology, Ningbo, China
- Andriy Zakutayev, National Renewable Energy Laboratory, USA
- Alex Zunger, Colorado University at Boulder, USA

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- Jun-Wei Luo, Institute of Semiconductors, CAS, China
- Lane Martin, University of California, Berkeley, USA
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- David Scanlon, University College London, UK
- Byungha Shin, Korea Advanced Institute of Science & Technology, Korea
- Su-Huai Wei, Eastern Institute of Technology, Ningbo, China
- Zhen-Yu Zhang, University of Science and Technology, China

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- Shiyu Chen, Fudan University, China
- Hui-Xiong Deng, Institute of Semiconductors, CAS, China
- Xin-Gao Gong, Fudan University, China
- Bing Huang, Beijing Computational Science Research Center, China
- Wu Li, Eastern Institute of Technology, Ningbo, China
- Jun-Wei Luo, Institute of Semiconductors, CAS, China
- Xiaodong Pi, Zhejiang University, China
- Chen Qiu, Eastern Institute of Technology, Ningbo, China
- Bo Shen, Peking University, China
- Guozhen Shen, Beijing Institute of Technology, China
- Xun Shi, Institute of Ceramics, CAS, China
- Man-Ling Sui, Beijing University of Technology, China
- Ning Tang, Beijing University
- Su-Huai Wei, Eastern Institute of Technology, Ningbo, China
- Zhongming Wei, Institute of Semiconductors, CAS, China
- Hong-Yu Wen, Institute of Semiconductors, CAS, China
- Hongjun Xiang, Fudan University, China
- Ji-Hui Yang, Fudan University, China
- Wanjian Yin, Soochow University, China
- Jingbi You, Institute of Semiconductors, CAS, China
- Pu Yu, Tsinghua University, China
- Lijun Zhang, Jilin University, China
- Wen-Qing Zhang, Southern University of Science and Technology, China
- Yong Zhang, Nanjing University, China
- Jian-Hua Zhao, Institute of Semiconductors, CAS, China
- Yixin Zhao, Shanghai Jiao Tong University, China

### Publication Committee

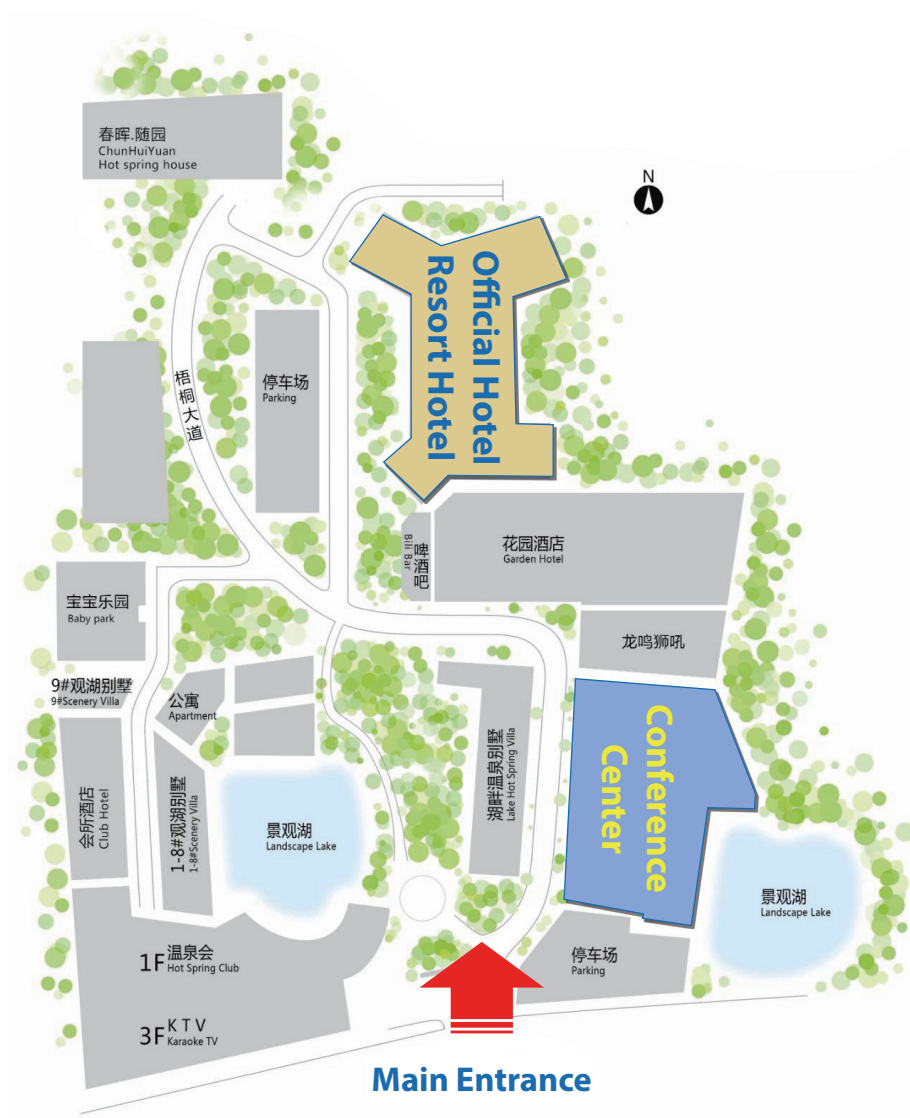
- Jun-Wei Luo, Institute of Semiconductors, CAS, China
- Hui-Xiong Deng, Institute of Semiconductors, CAS, China
- Su-Huai Wei, Eastern Institute of Technology, Ningbo, China

## VENUE INFORMATION

Beijing Chunhuiyuan International Conference Center is located in the Beijing Chunhuiyuan Resort, which is a comprehensive resort that integrates business meetings, tourism, leisure vacation, entertainment, and dining. Beijing Chunhuiyuan ICC is one of the buildings of this complex.

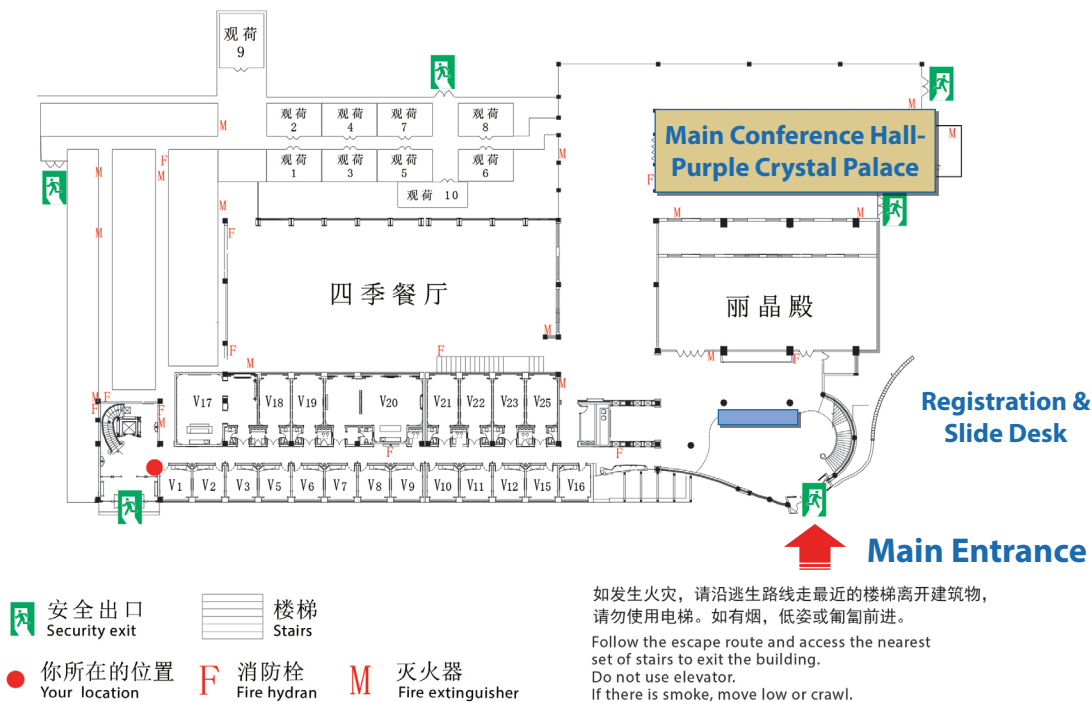
It is situated on the beautiful "First River of the National Gate" Wenyu Riverside. It covers an area of 1.8 million square meters, embracing "sky, earth, forest, water".

## FLOOR PLAN OF BEIJING CHUHUINYUAN RESORT

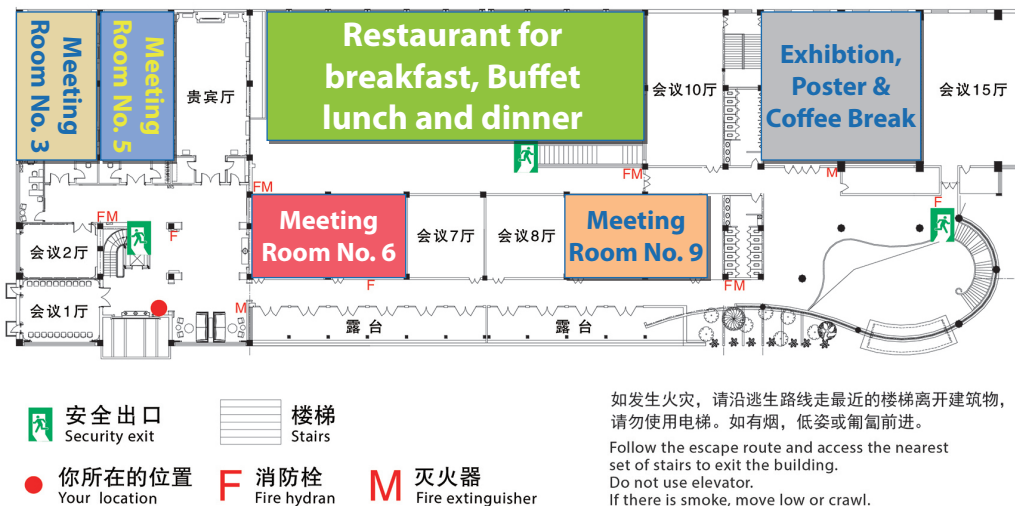


## FLOOR PLAN OF CONFERENCE CENTER

### 1F 消防疏散图 EVACUATION MAP



### 2F 消防疏散图 EVACUATION MAP



## EXHIBITORS LIST

Booth No.	Exhibitor
A01	北京龙讯旷腾科技有限公司 Beijing Lonxun Quantum Co.,Ltd.
B01	北京东科泓生科技有限公司 Beijing Coolight Technology Co., Ltd
B02	奥量光子（北京）科技有限公司 Ultrafast Quantum Photonic Co. Ltd
B03	北京锐雪科技有限公司 Beijing Reyshore-Tec Ltd.





## CONGRESS INFORMATION

### REGISTRATION

ICTMC-22 participants are asked to register at the registration desks. You could register at Lobby of Resort Hotel in the afternoon of 9<sup>th</sup> Sep. and could register at Lobby of Chunhuiyuan International Conference Center from 10<sup>th</sup> Sep. You will receive your name badge and your conference bag containing the program book and other items. The opening hours of the registration desk are as follows:

Date	Resort Hotel Lobby	Conference Center Lobby
Sept. 09 (Mon)	13:00-20:00	-
Sept. 10 (Tue)	-	07:30-18:00
Sept. 11 (Wed)	-	08:00-18:30
Sept. 12 (Thur)	-	08:00-12:00
Sept. 13 (Fri)	-	08:00-12:00

### SLIDES DESK

It is recommended that each speaker come to the Slides Desk to test the document as soon as your arrival, and copy your slides to your meeting room computer at least 30 minutes before the session. For speakers who do not copy the slides to his meeting room, the time for copying your slides to the computer will be included in your presentation time. The opening hours of the slides desks are as follows:

Date	Resort Hotel Lobby	Conference Center Lobby
Sept. 09 (Mon)	13:00-20:00	-
Sept. 10 (Tue)	-	07:30-18:00
Sept. 11 (Wed)	-	08:00-18:30
Sept. 12 (Thur)	-	08:00-12:00
Sept. 13 (Fri)	-	08:00-12:00

## POSTER & EXHIBITION SERVICE DESK

Poster authors could get the tape to put up their posters at the service desk. Before you put up your poster, please sign in to the poster list to confirm your participation. The poster & exhibition service desk is by the gate of poster & exhibition area.

Exhibitors could also get help from this service desk. The opening hours of the Service Desk are as follows:

Date	Conference Center (2F)
Sept. 09 (Mon)	From 16:00
Sept. 10 (Tue)	07:30-18:00
Sept. 11 (Wed)	08:00-18:30
Sept. 12 (Thur)	08:00-12:00
Sept. 13 (Fri)	08:00-12:00

## DINING INFORMATION

### Breakfast of Resort Hotel

This hotel has no breakfast restaurant, all in house guests need to go to the Gallery Restaurant on the second floor of the Conference Center for breakfast. Room card is required for dining, so please bring your room card when you have breakfast at Gallery Restaurant.

### Lunch & Dinner

Your conference registration fee includes buffet lunches from Sept. 10-12 and buffet dinners on Sept. 10 & 12.

The lunch and dinner restaurant is Gallery Restaurant, which is located on the second floor of Conference Center

Kindly note that the dining time is fixed. Please have your lunch according to the conference program.

Date	Lunch	Dinner
Sept. 10 (Tue)	12:00-14:00	17:30-19:00
Sept. 11 (Wed)	12:00-14:00	18:30-20:30
Sept. 12 (Thur)	12:00-14:00	17:30-19:00

### **Banquet**

The coupon for banquet of September 11 is separated from the combined coupons, the banquet is included in the conference registration fee. This is an excellent occasion to communicate with participants and speakers.

**Venue:** Purple Crystal Palace on the first floor of the Conference Center

**Date & Time:** 18:30-20:30, September 11, 2024

## **FACILITIES**

### **Wi-Fi**

Wi-Fi Internet access will be available free of charge to all participants.

The name of Wi-Fi is: CHY (do not need password)

### **Smoking Policy**

Chunhuiyuan Conference Center is a non-smoking facility participants are requested to refrain from smoking in indoor areas.

### **Dress Code**

You are welcome to wear smart casual or comfortable clothes.

### **Bank or ATM in the Resort Hotel**

ATM is available in the resort Hotel, you may use your bank card to withdraw cash from ATM.

There is also an Agricultural Bank of China near Chunhuiyuan ICC.

#### **Detail is as follows:**

Agricultural Bank of China (Weilaikexuecheng Branch)

**Location:** No. 3 Yingcai Nanjie Road, Shunyi District, Beijing City. (About 5 minutes by taxi from Chunhuiyuan ICC)

# ICTMC22 Program at a Glance

Time	Sept 9, 2024 (Monday)	Sept 10, 2024 (Tuesday)	Sept 11, 2024 (Wednesday)	Sept 12, 2024 (Thursday)	Sept 13, 2024 (Friday)						
08:00-08:30	13:00-20:00 On-site Registration	On-site Registration	Sign in	Sign in	Sign in						
08:30-08:45		Opening	4 parallel sessions		4 parallel sessions						
08:45-09:15		Keyno (30min*3)	Invited + Oral	Invited + Oral	Invited + Oral	Invited + Oral	Invited + Oral	Invited + Oral	Invited + Oral	Keynte (30min*3)	
09:15-09:45											
09:45-10:00											
10:00-10:15											
10:15-10:30		Coffee & Tea Break	10:10-10:20 Coffee & Tea Break	10:10-10:20 Coffee & Tea Break	10:10-10:20 Coffee & Tea Break	Coffee & Tea Break					
10:30-11:00		Keynote (30min*3)	10:20 4 parallel sessions	Invited + Oral	Invited + Oral	Invited + Oral	Invited + Oral	Invited + Oral	Invited + Oral	Invited + Oral	Keynote (30min*3)
10:30-11:00											
11:00-11:30											
11:30-12:00											
12:00-14:00		Lunch & Rest	Lunch & Rest	Lunch & Rest	Lunch & Rest						
14:00-14:30		4 parallel sessions	4 parallel sessions	4 parallel sessions	Excursion (Two options: 1. The Great Wall; 2. The Summer Palace.)						
14:30-15:00		Invited + Oral	Invited + Oral	Invited + Oral			Invited + Oral				
15:00-15:40		Invited + Oral	Invited + Oral	Invited + Oral			Invited + Oral				
15:40-15:50		15:40 Coffee & Tea Break	15:40 Coffee & Tea Break	15:40 Coffee & Tea Break							
15:50-17:30		4 parallel sessions	Poster Session Poster Award Review								
		Invited + Oral	Invited + Oral	Invited + Oral			Invited + Oral				
17:30-19:00		Dinner	18:30 Banquet (for all participants, including dinner and Poster Award Announcement)								
19:00-21:00		Free Hours (IAC Meeting)									

## SCIENTIFIC PROGRAM

### Opening & Keynote Session Purple Crystal Palace (1F)

Date	Time	Chair	Name	Affiliation	Title of the Talk
Sep.10	08:30-08:45	<b>Opening</b>			
	08:45-09:15	Xin-Gao Gong	Xian-Hui Chen	University of Science and Technology of China	Superconducting stripes and anisotropic TC in an oxide heterostructure EuO/KTO(110)
	09:15-09:45		Zhen-Yu Zhang	University of Science and Technology of China	Element-mutated ternary systems as topologically nontrivial two-dimensional magnets
	09:45-10:15		Lin-Wang Wang	Institute of Semiconductors, CAS	PWmat: the progress report of a GPU plane wave first principles calculation package
	10:15-10:30	<b>Coffee &amp; Tea Break</b>			
	10:30-11:00	Jian-Hua Zhao	Li-Dong Chen	Shanghai Institute of Ceramics,CAS	Semiconducting chalcogenides: ductility and thermoelectric properties
	11:00-11:30		Gerrit Ernst-Wilhelm Bauer	Tohoku University, Japan	Selected Topics in Magnonics and Ferronics
	11:30-12:00		Young Hee Lee	Sungkyunkwan University	Van der Waals-Layered Magnetic Semiconductors: Diluted Magnetic Semiconductors (DMSs)

# Meeting Room 3 (2F)

Topic: Computational material design and modeling						
Date	Time	Session Chair	Name	Affiliation	Title of the Talk	
Sep.10	14: 00-14: 20	Wanjian Yin	Jing Ma	Nanjing University	Stability Prediction of Gold Nanoclusters with Different Ligands and Doped Metals	
	14: 20-14: 40		Li-Min Liu	Beihang University	The Nature of Excess Electrons and their Effect on the Activity of Reduced Metal Oxides	
	14: 40-15: 00		Xiang-Mei Duan	Ningbo University	Microscopic Mechanisms of Photovoltaic Conversion and Material Design	
	15: 00-15: 20		Xin-Gang Zhao	Northeast Normal University	Screen d-electron ternary oxide memristors based on anti-doping principles	
	15: 20-15: 40		Jun-Jie Wang	Nanjing University	Machine learning accelerated crystal structure prediction of ternary and multinary compounds	
	15: 40-15: 50	Coffee & Tea Break				
	15: 50-16: 10	Lijun Zhang	Zhi-Mei Sun	Beihang University	Accelerating the Discovery and Design of Novel Materials by ALKEMIE	
	16: 10-16: 30		Zhu-Hua Zhang	Nanjing University of Aeronautics and Astronautics	Rich structures and functionalities at interfaces of 2D materials	
	16: 30-16: 50		Lei Shen	National University of Singapore (NUS)	Crystal Structure Relaxation with Machine Learning	
	16: 50-17: 10		Liang Ma	Southeast University	Controllable Nucleation Mechanism and Epitaxy Descriptor of Two-Dimensional Materials	
17: 10-17: 30	Li Huang		Southern University of Science and Technology	Magneto-Optical Properties and Hall Effects with Net Zero Magnetism		
Sep.11	08: 30-08: 50	Jihui Yang	Shi-Xuan Du	Institute of Physics,CAS	Rational Design of Ternary and Multinary Materials with Designed Properties	
	08: 50-09: 10		Xian-Bin Li	Jilin University	Computational Study of Multinary Chalcogenide Semiconductors for Low-Power Phase-Change Memory Applications	
	09: 10-09: 30		Bin Xu	Soochow University	Electric-field control of magnetism in BiFeO3-based multiferroics	
	09: 30-09: 50		Xie Zhang	Northwestern Polytechnical University	Computational screening of multinary compounds for deep-ultraviolet light emitters	
	09: 50-10: 10		Zhi-Xin Guo	Xi'an Jiaotong University	Efficient electrostatic control of 2D magnets in bilayer ternary compounds with enhanced interlayer magnetic coupling and its device application	
	10: 10-10: 20	Coffee & Tea Break				
	10: 20-10: 40	Xie Zhang	Wei-Chao Wang	Nankai University	Mn-based ternary mullites for environmental and energy applications	
	10: 40-11: 00		Bing Huang	Beijing Computational Science Research Center	Manipulation of Nonlinear Optical Properties in Semiconductors	
	11: 00-11: 20		Yi-Yang Sun	Shanghai Institute of Ceramics,CAS	Recent Progress on Studies of Chalcogenide Perovskites as Functional Materials	
	11: 20-11: 40		Jun Kang	Beijing Computational Science Research Center	Effect of site disorder on the defect properties of MgSnN2	
11: 40-12: 00	Tian-Qi Deng(oral)		Zhejiang University	Computational Survey of the Charge Carrier Scattering Mechanisms in Compound Semiconductors		

# Meeting Room 3 (2F)

Topic: Material growth and characterization techniques						
Date	Time	Session Chair	Name	Affiliation	Title of the Talk	
Sep.11	14: 00-14: 20	Bo Sheng	Qian Sun	Suzhou Institute of Nano-Tech and Nano-Bionics, CAS	Ga(Al, In)N-based Light Emitting Devices Grown on Si	
	14: 20-14: 40		Xiao-Juan Sun	Changchun Institute of Optics, Fine Mechanics and Physics, CAS	Growth and defect regulation of non-polar AlN-based materials	
	14: 40-15: 00		Yang Liu	Sun Yat-Sen University	Self-Screening Effect of Polarization Electric Field in bulk Gallium Nitride and its applications	
	15: 00-15: 20		Ping Wang	Peking University	Epitaxial Growth and Characterization of Emerging Sc-III-Nitride Ferroelectrics	
	15: 20-15: 40		Ya-Ping Wu	Xiamen University	Growth of Type-II Hexagonal and Rhombohedral Janus van der Waals Heterostructures with Enhanced Valley Polarization	
	15: 40-15: 50	Coffee & Tea Break				
	15: 50-18: 00	Poster Session				
Sep.12	08: 30-08: 50	Man-Ling Sui	Xue-Lin Yang	Peking University	Atomistic Understanding of Dislocation Climb in Nitride	
	08: 50-09: 10		Sen Huang	Institute of Microelectronics of Chinese Academy of Sciences	Threshold voltage instability in III-nitride heterostructure metal-insulator-semiconductor high-electron-mobility transistors	
	09: 10-09: 30		Ke Wang	Nanjing University	III nitride digital alloys and deep UV LEDs grown by molecular beam epitaxy	
	09: 30-09: 50		Rong-Fu Chen	City University of Hong Kong	3D atom dynamics for multi-component doped helix materials	
	09: 50-10: 10		Jian-Hua Zhao	Institute of Semiconductors, CAS	Molecular-beam epitaxy and optical properties of high-quality ultrathin homogeneous GaAs <sub>1-x</sub> Sb <sub>x</sub> ternary semiconductor nanowires	
	10: 10-10: 20	Coffee & Tea Break				
	10: 20-10: 40	Xue-Lin Yang	Xue-Dong Bai	Institute of Physics, CAS	Surface growth and structural manipulation by in-situ TEM	
	10: 40-11: 00		He Tian	Zhejiang University	In-situ manipulation of ferroelectric domain and domain walls	
	11: 00-11: 20		Rong Yu	Tsinghua University	Direct imaging and positioning interstitial atoms in solids	
	11: 20-11: 40		Jian-Jun Tian	University of Science and Technology Beijing	Colloidal fabrication of high-quality perovskite semiconductors for efficient devices	
11: 40-12: 00	Qi Chen		Beijing Institute of Technology	The heterogeneity in perovskite materials and solar cells		

# Meeting Room 5 (2F)

Topic: Light emitting materials and light manipulation						
Date	Time	Session Chair	Name	Affiliation	Title of the Talk	
Sep.10	14:00-14:20	Zhongming Wei	Ai-Wei Tang	Beijing Jiaotong University	Tunable Luminescence of Narrow-Bandwidth I-III-VI Type Semiconductor Nanocrystals for QLEDs	
	14:20-14:40		Jian-Xin Tang	Macau University of Science and Technology	Synergetic Interface Engineering on Blue Perovskite Light-Emitting Diodes	
	14:40-15:00		Rong-Jun Xie	Xiamen University	Luminescent materials for advanced displays	
	15:00-15:20		Guo-Fa Cai	Henan University	Electrochromic Materials and Multifunctional Large-size Device	
	15:20-15:40		Yang Chai	The Hong Kong Polytechnic University	Bioinspired in-sensor computing for artificial vision	
	15:40-15:50	Coffee & Tea Break				
	15:50-16:10	Ai-Wei Tang	Liang Li	Soochow University	Perovskite Optoelectronic Devices	
	16:10-16:30		Hui Huang	University of Chinese Academy of Sciences	Precise and Scalable Synthesis of Conjugated Polymers	
	16:30-16:50		Hua Li	Shanghai Institute of Microsystem and Information Technology, CAS	GaAs/AlGaAs semiconductor laser based terahertz frequency combs	
	16:50-17:10		Shao-Teng Wu	Institute of Semiconductors, CAS	Research on infrared SiGeSn LED on 12 inches silicon	
17:10-17:30	Yue Zhao(oral)		Harbin Institute of Technology	High Performance All-Inorganic Perovskite Photodetectors and Corresponding Arrays Imaging System		
Sep.11	08:30-08:50	Jian-Wei Wang	Yi-Zheng Jin	Zhejiang University	Device physics and material chemistry of quantum-dot light-emitting diodes	
	08:50-09:10		Zhi-Feng Shi	Zhengzhou University	Lead-free halide perovskites luminescent materials and devices	
	09:10-09:30		Ting Wang	Institute of Physics, CAS	III-V Quantum Dot Comb Laser on Silicon for Integrated Optical I/O	
	09:30-09:50		Xing-Jun Wang	Peking University	Silicon photonics and system	
	09:50-10:10		Han Zhang(oral)	Shanghai Institute of Ceramics, CAS	Exploration of New Chalcogenide Perovskite Materials for Optoelectronic Applications	
	10:10-10:20	Coffee & Tea Break				
	10:20-10:40	Yi-Zheng Jin	Jian-Wei Wang	Peking University	Large-scale integrated quantum photonics	
	10:40-11:00		Xue Bai	Jilin University	Lanthanide based materials and optoelectronic devices	
	11:00-11:20		Jing-Xuan Wei	University of Electronic Science and Technology of China	Novel Polarization-sensitive Photodetectors Based on Photonic-Electronic Nanostructures	
	11:20-11:40		Chang-Xi Zheng	Westlake University	Imaging deep ultraviolet photon-matter interaction using low-temperature quantum electron microscopy	
11:40-12:00	Yu-Qing Sun(oral)		Hebei Normal University	First-principles calculation of effect of Bi doping on magnetic and optical properties of LaFeO <sub>3-x</sub>		



# Meeting Room 5 (2F)

Topic: Complex wide-band-gap materials						
Date	Time	Session Chair	Name	Affiliation	Title of the Talk	
Sep.11	14: 00-14: 20	Xiaodong Pi	Jian-Dong Ye	Nanjing University	An avalanche-and-surge robust NiO/Ga2O3 p-n heterojunction power diode	
	14: 20-14: 40		Xiao Yu	Hangzhou Institute of Technology, Xidian University	Impact of Oxygen Vacancy on Ferroelectric Characteristics and Reliability of Hf0.5Zr0.5O2 (HZO) Thin Films	
	14: 40-15: 00		Wen-Bin Li	Westlake University	Origin of the Unusually High Electrical Conductivity of the Delafossite Metal PdCoO2	
	15: 00-15: 20		Yu-Ning Wu	East China Normal University	Simulations of the irradiation damage of wide-bandgap semiconductors	
	15: 20-15: 40		Xue-Fen Cai	Shenzhen University	Bismuth-alloyed Ga2O3 as a novel p-type transparent conducting oxide	
	15: 40-15: 50	Coffee & Tea Break				
	15: 50-18: 00	Poster Session				
Sep.12	08: 30-08: 50	Jian-Dong Ye	Hong-Lei Wu	Shenzhen University	Impact of different energy level of aluminum nitride on photodetectors	
	08: 50-09: 10		Peng Zhang	Shenzhen University	Theoretical exploration of electrider materials with exotic physical properties	
	09: 10-09: 30		Jin-Song Xia	Huazhong University of Science and Technology	Photonic Devices based on Thin-Film Lithium Niobate	
	09: 30-09: 50		Ya-Dong Xu	Northwestern Polytechnical University	In Pursuit of high resolution CsPbBr3 Gamma-ray Detectors by Optimization of Contact and Configuration	
	09: 50-10: 10		Yan-Jun Fang	Zhejiang University	Suppression of Ion Migration in Halide Perovskites for Sensitivity and Stable X-ray Detectors	
	10: 10-10: 20	Coffee & Tea Break				
	10: 20-10: 40	Peng Zhang	Rong Wang	Zhejiang University	Tailoring the kinetic and electronic properties of dislocations in 4H-SiC by doping	
	10: 40-11: 00		Hong-Liang Zhang	Xiamen University	The electronic structure and band alignment (AlxGa1-x)2O3/Ga2O3 heterojunctions	
	11: 00-11: 20		Liang Wu	Hangzhou Dianzi University	Progress and device prospects on bulk AlN crystal growth by PVT method	
	11: 20-11: 40		Jing-Xiu Yang	Jilin Jianzhu University	Manipulation of Band Structure and Defect Properties in Semiconductor Materials	
11: 40-12: 00	Hai-Wen Dai		Nanyang Technological University	Advancing Data-Driven Inorganic Materials Discovery: Insights from a Successful Case and Challenges Posed by Disordered Structures		

# Meeting Room 6 (2F)

Topic: Photocatalysis, thermoelectrics, and energy storage						
Date	Time	Session Chair	Name	Affiliation	Title of the Talk	
Sep.10	14: 00-14: 20	Wenqing Zhang	Yuan-Hua Lin	Tsinghua University	High performance dielectric capacitors	
	14: 20-14: 40		Ping Wei	Wuhan University of Technology	Optimal design and performance evaluation of stable interfacial barrier layer for Bi <sub>2</sub> Te <sub>3</sub> -based thermoelectric devices	
	14: 40-15: 00		Yuan Deng	BeiHang University	Multifield-Induced Fabrication Techniques for Bi <sub>2</sub> Te <sub>3</sub> -Based Thermoelectric Thick Films and Microdevices for Innovative Applications	
	15: 00-15: 20		Li-Wen Sang	Fudan University	Homoepitaxial growth of p-GaN for pMOS capacitors	
	15: 20-15: 40		Bao-Ying Dou(oral)	Henan University	Nonradiative Recombination in Cu(In,Ga)Se <sub>2</sub> Alloys	
	15: 40-15: 50	Coffee & Tea Break				
	15: 50-16: 10	Xun Shi	Chen-Guang Fu	Zhejiang University	Topological Heusler magnets for transverse thermoelectric	
	16: 10-16: 30		Tian-Ran Wei	Shanghai Jiao Tong University	Superior plasticity and thermoelectric performance of Ag <sub>2</sub> S-Ag <sub>2</sub> Se-Ag <sub>2</sub> Te multinary materials	
	16: 30-16: 50		Qian Zhang	Harbin Institute of Technology,Shenzhen	High performance Mg <sub>3</sub> (Bi,Sb) <sub>2</sub> -based thermoelectric generators	
	16: 50-17: 10		Pan Xiong	Nanjing University of Science & Technology	Confined Ion Transport in Two-Dimensional Materials and High-Efficiency Energy Utilization	
	17: 10-17: 30		Qian-Hui Lou(oral)	Zhejiang University	High Defect Tolerance in Heavy-band Thermoelectrics	
Sep.11	08: 30-08: 50	Wu Li	Li-Ming Yang	Huazhong University of Science and Technology	The electronic structure, magnetism, and it's strain modulation on A <sub>3</sub> BX <sub>2</sub> compounds	
	08: 50-09: 10		Jia Li	Tsinghua Shenzhen International Graduate School	Molecular Understanding of the Critical Role of Solid-Liquid Interface on Electrocatalysis	
	09: 10-09: 30		Jia-Zhen Wu	Southern University of Science and Technology	Ru/Si 2D superlattice for alkaline hydrogen evolution reaction	
	09: 30-09: 50		Jian-Ping Xiao	Dalian University of Chemical Physics,CAS	Computational Catalyst Design Based on Energetic Descriptors and Reaction Phase Diagram Analysis Accelerated by Machine Learning	
	09: 50-10: 10		Xiang-Yue Meng(oral)	University of Chinese Academy of Sciences	Lead free perovskite solar cells	
	10: 10-10: 20	Coffee & Tea Break				
	10: 20-10: 40	Li-Ming Yang	Si-Qi Shi	Shanghai University	Design and Discovery of Novel Battery Materials	
	10: 40-11: 00		Hua-Bin Zhang	KAUST Catalysis Center	Stories about single atom catalysis	
	11: 00-11: 20		Li-Dong Zhao	BeiHang University	Advanced thermoelectric cooling materials	
	11: 20-11: 40		Wan-Jian Yin	Soochow University	Expanding Multinary Oxide Perovskites for High-Performance Catalysts by Symbolic Regression	
	11: 40-12: 00		Li-Rong Hu(oral)	Zhejiang University	p-type Dopability in Half-Heusler Thermoelectric Semiconductors	

# Meeting Room 6 (2F)

Topic: Photovoltaic materials and applications					
Date	Time	Session Chair	Name	Affiliation	Title of the Talk
Sep.11	14: 00-14: 20	Shiyu Chen	Yi Zhang	Nankai University	Qualified Absorber Layer Growth to Attain High Efficient Chalcogenide Thin Film Solar Cells
	14: 20-14: 40		Da-Long Zhong	National Institute of Clean-and-Low-Carbon Energy	Thin-Film Photovoltaic Technology Advancements and Industrialization Challenges: Sphalerite, Chalcopyrite, and Perovskite
	14: 40-15: 00		Si-Xin Wu	Henan University	Defect engineering of kesterite photovoltaics
	15: 00-15: 20		Fang-Yang Liu	Central South University	Bulk and Interface Modification for Copper-Zinc-Tin-Sulfide-Selenide Photovoltaic Thin Films
	15: 20-15: 40		Jian-Jun Li	Institute of Metal Research,CAS	Microscopic carrier loss mechanisms in kesterite Cu <sub>2</sub> ZnSn(S,Se) <sub>4</sub> thin film solar cells
	15: 40-15: 50	Coffee & Tea Break			
	15: 50-18: 00	Poster Session			
Sep.12	08: 30-08: 50	Jingbi You	Sheng-Zhong Liu	Dalian University of Chemical Physics,CAS	Perovskite – a wonder material for solar cells
	08: 50-09: 10		Yi-Xin Zhao	Shanghai Jiao Tong University	Low dimensional perovskite and surface termination to passivate and stabilize perovskite photovoltaics.
	09: 10-09: 30		Qing Zhao	Peking University	Ion transport in micro-nano structures and related device applications
	09: 30-09: 50		Meng-Lin Huang	Fudan University	Defect correlation reveals critical defects in low-symmetry materials
	09: 50-10: 10		Biao Zeng (oral)	Shanghai Institute of Ceramics, CAS	CVD Synthesis of Millimeter-Scale BiSCl Nanorods and Bandgap Tuning via Structural Arrangement
	10: 10-10: 20	Coffee & Tea Break			
	10: 20-10: 40	Yixin Zhao	Ping-Qi Gao	Sun Yat-Sen University	Indium-saving transparent electrode towards sustainable development of silicon heterojunction solar cells
10: 40-11: 00	Jun-Liang Yang		Central South University	Printing Organic and Perovskite Solar Cells and their Modules	
11: 00-11: 20	Wei-Min Li		Shenzhen Institute of Advanced Technology, CAS	Over 20%-efficiency flexible and bending durable CIGS solar cell on stainless steel substrate through diffusion barrier insertion	
11: 20-11: 40	Zai-Xing Yang		Shandong University	Low-dimensional antimonide and optoelectronic devices	
11: 40-12: 00	Ying Li		Beijing Institute of Technology	Study on Bionic Visual Sensors Based on Lead-free Perovskite Materials	

# Meeting Room 9 (2F)

Topic: Spintronic, multiferroic, and other magnetic compounds						
Date	Time	Session Chair	Name	Affiliation	Title of the Talk	
Sep.10	14: 00-14: 20	Pu Yu	Maciej Sawicki	Maciej Sawicki	Towards Electric-Field Manipulation of Magnetization in Insulating Dilute Ferromagnets	
	14: 20-14: 40		"Nguyen Duy KHANH"	Institute for Solid State Physics (ISSP), The University of Tokyo, Chiba, Japan	Topological transport behavior in intercalated van der Waals antiferromagnets	
	14: 40-15: 00		Yong-Bing Xu	Nanjing University	Manipulation of spin ordering in 2D magnets	
	15: 00-15: 20		Chun-Gang Duan	East China Normal University	Ternary and multinary ferrovalley materials	
	15: 20-15: 40		Jin-Xing Zhang	Beijing Normal University	Artificial Symmetry Design for Magnetoelectric Phase Transition	
	15: 40-15: 50	Coffee & Tea Break				
	15: 50-16: 10	Chun-Gang Duan	Jin-Bo Yang	Peking University	Development of Iron-rich Rare-earth permanent magnetic materials	
	16: 10-16: 30		Hong-Jun Xiang	Fudan University	Property analysis and simulation package for materials (PASP) and its applications to magnetic and ferroelectric materials	
	16: 30-16: 50		Shuai Dong	Southeast University	Alterferroicity	
	16: 50-17: 10		Pu Yu	Tsinghua University	A correlated ferromagnetic polar metal by design	
17: 10-17: 30	You-Wen Long		Institute of Physics,CAS	Charge and spin states of PbFeO3 and PbCoO3 prepared under high pressure		
Sep.11	08: 30-08: 50	Chang-Song Xu	Chang-Qing Jin	Institute of Physics,CAS	New Spintronic Materials: Design , Synthesis & Characterizations	
	08: 50-09: 10		Ning Tang	Peking University	Spin properties of the two-dimensional electron gas in GaN-based heterostructures	
	09: 10-09: 30		Gang Xiang	Sichuan University	Transition Metal-doped Gallium Oxide Magnetic Semiconductor Thin Films: Fabrication, Characterizations and Potential Application in Magnetic Memristors	
	09: 30-09: 50		Zhi-Min Liao	Peking University	Control over Berry curvature dipole and orbital magnetic moments	
	09: 50-10: 10		Jian Zhou	Xi'an Jiaotong University	Neel vector tuning hidden bulk photocurrent generation in Mn-based ternary antiferromagnets	
	10: 10-10: 20	Coffee & Tea Break				
	10: 20-10: 40	Chang-Qing Jin	Tian-Xiang Nan	Tsinghua University	Control of magnon spin transport in antiferromagnetic and multiferroic materials	
	10: 40-11: 00		Yu-Rong Yang	Nanjing University	External field effects of ferroelectrics from first principles	
	11: 00-11: 20		Chang-Song Xu	Fudan University	Fractional Quantum Ferroelectricity	
	11: 20-11: 40		Zhi-Qi Liu	BeiHang University	High-temperature ferromagnetism in ternary oxide La2CoO4±x thin films and its electrochemical applications	
11: 40-12: 00	Da-Hai Wei		Institute of Semiconductors, CAS	Progresses of room temperature magnetic semiconductors based on Antimonides and Germanide		

# Meeting Room 9 (2F)

Topic: Miscellaneous						
Date	Time	Session Chair	Name	Affiliation	Title of the Talk	
Sep.11	14: 00-14: 20	Huixiong Deng	Hang-Hui Chen	NYU Shanghai	A first-principles study of nickelate superconductors	
	14: 20-14: 40		Liang Qiao	University of Electronic Science and Technology of China	Critical Role of H for Superconductivity in Infinite-layer Nickelates	
	14: 40-15: 00		Xin Yang	Center for High Pressure Science&Technology Advanved Research	Theoretical Design of High-temperature Superconductivity in Metal Borides	
	15: 00-15: 20		Zhe-Shuai Lin	Technical Institute of Physics and Chemistry,CAS	Isotropic Zero Thermal Expansion and Good Optical Transparence in Sodalite Framework Crystals	
	15: 20-15: 40		Jun-Yi Zhu	The Chinese University of Hong Kong	Revised Electron counting models based on six-fold coordination and layers and its application in the phase change in transition metal oxides	
	15: 40-15: 50	Coffee & Tea Break				
	15: 50-18: 00	Poster Session				
Sep.12	08: 30-08: 50	Bing Huang	Wei Ji	Renmin University of China	Coexistence of ferromagnetism and ferroelectricity in van der Waals bilayers	
	08: 50-09: 10		Yi Du	BeiHang University	2D Frustrated Materials with Exotic Electronic Flat Bands	
	09: 10-09: 30		Song Li	Winger physics Center	Quantum Emission from Coupled Spin Pairs in hBN	
	09: 30-09: 50		Shi Liu	Westlake University	Understand Ferroelectrics with Universal Force Field	
	09: 50-10: 10		Bo-Nan Zhu	Beijing Institute of Technology	Exploring earth-abundant Li-ion cathode materials using random structure searching	
	10: 10-10: 20	Coffee & Tea Break				
	10: 20-10: 40	Wei Ji	Jun Di	Nanjing University of Science & Technology	2D atomic layer for photocatalytic CO2 reduction	
	10: 40-11: 00		Li-Hui Song	Zhejiang University	Research on the Irradiation Effects of Silicon Carbide	
	11: 00-11: 20		Chen Zhang	Institute of Semiconductors, CAS	Theoretical understanding of correlation between magnetic phase transition and the superconducting dome in high-Tc cuprates	
	11: 20-11: 40		Gao-Feng Teng(oral)	Beijing Computational Science Research Center	"Origin of the contrasting magnetic stability of antiferromagnetic CuMnAs and CuMnSb"	
11: 40-12: 00	Han-Pu Liang(oral)		Beijing Computational Science Research Center	Critical Role of Configurational Disorder in Stabilizing Chemically Unfavorable Coordination in Complex Compounds		

## Keynote Session & Closing Purple Crystal Palace (1F)

Date	Time	Chair	Name	Affiliation	Title of the Talk
Sep.13	08:30-09:00	Jun-Wei Luo	Hideo Hosono	Tokyo Institute of Technology, Japan	Recent Advances in Materials and Application of Electrides
	09:00-09:30		Feng-Qi Liu	Institute of Semiconductors, CAS	Realization of Quantum Dot Cascade Laser Structure
	09:30-10:00		Yong Zhang	University of North Carolina at Charlotte	II-VI based organic-inorganic hybrid superlattices: structure, stability, and properties
	10:00-10:15	<b>Coffee &amp; Tea Break</b>			
	10:15-10:45	Su-Huai Wei	David Cahen	Weizmann Institute	Structural Disorder in Photovoltaic Materials
	10:45-11:15		Qing-Bo Meng	Institute of Physics,CAS	The Pathway to >15% Efficiency Emerging Kesterite Solar Cells
	11:15-11:45		Mikhail Otrokov	Institute of Nanoscience and Materials of Aragon in Zaragoza (Spain)	Intrinsic Magnetic Topological Insulators of the MnBi <sub>2</sub> Te <sub>4</sub> Family
	11:45	<b>Closing</b>			

## KEYNOTE SPEAKER BIOGRAPHIES & ABSTRACTS



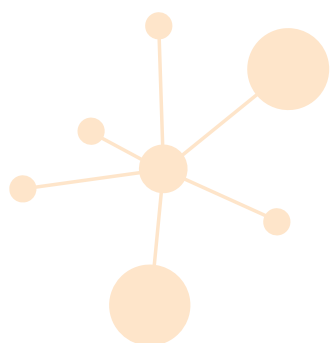
### Xian-Hui Chen

University of Science and Technology of China

Professor Xianhui Chen obtained his doctorate degree from University of Science and Technology of China (USTC) in 1992. Now he is a distinguished professor at USTC, an academician of the Chinese Academy of Sciences. His research interests focus on the exploration of novel superconducting, strong electron-correlated and topological quantum materials and the related physics therein. Professor Xianhui Chen has published more than 500 SCI papers. He won the First Prize of State Natural Science Award in 2013, the Bernd T. Matthias Prize in Superconducting Materials in 2015, the Ho Leung Ho Lee Foundation Physics Prize in 2017, the TWAS Prize in Physics in 2019 and the Future Science Prize Physical Science Prize in 2023, etc..

### **Superconducting stripes and anisotropic TC in an oxide heterostructure EuO/KTO (110)**

University of Science and Technology of China  
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#### **Abstract:**

In this talk I will introduce our recent progress on the study of the interface between high-quality EuO (111) thin film and KTO (110) substrate. Both oxides are insulating, yet the interface is metallic and shows superconductivity with onset transition temperature  $T_{\text{onset } c} = 0.6\text{-}1.4$  K depending on the carrier density. The 2D nature of superconductivity is verified by the large anisotropy of the upper critical field and the characteristics of a BKT transition. By applying gate voltages,  $T_{\text{onset } c}$  can be largely tuned with an enhancement of  $\sim 70\%$ ; such an enhancement can be possibly associated with a boosted spin-orbit coupling (SOC) energy. Further analysis based on the upper critical field ( $H_{c2}$ ) and magnetoconductance reveals complex nature of SOC at the EuO/KTO (110) interface with different dominant scattering mechanisms in the superconducting and normal states. Our results demonstrate that the SOC should be considered an important factor in determining the 2D superconductivity at oxide interfaces.



## Zhen-Yu Zhang

University of Science and Technology of China

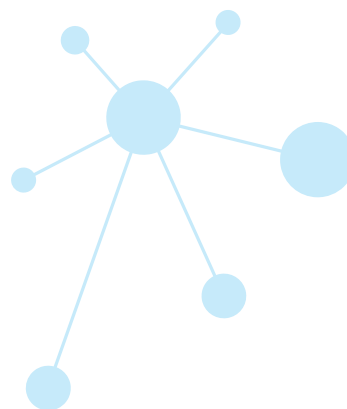
Prof. Zhang received his B.S. degree from Wuhan University in 1982 and PhD degree from Rutgers University in 1989, both in physics. He was a Distinguished Research Scientist at Oak Ridge National Laboratory and Chair of Excellence Professor of Physics at the University of Tennessee, USA before joining the University of Science and Technology of China (USTC) in January 2011. He is now a Distinguished Chair and Yan Jici Professor of Physics at USTC and serves as co-founding Director of the International Center for Quantum Design of Functional Materials (ICQD), USTC. His research interests lie in the fields of theoretical understanding of the formation, stability, properties, and potential applications of low-dimensional materials that exhibit global or macroscopic quantum properties. He has authored/coauthored over 300 peer-reviewed papers, and has disseminated the research findings in over 300 invited/keynote/plenary talks and lectures. He is a fellow of the American Physical Society, and has served or currently serves on the editorial boards of several professional journals.

### **Element-mutated ternary systems as topologically nontrivial two-dimensional magnets**

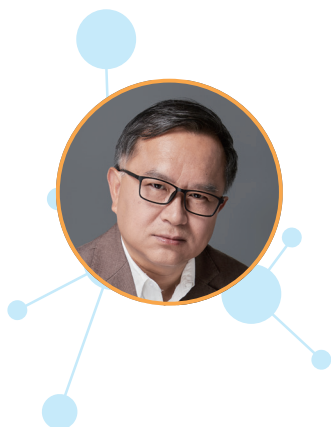
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In this talk, I will present results from our recent theoretical and experimental studies of two-dimensional magnets, focusing on how to convert topologically trivial binary systems into ternary materials with electronically and magnetically nontrivial properties via proper element mutation.







## Lin-Wang Wang

Institute of Semiconductors, CAS

Lin-Wang Wang graduated from Shanghai Jiao Tong University in 1985 and graduated from Cornell University in the United States in 1991 with a doctorate in science. From 1992 to 1999, he worked at the U.S. Renewable Energy Laboratory, holding postdoctoral and researcher positions respectively. From 1999 to 2021, he worked at the Lawrence Berkeley National Laboratory in the United States as a researcher and senior researcher. From 2022 to present, he serves as a researcher at the Institute of Semiconductors, Chinese Academy of Sciences. Dr. Wang is mainly engaged in algorithm research for large-scale material calculations. He has achieved a number of original research results with important international influence in semiconductor low-dimensional structures, computational materials science, and energy materials science. He has developed more than ten algorithms and material calculation and device simulation programs, including PEtot, Escan, LCBB, LS3DF, etc. He was elected as the American Physical Society Fellow (APS Fellow) in 2006 and has been provided the international high-performance computing Gordon Bell Award. Dr. Wang has published more than 400 SCI papers, including 10 Science and Nature papers, and more than 80 PRL, JACS and NanoLett level papers. The total number of citations of his paper is more than 40,000 times, and the H-index is 100. He is one of the original developers of the now commercialized PWmat code.



### **PWmat: the progress report of a GPU plane wave first principles calculation package**

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PWmat is a GPU plane wave pseudopotential first principles calculation package. After ten year's development, it has acquired many different features. Now, besides plane wave basis, it also has Gaussian basis, as well as the semi-empirical DFTB method. Besides the usual ab initio molecular dynamics, it can also perform real time time-dependent density functional method calculations. It has the nonequilibrium Green's function method for quantum transport. For larger than 10,000 atom systems, it has the O(N) method and charge patching method for nanostructure calculations. Its fixed potential calculation is popular for electric chemistry study. The PWmat has been implemented in GPU, CPU, DCU and window operation systems. In this talk, I will review these progresses in PWmat, let the audience know its current capabilities and our future plan.




### Li-Dong Chen

Shanghai Institute of Ceramics, CAS

Prof. Lidong Chen received his doctor degree in Materials Science from Tohoku University in 1990. After being chief engineer at Riken Cooperation and postdoctoral appointment at Japan National Aerospace Laboratory, he had worked at the Institute for Materials Research, Tohoku University, as research associate and associate professor. He joined Shanghai Institute of Ceramics, Chinese Academy of Sciences as professor in 2001. Prof. L.D. Chen has published over 300 authored or co-authored papers in the area of thermoelectrics. Currently he serves as Co-Editor-in-Chief of npj Computational Materials. He was elected as a member of Chinese Academy of Sciences (Academician) in 2023.

#### **Semiconducting chalcogenides: ductility and thermoelectric properties**

State Key Laboratory of High Performance Ceramics and Superfine Microstructure,  
Shanghai Institute of Ceramics, CAS, Shanghai 200050, China  
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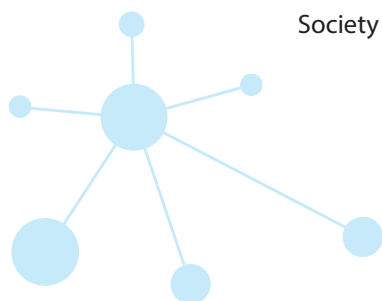
Flexible thermoelectrics provides a different solution for developing portable and sustainable flexible power supplies. The discovery of Ag<sub>2</sub>S-based ductile semiconductors has driven a shift in the potential for flexible thermoelectrics, while it is still a big challenge to develop ductile materials with high thermoelectric performance. We have put our efforts on the synergistic modulation of thermoelectric properties and ductility of Ag<sub>2</sub>S-based chalcogenides. By partially substituting S with Se and/or Te, a series of n-type thermoelectric materials with relatively good ductility have been developed. Furthermore, based on systematic study on the composition-performance phase diagram in AgCu(Se,S,Te) pseudo-ternary solid solutions, a series of high-performance p-type ductile thermoelectric materials have been discovered. The maximum zT values in both n- and p-type ductile materials reach at >0.6 at room temperature. Ring-shape TE devices and flexible TE devices are further fabricated demonstrating great potentials for the applications in flexible electronics.



## Gerrit Ernst-Wilhelm Bauer

Tohoku University, Japan

Gerrit Ernst-Wilhelm Bauer (1956) holds an Engineering Degree (1980) in Chemical Technology from Twente University (The Netherlands) and Doctor Degree in Physics (1984) from the Technical University Berlin (Germany) for research carried out at the Hahn-Meitner-Institute of Nuclear Research. After a Feodor Lunen/JSPS postdoc at the Institute for Solid State Physics of the University of Tokyo (1984-86), he was a member of the Scientific Staff of the Philips Research Laboratories (1986-92), Professor of Physics at the Delft University of Technology 1992-2022 (part-time since 2011), Professor at the Institute for Materials Research of Tohoku University 2011-2022, and part-time Professor at Groningen University 2018-2022. Since 2021 he is a Professor at the Advanced Institute for Materials Research (AIMR) of the World Premier International Research Centers Initiative (WPI) at Tohoku University and since 2022 jointly appointed as Chair Professor at the Kavli Institute of Theoretical Sciences (KITS) of the University of the Chinese Academy of Sciences, Beijing, China. He received the Wilhelm-Conrad-Röntgen Award from Würzburg University (2000), the Outstanding Referee Award by the American Physical Society (2008), and the Lars Onsager Medal from the Norwegian University of Science and Technology (2009). He became Fellow of the American Physical Society in 2010, Distinguished Lecturer of the IEEE Magnetics Society in 2012, Fellow of the Japan Society for Applied Physics 2022, and Humboldt Research Awardee in 2023.



### Selected Topics in Magnonics and Ferronics

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The duality between electric and magnetic dipoles in electromagnetism only partly applies to condensed matter. In particular, the elementary excitations of the magnetic and ferroelectric orders, namely magnons and ferrons, differ in many respects. I will compare the basic physics underlying the advanced field of “magnonics” with that of the emerging field of “ferronics”<sup>[1]</sup> and share recent insights.

### Reference:

[1] G.E.W. Bauer, P. Tang, R. Iguchi, J. Xiao, K. Shen, Z. Zhong, T. Yu, S.M. Rezende, J.P. Heremans, and K. Uchida, Perspective: Polarization transport in ferroelectrics, *Phys. Rev. Appl.* 20, 050501 (2023).





### Young Hee Lee

Sungkyunkwan University

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. Currently, he is the Director of Center for Integrated Nanostructure Physics, Institute for Basic Science at SKKU. He serves for an Associate Editor of ACS Nano. Prof. Lee's work has focused on understanding the fundamental properties of nanostructures in 0D, 1D, 2D and their hybrid heterostructures, design and synthesis of various heterostructures to implement unique physical and chemical properties. His research covers carrier dynamics, carrier multiplication phenomena, hot carrier solar cell, thermoelectrics, quantum mechanical tunneling phenomena, and nanocarbon-based soft electronics. His pioneering works on synthesis and engineering of electronic and atomic structures of carbon nanotubes and graphene, other 2D materials and their applications to electronic devices, and energy harvesting have led not only nanoscience but also nanotechnology industry in Korea. He has published more than 659 scientific papers in international journals and his total citation number exceeds over 80,000 times with H-index of 134 (Google Scholar, Mar. 2024).

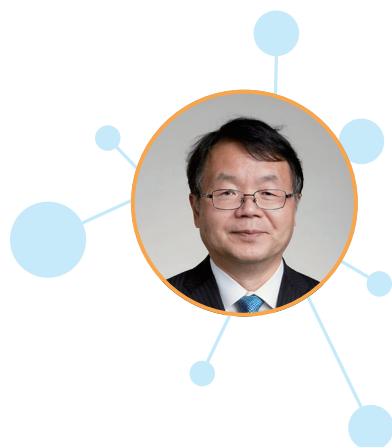


#### **Van der Waals-Layered Magnetic Semiconductors: Diluted Magnetic Semiconductors (DMSs)**

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Ferromagnetism in van der Waals two-dimensional (2D) materials has been reported recently. Intrinsic CrI<sub>3</sub> and CrGeTe<sub>3</sub> semiconductors reveal ferromagnetism but the T<sub>c</sub> is still low below 60K. In contrast, monolayer VSe<sub>2</sub> is ferromagnetic metal with T<sub>c</sub> above room temperature but incapable of controlling its switching via gating due to metallic nature. Moreover, the long-range ferromagnetic order in diluted metal chalcogenide semiconductors has not been demonstrated at room temperature. The key research target is to realize the long-range order ferromagnetism, T<sub>c</sub> over room temperature, and semiconductor with gate tunability. In this talk, we introduce magnetic dopant, vanadium in semiconducting WSe<sub>2</sub> and manifest T<sub>c</sub> at room temperature and gate tunability at low doping concentration. We further explore different doping concentrations including highly degenerate regime and demonstrate unconventional magnetic order by random telegraph spin noises via interlayer coupling and more recent progresses.



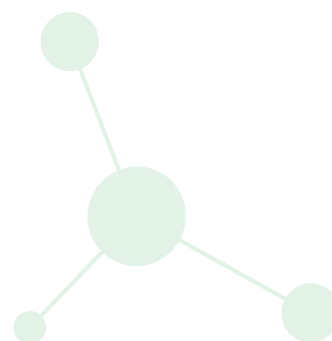


### Hideo Hosono

Tokyo Institute of Technology, Japan

Hideo Hosono is an institute professor and the founding director of Materials Research Center for Element Strategy at Tokyo Institute of Technology and a concurrent distinguished fellow and a group lead at NIMS. He received his Ph.D at 1982 in Applied Chemistry from Tokyo Metropolitan University, and became a Professor of Tokyo Tech in 1999. Dr. Hosono proposed a design concept for transparent amorphous oxide semiconductors (TAOSs) with large electron mobility in 1996 and reported c- and a-IGZO (InGaZnOx)-thin film transistors in 2003 -2004. IGZO-TFTs are now used in the state of the art displays to drive them. In 2008 his group discovered an Iron-pnictide high-Tc superconductor. The paper reporting this discovery was ranked as the most cited paper among all papers published in 2008 and chosen as the breakthrough of the year 2008 by the Science Magazine. He is a pioneer of RT stable electrified materials and their applications including catalyst for ammonia synthesis under mild conditions. He has received international awards including the Japan Prize, Von Hippel Prize (MRS), J.C.McGroddy Prize(APS), Jan Raychman Prize(SID), B.T.Matthias Prize and Thomson Reuters Citation Laureate in Physics. He is a foreign member of the Royal Society(London). His major concern is design and exploration of electro-active materials (semiconductors, superconductors and catalysis).

### Recent Advances in Materials and Application of Electrifieds





### Feng-Qi Liu

Institute of Semiconductors, CAS

Feng-Qi Liu received the Ph.D. degree in condensed matter physics from Nanjing University, Nanjing, China, in 1996. Since then, he joined Institute of Semiconductors, Chinese Academy of Sciences, where his work has concentrated on the MBE growth and fabrication of high-performance mid-infrared and terahertz quantum cascade lasers (QCLs). He received the National Natural Science Foundation for Distinguished Young Scholars in 2005, and the New Century National Hundred, Thousand and Ten Thousand Talent Project in 2007. He developed a series of room temperature (RT) operated high-performance QCLs with emitting wavelength in the range of 3.5–16 microns, innovated the first quantum dot cascade lasers by two-step strain compensation active region design, developed high power terahertz QCLs with emitting frequencies between 2.95–5.4 THz, developed a series of quantum dot cascade detectors with very low dark current and background noises, high operating temperature, and high detectivities.

#### Realization of Quantum Dot Cascade Laser Structure

Feng-Qi Liu<sup>\*1,2</sup>, Ning Zhuo<sup>1</sup> and Jin-Chuan Zhang<sup>1</sup>

1 Key Laboratory of Semiconductor Materials Science, Institute of Semiconductors,  
Chinese Academy of Sciences, 100083, Beijing, China

2 College of Materials Science and Opto-Electronic Technology, University of Chinese  
Academy of Sciences, Beijing 100049, China

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Mid-infrared quantum cascade lasers (QCLs) have experienced tremendous improvement in terms of output power and efficiency in the past years. Wavelength tunable QCLs have found various applications, such as air-pollution, industrial-discharge, and toxicant detection. In these application scenarios, high efficiency of QCL is a basic requirement. Due to the essence of the extremely short non-radiative lifetimes commonly associated with the intersubband transitions in the quantum wells, the room temperature wall plug efficiency of QCL is no more than 30%. Quantum dot cascade laser (QDCL), in which quantum well active region is replaced by quantum-dot active region, is predicted as high wallplug efficiency and broad tunability. However, the design and growth of QDCLs is extremely difficult. In this talk we demonstrate the development of QDCLs by two-step strain-compensation active region design and material growth technique. The QDCLs based on three-layer QDs active region, two-layer QDs active region, and single-layer QD active region have been exploited. The QDCL with structure based on two-layer QD active region presents room temperature continuous wave lasing at wavelength of around 7 $\mu$ m, proving a feasible route for developing QDCLs.



## Yong Zhang

University of North Carolina at Charlotte

Yong Zhang is the Bissell Distinguished Professor in the Department of Electrical and Computer Engineering at The University of North Carolina at Char. He earned his B.S. and M.S. degrees in Physics from Xiamen University, followed by a Ph.D. in Physics from Dartmouth College. Prior to joining UNC-Charlotte in 2009, Dr. Zhang served as a Senior Scientist at National Renewable Energy Laboratory (NREL). His research spans electronic and optical properties of semiconductors and related nanostructures, organic-inorganic hybrid materials, impurity and defects in semiconductors, and innovative materials and device architectures for applications in optoelectronics, energy, and electronic-photonic integrated circuits. He has over 270 publications, 6 patents, and more than 10,600 citations. He is a Fellow of American Physical Society.

### II-VI based organic-inorganic hybrid superlattices: structure, stability, and properties

The University of North Carolina at Charlotte

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A group of organic-inorganic hybrid nanostructures, for instance,  $\text{ZnTe}(\text{ML})_{0.5}$ , where  $\text{ML} = \text{C}_n\text{N}_2\text{H}_{2n+4}$  ( $n = 0, 2-4$ ), have been shown to exhibit nearly perfect crystal structures, manifesting as high crystallinity comparable to that of a typical high quality III-V or II-VI binary and better than any known semiconductor superlattices. For instance,  $\beta\text{-ZnTe}(\text{C}_2\text{N}_2\text{H}_8)_{0.5}$ , as shown in the graph, has a 20-30" XRD rocking-curve linewidth, below 1  $\text{cm}^{-1}$  low-temperature Raman linewidth, and band-edge free exciton emission ( $\sim 3.56$  eV) without below-bandgap emission. More interestingly, it offers various highly desirable properties, e.g., room temperature excitonic emission due to a large exciton binding energy estimated to be around 300 meV, strongly enhanced optical absorption as high as 106  $\text{cm}^{-1}$ , close to 100% internal quantum efficiency in room-temperature photoluminescence, zero-thermal expansion over a broad temperature range, and much reduced density and dielectric constants. Uniquely, it is the only hybrid that exhibits an over-15-year shelf life, benefiting from a relatively large formation energy and kinetic barrier. On the one hand, it offers a new approach to form perfect heterostructures beyond the conventional wisdom of requiring lattice match; on the other hand, the novel properties suggest many potential applications, such as room-temperature exciton-polariton condensation, efficient UV emission and detection, transparent p-type conductive material. It serves as unique platform to explore a number of basic topics of solid-state physics.



## David Cahen

Weizmann Institute

David Cahen was born and raised in the Netherlands. After high school he moved to Israel, where he studied chemistry & physics at the Hebrew Univ. of Jerusalem (HUJI; B.Sc.). He continued then to a materials research Ph.D. at Northwestern, including a half year winter break at Stanford. He returned to Israel for his PD in biophysics (of photosynthesis) at the HUJI and the Weizmann Inst. of Science (WIS). He joined the WIS faculty in 1976, working on photoelectrochemical solar cells, including such cells with built-in storage. Nowadays he focusses on opto(bio)electronic materials chemistry & physics, emphasizing what can make such materials sustainable, which explains his interest in self-healing of materials, and, quite distinctly, proteins as (opto)electronic materials. An AVS, MRS and Helmholtz Int'l fellow and visiting prof at Chiba Univ., he is also active in energy & sustainability (E&S) research (founder and 1st director of WIS' integrated effort in the field) and education (organizes and teaches local and int'l courses; co-edited and wrote textbook on Materials for E&S), and in science for peace efforts. From 2017-2022 he headed a group at near-by Bar-Ilan Univ.

### Structural Disorder in Photovoltaic Materials

Weizmann Institute of Science, Rehovot Israel

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With few exceptions today's leading PV materials appear to thrive on structural disorder, static and/or dynamic. Exceptions are Si, Ge, GaAs and InP, leaving ternary and multinary PV compounds with disorder. Dynamic disorder came to the fore with the Pb-halide perovskites (HaPs), where it explains some amazing optoelectronic properties, critical for PV, LED and detectors. Two phenomena that are used to explain these properties, viz. self-healing and defect tolerance, involve lattice dynamics. Both can be traced to early work on chalcopyrites!

Static disorder in the most successful HaP for PV, has been less in the limelight but is prevalent in the preferred (A<sub>1</sub>A<sub>2</sub>A<sub>3</sub>) Pb (X<sub>1</sub>X<sub>2</sub>)<sub>3</sub> composition. Here HaPs resemble other PV materials: static disorder is more the rule than the exception for compound semiconductors (to be) used in commercial PV cells. Dynamic disorder may also be relevant for organics in OPV and Cu<sup>+</sup> mobility introduces some dynamics in CIGS.

Static disorder can be a given as for kesterites, Cu<sub>2</sub>ZnSnS<sub>4</sub>, amorphous silicon, a-Si: H, and on the multi-material level, dye-sensitized cells. In others, though, it entered gradually, via optimization efforts, mostly of the optical bandgap or the stability of the materials.

I will illustrate this thesis with examples and give simple explanations for the power of dynamic disorder.





### Qing-Bo Meng

Institute of Physics, CAS

Qingbo Meng is currently a full professor at Institute of Physics (IOP), Chinese Academy of Sciences (CAS), Director of Center for Clean Energy, IOP, and a director member of Chinese Renewable Energy Society. He received his PhD degree in 1997 from Changchun Institute of Applied Chemistry, CAS. From 1997 to 1999, he was a postdoctoral fellow in IOP. From 1999 to 2002, he was a STA Fellow and Researcher of the University of Tokyo and KAST in Japan. He obtained "Distinguished Young Scholar Fund" from NSFC in 2007 and was selected as the project leader of the Fund for Creative Research Groups of China in 2014. He was awarded to "the Special Allowance of the State Council" in 2010 and "The president Award of the Tokyo University Science" in 2011. His current research interest focuses on solar energy materials & devices, including new generation thin film solar cells (such as perovskite solar cells, Kesterite solar cells) and artificial photosynthesis. He has published over 300 papers, which were cited about 18000 times (h-index 80). He has authorized over 80 patents, and over 15 of them have been transferred to industry.

#### The Pathway to >15% Efficiency Emerging Kesterite Solar Cells

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#### Abstract:

We have conducted systematical investigations into the charge dynamics in CZTSSe solar cells and found that the charge loss in this device mainly lies in the bulk nonradiative recombination arising from the deep electronic defects and microstructural distortions.<sup>1</sup> This finding has guided us to introduce a series of regulations on metal-molecular coordination in environment-friendly aqueous solution system, film growth mode, and crystal growth kinetics of CZTSSe to improve the film microstructure and phase evolutions.<sup>2-5</sup> Especially, we have explored three routes to control the reaction kinetics of the CZTSSe selenization.<sup>4-6</sup> In route 1, we introduced high environment pressure in the selenization chamber, which could delay the Se volatilization and dilute the Se vapor on the surface region of the precursor film. This would subsequently decrease the reaction activity between the Se and the metal elements in the film and thus could suppress the rapid formation of binary or ternary secondary phases. In route 2, we developed a dual-zone selenization strategy and introduced a solid-liquid/solid-vapor synergistic selenization approach. We firstly pre-deposited liquid Se onto the surface of the precursor film. The liquid Se could provide very high Se concentration to drive the direct and fast formation of the Kesterite phase. In route 3, we developed a multinary alloying strategy to regulate the stability of intermediate phases to facilitate the phase evolution and cation exchange process. These efforts finally helped us to realized efficiencies of >15% in Kesterite solar cells. Overall, this efficiency breakthrough brings new opportunities for the development of emerging inorganic thin-film solar cell systems, with CZTSSe as a representative.



### Mikhail Otrokov

Institute of Nanoscience and Materials of Aragon in Zaragoza (Spain)

Mikhail Otrokov (1984) obtained his PhD in Condensed Matter Physics in 2011 at Tomsk State University (Russia). Soon after that he moved to San Sebastian (Spain) as a post-doctoral researcher, first at the Donostia International Physics Center and then at the Materials Physics Center. In 2018, he got an independent Research Fellow position in Ikerbasque - Basque Foundation for Science in San Sebastian (Spain). Since 2023, he is a research scientist in the Institute of Nanoscience and Materials of Aragon in Zaragoza (Spain). His expertise is the computational materials science using the density functional theory, with the current research activity mainly focused on magnetic topological insulators, although he is also interested in the electronic structure and magnetism of 2D materials, metal-organic systems, rare-earth intermetallics, and others. His paper on the discovery of the first intrinsic magnetic topological insulator was distinguished by the "Frontiers of Science Award" in 2023.

#### Intrinsic Magnetic Topological Insulators of the $\text{MnBi}_2\text{Te}_4$ Family

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Recently,  $\text{MnBi}_2\text{Te}_4$  has been theoretically predicted and then experimentally confirmed to be the first intrinsic antiferromagnetic topological insulator (AFMTI). This opens a new field that focuses on intrinsically magnetic stoichiometric compounds: several  $\text{MnBi}_2\text{Te}_4$ -derived MTIs were synthesized right away, such as  $(\text{MnBi}_2\text{Te}_4)\cdot n(\text{Bi}_2\text{Te}_3)$ ,  $\text{MnBi}_{2-x}\text{SbxTe}_4$ ,  $(\text{MnSb}_2\text{Te}_4)\cdot n(\text{Sb}_2\text{Te}_3)$ ,  $\text{Mn}_2(\text{Bi,Sb})_2\text{Te}_5$ , and  $\text{MnBi}_2\text{Se}_4$ . As a result,  $\text{MnBi}_2\text{Te}_4$  and related compounds have been predicted to be a platform for realizing high-order topological insulator and superconductor states, Weyl semimetal phase, skyrmions, quantized magnetoelectric coupling, and Majorana fermions. Moreover,  $\text{MnBi}_2\text{Te}_4$ -based systems are predicted and/or observed to show 12 different types of Hall effect, some of them are fundamentally new, such as the layer Hall effect. A number of technological applications have also been envisioned, in particular, chiral interconnect devices based on the high-Chern-number topological heterostructures.

Concerning current challenges of this field, we will discuss the issue of the Dirac point gap in the  $\text{MnBi}_2\text{Te}_4$  topological surface state that caused a lot of controversy. While the early experimental measurements reported on large gaps, in agreement with *ab initio* calculations, a number of further studies claimed to observe a gapless dispersion of the  $\text{MnBi}_2\text{Te}_4$  Dirac cone. A number of possible theoretical explanations of this unexpected behavior have been put forward, which we will discuss in the context of the available experimental data.

We acknowledge the support by MCIN/AEI/10.13039/501100011033/ (Grant PID2022-138210NB-I00) and "ERDF A way of making Europe", by Ayuda CEX2023-001286-S financiada por MICIU/AEI/10.13039/501100011033, as well as MCIN with funding from European Union Next Generation EU (PRTR-C17.11) promoted by the Government of Aragon.

## INVITED SPEAKER BIOGRAPHIES

### Topic 1: Computational material design and modeling



#### Jing Ma

Nanjing University

Jing Ma is a professor of chemistry (since 2005). She has received several awards, including Outstanding Young Chemist Award of Chinese Chemical Society and Chinese Young Women Scientists Awards. Her research is concentrated on the electrostatic polarization in low-scaling QM calculations and force field simulations of oligomers and stimuli-responsive materials with unique optical and electrical properties. Recently she is also interested in the material datasets and data-driven material designs. She is Senior Editor for the *Langmuir* (2024-present), Member of the Editorial Advisory Board for the *Journal of Chemical Theory and Computation* (2019-present).

**Title:** Stability Prediction of Gold Nanoclusters with Different Ligands and Doped Metals

#### Li-Min Liu

Beihang University

Li-Min Liu received his Ph.D. from Institute of Metal Research, Chinese Academy of Sciences in 2006. During his Ph.D. study, he visited Queen's University of Belfast, UK, for a year. Then he worked in Fritz-Haber-Institut (Germany), University College London (UK), and Princeton University. During 2011–2017, he took a tenure-track position in CSRC. Since Sep. 2017, he joined School of Physics, Beihang University. He was granted "the 1000-plan for young talents" and "the National Science Fund for Distinguished Young Scholars". His research interests focus on energy-related materials.

**Title:** The Nature of Excess Electrons and their Effect on the Activity of Reduced Metal Oxides





### Xiang-Mei Duan

Ningbo University

Xiangmei Duan, professor, PhD supervisor. She has been engaged in the multi-scale simulation and design of new materials, and has made a series of research achievements in new semiconductor materials, physical property control of low-dimensional materials, and single-atom catalysis, and has published 90 papers in international academic journals.

**Title:** Microscopic Mechanisms of Photovoltaic Conversion and Material Design

### Xin-Gang Zhao

Northeast Normal University

Xin-Gang Zhao is a full professor at Northeast Normal University since 2023 and is one of Outstanding Young Scientist Overseas. He worked as a research associate with Prof. Alex Zunger at the University of Colorado Boulder after earning his PhD from Jilin University in 2017. His research focuses on the design of functional materials, particularly optoelectronic semiconductors. He uses high-throughput DFT calculations and machine learning to explore structure-property relationships and develop material design methods. Currently, he is interested in the effects of microstructure changes on carrier transport in semiconductors. He has published over 30 high-quality papers, with more than 2,800 citations. Additionally, he is a guest editor for InfoScience.

**Title:** Screen d-electron ternary oxide memristors based on anti-doping principles



### Jun-Jie Wang

Nanjing University

Junjie Wang received his Bachelor's degree in Physics from Nanjing University in 2018 and his Ph.D. in 2023. He is currently conducting postdoctoral research at Nanjing University. His current research field is computational condensed matter physics, with a primary focus on high-pressure physics, machine learning force fields, and crystal structure search.

**Title:** Machine learning accelerated crystal structure prediction of ternary and multinary compounds





### Zhi-Mei Sun

Beihang University

Dr. Zhimei Sun is a Cheung Kong Scholar Chair Professor at School of Materials Science and Engineering of Beihang University, China. She received her PhD at Institute of Metal Research (CAS) in 2002, and after which she has been worked at RWTH Aachen University (Germany) and Uppsala University (Sweden) from 2002 to 2007, and at Xiamen University (China) from 2007 to 2013. Since August 2013 she has been working at Beihang University (China). Her research interest is AI accelerated materials discovery and property design, and the materials involve phase-change memory materials, structural materials and 2D transition metal carbides/borides, etc.

**Title:** Accelerating the Discovery and Design of Novel Materials by ALKEMIE

### Zhu-Hua Zhang

Nanjing University of Aeronautics and Astronautics

Zhuhua Zhang, Professor of Nanjing University of Aeronautics and Astronautics, Deputy Director of National Key Laboratory of Aerospace Structural Mechanics and Control, Deputy Director of International Frontier Science Research Institute. He is mainly working on the physical mechanic properties of low-dimensional functional materials and structural materials. He has stayed in the list of China's highly cited scholars in since 2020. He presided over the National Outstanding Youth Science Fund project, and the international (regional) cooperation and exchange project of the Foundation Committee. He was selected as the Youth Project of the National High-level Talent Program (2017), Jiangsu Distinguished Professor and Jiangsu "Double and Creative Talent" (2019). He has won the Chinese Mechanics Society Youth Science and Technology Award (2021), the Fok Yingdong Education Foundation Young Teachers Award (2020).

**Title:** Rich structures and functionalities at interfaces of 2D materials



### Shen Lei

National University of Singapore (NUS)

Dr. Shen Lei is a senior lecturer in the Department of Mechanical Engineering and Engineering Science Programme at the National University of Singapore (NUS). He obtained his PhD from NUS. As the sole recipient of the Lee Kuan Yew Postdoctoral Fellowship at NUS in 2014, he joined NUS as a lecturer. His interest lies in cross-disciplinary computational materials and physics, focusing on applying material fundamental properties for advanced technologies and predicting advanced materials based on the materials genome, high-throughput calculations, and machine learning.

**Title:** Crystal Structure Relaxation with Machine Learning



### Liang Ma

Southeast University

Liang Ma received his bachelor's and Ph.D. degrees in physics from Southeast University in 2009 and 2015, respectively. He then pursued postdoctoral research at the Department of Chemistry of University of Nebraska-Lincoln with Prof. Xiao Cheng Zeng. At the end of 2018, he joined the School of Physics of Southeast University as faculty member. Now, he is a specially appointed young principal professor at Southeast University. His research interest mainly focuses on the multiscale simulation studies for the rational design, growth mechanism and property modulation of low-dimensional materials. He has so far published more than 60 scientific papers in high-end journals, including Nature (2), Nat. Nanotech nol. etc., with citations > 4000 and H-index of 29.

**Title:** Controllable Nucleation Mechanism and Epitaxy Descriptor of Two-Dimensional Materials

### Li Huang

Southern University of Science and Technology

Dr. Li Huang is currently an associate professor in Physics department of Southern University of Science and Technology. She got her Ph.D. in 2006 from Fudan University. Before joined SUSTech, she had been a postdoc at Georgia Institute of Technology and Ames National Laboratory. Her research field is computational condensed matter physics. Recently, her research focuses on the physical properties and manipulations of low-dimensional quantum materials and novel energy materials based on first-principles calculations and effective model analysis.

**Title:** Magneto-Optical Properties and Hall Effects with Net Zero Magnetism



### Shi-Xuan Du

Institute of Physics, CAS

Shixuan Du contributed many influential works on the nature of molecular assembly, on surface reaction, novel two dimensional atomic crystals, and the growth mechanism of low-dimensional materials using first-principle calculations. She is the winner of the National Science Fund for Distinguished Young Scholars and the editorial board member of Journal of Physics, Condensed Matter. She got the Award of the Chinese Young Women in Science Fellowship. As a Major Contributor, she won the 2013's Outstanding Science and Technology Achievement Prize of the Chinese Academy of Sciences.

**Title:** Rational Design of Ternary and Multinary Materials with Designed Properties



### Xian-Bin Li

Jilin University

Prof. Xian-Bin Li is the leader of Lab of Computational Semiconductor Physics and the head of Department of Microelectronics Science and Engineering, Jilin University, China. He mainly focuses on the key scientific problems related to microelectronics and optoelectronics including physics of phase-change memory materials, physics of defects in semiconductors, and physics of light-matter interaction. He now also serves as the vice chair of National Youth Forum on Optics, China.

**Title:** Computational Study of Multinary Chalcogenide Semiconductors for Low-Power Phase-Change Memory Applications

### Bin Xu

Soochow University

Prof. Bin Xu is currently working at the School of Physical Science and Technology of Soochow University. He has conducted postdoctoral and research assistant professor work at the University of Texas at Arlington, the University of Liège in Belgium, and the University of Arkansas in the United States. In 2019, he joined Soochow University. He is dedicated to the development and application of first-principles computational methods, focusing on fundamental research on various material properties such as ferroelectricity, multiferroicity, electron-phonon coupling, and transport.

Title: Electric-field control of magnetism in BiFeO<sub>3</sub>-based multiferroics



### Xie Zhang

Northwestern Polytechnical University

Xie Zhang, Professor in the School of Materials Science and Engineering at the Northwestern Polytechnical University and recipient of the National Talented Youth Program of China. He further worked as a postdoctoral researcher at MPIE (2015-2016) and at the University of California Santa Barbara (UCSB). Dr. Zhang focuses on computational design of advanced structural and energy materials. In recent years, he has published a series of high-profile papers in Nature Materials, Nature Computational Science, Physical Review Letters etc. He received the Outstanding Research Achievements award by the UCSB SSLEEC in 2018 and the Early Career Award in High-performance Scientific Computing by NERSC in 2019.

**Title:** Computational screening of multinary compounds for deep-ultraviolet light emitters



### Zhi-Xin Guo

Xi'an Jiaotong University

Zhi-Xin Guo is now an associate professor in Xi'an Jiaotong University. His primary research interest lies in computational condensed matter physics, with a particular focus on addressing power consumption issues in high-performance integrated circuit chips due to the miniaturization and increased density of electronic components. His work centers on the quantum regulation of interfacial information transmission performance in devices. He has proposed methods to reduce power consumption in information transmission by synergistically utilizing various interfacial quantum effects such as quantum confinement, orbital hybridization, and charge transfer. These approaches aim to solve the challenges of high-density and low-power information transmission in chips.

**Title:** Efficient electrostatic control of 2D magnets in bilayer ternary compounds with enhanced interlayer magnetic coupling and its device application

### Wei-Chao Wang

Nankai University

Weichao Wang is a professor of electronic information and optical engineering at Nankai University in China. He is a Fellow of the Royal Society of Chemistry and has been selected as a leading talents of the National Talents Program. He has published more than 180 papers in international authoritative journals such as Science, Advanced Materials, and Journal of the American Chemical Society, and has been cited more than 9500 times. His research interests focus on ternary oxide catalysis chemistry in the application of environmental treatment and energy conversion and storage.

**Title:** Mn-based ternary mullites for environmental and energy applications



### Bing Huang

Beijing Computational Science Research Center

Bing Huang, professor of Beijing Computational Science Research Center. His research interests include Computational Condensed Matter Physics, Semiconductor Physics and Light-Matter Interactions.

**Title:** Manipulation of Nonlinear Optical Properties in Semiconductors







### Yi-Yang Sun

Shanghai Institute of Ceramics, CAS

Yi-Yang Sun received his bachelor (1996), master (1999) and doctoral (2004) degrees from Jilin University, Xiamen University and National University of Singapore (NUS), respectively. From 2004 to 2010, he did postdoctoral research at NUS, Renewable Energy National Laboratory (NREL) and Rensselaer Polytechnic Institute (RPI). From 2010 to 2017, he worked as a research assistant professor and later research scientist in the Department of Physics, RPI. Since 2017, he has been a professor at Shanghai Institute of Ceramics, Chinese Academy of Sciences. His research focuses on the study of material properties based on first-principles calculations and design of novel functional materials.

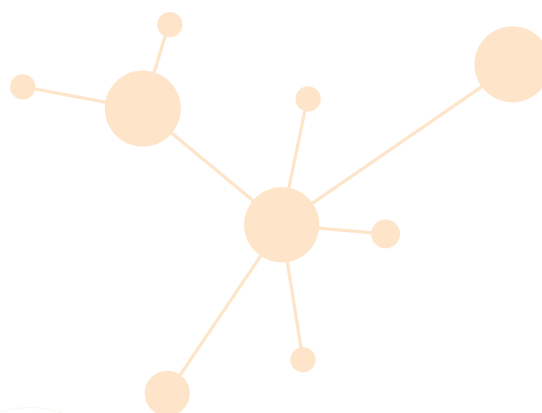
**Title:** Recent Progress on Studies of Chalcogenide Perovskites as Functional Materials

### Jun Kang

Beijing Computational Science Research Center

Jun Kang is an assistant professor in the Materials and Energy Division at the Beijing Computational Science Research Center (CSRC). He obtained his PhD degree at the Institute of Semiconductors, Chinese Academy of Sciences in 2014. Before moving to CSRC in 2019, he conducted post-doctoral research at the University of Antwerp and Lawrence Berkeley National Laboratory. His research interests include computational studies on defect and doping properties of semiconductors, and electronic structure of low-dimensional materials.

**Title:** Effect of site disorder on the defect properties of  $\text{MgSnN}_2$



## Topic 2: Material growth and characterization techniques



### Qian Sun

Suzhou Institute of Nano-Tech and Nano-Bionics, CAS

Prof. Qian Sun received his Ph.D. degree in Electrical Engineering from Yale University. He was with Bridgelux Inc., Livermore, California, where he made the key contribution to the R&D of 160 lm/W GaN-based LED grown on 8-inch Si substrates. He currently is a professor at Suzhou Institute of Nano-Tech and Nano-Bionics (SINANO), CAS, Suzhou, China. He currently holds 20 PCT patents and over 50 China patents, and has authored/co-authored about 120 peer-reviewed articles published on international journals, including Nature Photonics and Light: Science & Applications. He was the recipient of the Distinguished Youth Award (2023) and Exceptional Youth Award (2015) from NSFC, the National Technological Invention Award (2015) from the Chinese Central Government, the National Young Talents Award (2011) from the Chinese Central Government, Henry Prentiss Becton Prize (2010) from Yale University, and Guo Moruo Presidential Award (2002) from USTC.

**Title:** Ga(Al, In)N-based Light Emitting Devices Grown on Si

### Xiao-Juan Sun

Changchun Institute of Optics, Fine Mechanics and Physics, CAS

Xiaojuan Sun is a professor worked in Changchun Institute of Optics, Fine Mechanics and Physics, Chinese Academy of Science (CIOMP, CAS). She received Ph.D. degree in Condensed Matter Physics from CIOMP, CAS. She focuses on the physics, the III-nitride materials and photoelectric devices.

**Title:** Growth and defect regulation of non-polar AlN-based materials





### Yang Liu

Sun Yat-Sen University

Yang Liu, received the Ph.D degree in microelectronics and solid state electronics, Jilin University, 2000. In 2001, he worked on GaN materials and devices in Nagoya Institute of Technology, Nagoya, Japan, which is globally famous for their cutting edge GaN-on-Si technique. Since 2007, Dr. LIU, joined Sun Yat-sen University, Guangzhou, China, as a professor and the director of Guangdong research center of engineering technology for wide gap semiconductor GaN based power electronic materials and devices. Currently, he has two research directions, one is focusing on the design and reliability analysis of GaN based lateral structure power devices toward industrial and Electric Vehicle applications, the other is solution of basic material issues for vertical structure GaN power device application.

**Title:** Self-Screening Effect of Polarization Electric Field in bulk Gallium Nitride and its applications

### Ping Wang

Peking University

Ping Wang is an Assistant Professor in the School of Physics at Peking University, where he has been since 2023. He received his B.S. degree from Tianjin University in 2012, and completed his Ph.D. in Condensed Matter Physics at Peking University in 2017. From 2018 to 2023, he served as a Postdoctoral Research Fellow at the University of Michigan, Ann Arbor. His research focuses on nitride-based wide bandgap semiconductors and the development of emerging III-V ferroelectric semiconductors.

**Title:** Epitaxial Growth and Characterization of Emerging Sc-III-Nitride Ferroelectrics



### Xue-Lin Yang

Peking University

Xuelin Yang received his PhD from Peking University in 2009. From 2009 to 2012, he joined the University of Tokyo as a post doctor. He is currently a professor of engineering at Peking University. He was a recipient of the National Excellent Youth Science Foundation. He co-authored more than 150 papers and hold on 20 patents on epitaxial growth technology. His current research interests include MOCVD epitaxial growth of GaN thick films and their heterostructures on Si substrates, exploring the defect physics in GaN based materials.

**Title:** Atomistic Understanding of Dislocation Climb in Nitride



### Ya-Ping Wu

Xiamen University

Dr. Yaping Wu is now a professor and doctoral supervisor at the Department of Physics, Xiamen University. She has long been dedicated to the research of new structural materials and new functional devices, including wide bandgap semiconductor optoelectronic devices, quantum structures and devices, two-dimensional materials, and spintronics. She has presided over and undertaken more than 20 scientific and technological projects, has published over 100 SCI papers in authoritative journals, and holds more than 30 authorized patents. She currently serves as the director of the Engineering Research Center of Micro-Nano Optoelectronic Materials and Devices of the Ministry of Education, a member of the China Vacuum Society, and holds positions of editorial board member and advisory committee member for academic journals such as InfoMat, InfoScience, and Journal of Semiconductors.

**Title:** Growth of Type-II Hexagonal and Rhombohedral Janus van der Waals Heterostructures with Enhanced Valley Polarization

### Sen Huang

Institute of Microelectronics of Chinese Academy of Sciences

Sen Huang received the Ph.D degree from Peking University, Beijing, China, in 2009. He is currently a Professor with the Institute of Microelectronics of Chinese Academy of Sciences (CAS) and the University of CAS, Beijing, China. He has ever been supported by excellent youth fund of National Natural Science Foundation of China. His research interest includes advanced design, fabrication and characterization technologies for III-V power semiconductor devices. He has led the research and development of several advanced technologies for GaN-based electronic devices, including ultrathin-barrier AlGa<sub>N</sub>/GaN heterostructure for fabrication of (Al)Ga<sub>N</sub>-recess-free enhancement-mode devices, O<sub>3</sub>-sourced atomic layer deposition of Al<sub>2</sub>O<sub>3</sub> gate dielectric, and high temperature low damage gate recess, etc.

**Title:** Threshold voltage instability in III-nitride heterostructure metal-insulator-semiconductor high-electron-mobility transistors





### Ke Wang

Nanjing University

Ke Wang is a professor at Nanjing University, where he holds a joint appointment in the School of Electronic Science and Engineering and the School of Physics. From 2008 to 2013, he was a JSPS Postdoc and senior researcher at Ritsumeikan University in Japan. In 2013, he went to Chiba University in Japan as an associate professor. He then joined RIKEN in Sendai as a senior research scientist in 2016. In 2019, he joined Nanjing University. His research works have involved epitaxial growth, fabrication and characterization of III-V nitride semiconductor materials and devices, such as deep UV emitters, high power high frequency electronic devices, quantum cascaded devices, photocathodes, etc.

**Title:** III nitride digital alloys and deep UV LEDs grown by molecular beam epitaxy



### Rong-Fu Chen

City University of Hong Kong

Professor Fu-Rong Chen received his PhD in Materials Science at Stony Brook University, USA in 1986. And he joined MSE Department of City University of Hong Kong at 2018. His research interests are in low dose 3D atomic resolution dynamics, soft materials dynamics imaging, quantum electron microscopy and solar energy tunable (SET) glass. Professor Chen is the recipient of many awards and honors, including Microscopy Society of American Innovation award for Design of Ultrafast/ Ultra-High Voltage Desktop Electron Microscope in 2019 and The Distinguished Professor of Tsing Hua University in 2012. He published more than 300 SCI papers in high impact journals. In average, he received 5 invitation talks for international conference per year. He has established two high technology companies, electrochromics energy saving smart glass and table-top electron microscope.

**Title:** 3D atom dynamics for multi-component doped helix materials



### Jian-Hua Zhao

Institute of Semiconductors, CAS

Jianhua Zhao is a professor at the Institute of Semiconductors. Her current interests include semiconductor spintronics and low-dimensional semiconductor physics, covering MBE growth of semiconductor and magnetic films, and low-dimensional semiconductor topological quantum computing structures; design, fabrication and underlying physics of novel devices such as magnetic memories and sensors. She has published more than 300 papers as the first author or co-author, and delivered more than 130 invited talks at conferences or workshops. She received the Asian Union of Magnetic Societies Award in 2022, Huang-Kun Physics Prize in 2017, Second Prize of National Technology Invention in 2000. She serves as a Member of Magnetism Commission of IUPAP (2018-2024), also the MMM Advisory Committee (MMM AdCom) Member (2018-2024).

**Title:** Molecular-beam epitaxy and optical properties of high-quality ultrathin homogeneous  $\text{GaA}_{1-x}\text{Sb}_x$  ternary semiconductor nanowires

### Xue-Dong Bai

Institute of Physics, CAS

Xuedong Bai is a professor at Institute of Physics, Chinese Academy of Sciences (CAS). Dr. Bai's research interest is focused on in-situ TEM method and its applications on materials science. He is the co-author of over 280 papers in peer-reviewed journals, including 8 in Nature, 2 in Science, 15 in Nature serials, 10 in JACS, 5 in PRL, and 7 in Adv. Mater.. He delivered over 70 keynote/invited talks at international conference. His H-index is 73 with over 20,000 citations (WOS). Xuedong Bai was named a number of academic awards, including Hu Gang-Fu Physics Award (Chinese Physics Society, 2015), the 2nd Place of the National Science and Technology Award (2011), and Distinguished Young Researcher Foundation (NSFC, 2007) etc..

**Title:** Surface growth and structural manipulation by in-situ TEM





### He Tian

Zhejiang University

He Tian joined the School of Materials Science & Engineering at Zhejiang University (China) in 2014 as a professor. His main research focuses on the application and development of advanced electron microscopy. His research interests include transition metal oxides, multiferroic materials, and ferroelectric nano-devices. Using in-situ techniques to control charged domain walls and polar structures, investigate the dynamic switching mechanism and topological transformations. He Tian has published 3 in Nature, 2 in Science, and more than 100 SCI articles in Nature Photonics, Nature Nanotechnology, etc.

**Title:** In-situ manipulation of ferroelectric domain and domain walls

### Rong Yu

Tsinghua University

Professor Rong Yu of Tsinghua University graduated from Zhejiang University in 1996 and received his Ph.D. degree from Institute of Metals, Chinese Academy of Sciences in 2002. Before joining Tsinghua University in 2008, he worked as a postdoctoral researcher at Lawrence Berkeley National Laboratory and the University of Cambridge. He has been engaged in the research of electron microscopy and microstructure of materials. He invented some electron microscopy methods, including adaptive-propagator ptychography, local-orbital ptychography, and local orbital tomography, and studied crystal structure and defects, electronic structure and magnetic structure of materials at the atomic scale, and carried out the research on rare earth permanent magnet materials.

**Title:** Direct imaging and positioning interstitial atoms in solids



### Jian-Jun Tian

University of Science and Technology Beijing

Jianjun Tian is a professor, and vice-dean of Institute for Advanced Materials and Technology, University of Science and Technology Beijing. Current research focuses on fabrication of semiconductor nanocrystals and films, and their applications in light emitting, solar cells and photodetectors. He published more than 200 peer-reviewed papers in *Science*, *Nat. Comm.*, *Adv. Mater.*, *Angew. Chem.*, *Nano Lett.*, *Adv. Funct. Mater.* etc.

**Title:** Colloidal fabrication of high-quality perovskite semiconductors for efficient devices





### Qi Chen

Beijing Institute of Technology

Prof. Qi Chen holds both his B.S and M.S degrees in Tsinghua University, and received his PhD degree at University of California, Los Angeles (UCLA). From 2013-2016, he worked as a postdoc fellow at California Nanosystem Institute (CNSI), UCLA. Now he is the professor in Beijing Institute of Technology. His research focuses on hybrids materials design, processing and applications in opto-electronics and for energy harvesting and storage. To date, he has published over 100 SCI papers with total citation of 30000, including Science, Nature Communications, etc. Currently, he is working on the fundamental research and development of perovskite solar cells for commercialization.

**Title:** The heterogeneity in perovskite materials and solar cells

## Topic 3: Material growth and characterization techniques

### Yi Zhang

Nankai University

Prof. Yi Zhang joined the School of Electronic Information and Optical Engineering at Nankai University. In December 2016, he was selected as one of the top 100 young discipline leaders at Nankai University. Currently he is the deputy Director of the Institute of Optoelectronic Thin Film Devices and Technology and the deputy Director of the Tianjin Key Laboratory of Optoelectronic Thin Film Devices and Technology. As the project leader, he has been in charge of the National Key Research and Development Program, and the National Natural Science Foundation of China. In 2022, CZTSSe solar cells with an efficiency of 14.4% were developed, entering the international leading level. As the founder he and other international scientists have initiated and organized an influential Asia Pacific seminar on copper based thin-film optoelectronic devices in this field.

**Title:** Qualified Absorber Layer Growth to Attain High Efficient Chalcogenide Thin Film Solar Cells







### Si-Xin Wu

Henan University

Sixin Wu received his Ph.D. degree in Shanghai Institute of Optics and Fine Mechanics in 1999. From 2000 to 2006, he worked as postdoctoral researcher at Tohoku University and National Institute for Materials Science, Tsukuba, Japan, University of Texas at Arlington, USA. He is currently a professor at the Key Laboratory for Special Functional Materials of the Ministry of Education, Henan University, China. At present, he is mainly engaged in the research of inorganic thin film photovoltaic devices.

**Title:** Defect engineering of kesterite photovoltaics

### Fang-Yang Liu

Central South University

Fangyang Liu returned to Central South University as a full professor in 2017. He is currently serving as the Vice Dean of the School of Metallurgy and Environment, Director of the Department of New Energy Materials and Devices, and Director of the Engineering Research Center for Advanced Battery Materials at the Ministry of Education. He is a recipient of the National "Ten Thousand Talents Program" for Young Top-notch Talent, Hunan Province Science and Technology Innovation Leading Talent, and is the Chief Scientist for National Key R&D Projects. His research focuses on non-ferrous metallurgical materials, energy-efficient conversion, and safe storage materials. In recent years, he has published over 80 SCI papers as the first or corresponding author in leading journals. He also holds 38 authorized patents and has led multiple major technological innovation projects.

**Title:** Bulk and Interface Modification for Copper-Zinc-Tin-Sulfide-Selenide Photovoltaic Thin Films



### Jian-Jun Li

Institute of Metal Research, CAS

Dr. Jianjun Li is a full professor at Institute of Metal Research (IMR) Chinese Academy of Science. He was a lecturer and an Australian Centre of Advanced Photovoltaic (ACAP) Research Fellow at the School of Photovoltaics and Renewable Energy Engineering (SPREE), University of New South Wales between 2019 to 2023. He received Ph.D. from the Institute of Photoelectronic Thin Film Devices and Technology, Nankai University, China in 2016. His research focuses on materials science and engineering, device physics, and characterization of emerging inorganic photovoltaic materials like chalcopyrite, kesterite, antimony chalcogenides, and their other photoelectronic applications. He has published 45 peer-reviewed journal papers, including Nature Energy, Advanced Materials, and Advanced Energy Materials, with an H-index of 25.

**Title:** Microscopic carrier loss mechanisms in kesterite  $\text{Cu}_2\text{ZnSn}(\text{S},\text{Se})_4$  thin film solar cells



### Meng-Lin Huang

Fudan University

Menglin Huang received his Ph.D. degree in Electronic Physics at East China Normal University in 2021 under the supervision of Prof. Shiyou Chen. Since then, He worked as a postdoctoral researcher in the School of Microelectronics at Fudan University. His research focuses on the use of first-principles simulation to study the point defects in materials and their influences on device reliabilities.

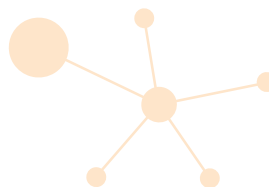
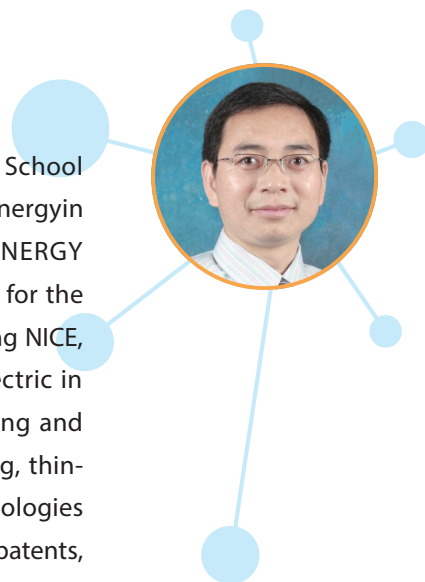
**Title:** Defect correlation reveals critical defects in low-symmetry materials

### Da-Long Zhong

National Institute of Clean-and-Low-Carbon Energy

Dr. Dalong Zhong obtained his Ph.D. in Materials Science from the Colorado School of Mines in 2001. He joined the National Institute of Clean-and-Low-Carbon Energy in Beijing in 2018 and is currently serving as a Chief Scientist of the CHN ENERGY Investment Group. He also holds positions as a member of the editorial board for the Clean Energy journal, and an adjunct professor at Fudan University. Before joining NICE, he held various leadership roles at the Global Research Center of General Electric in the United States. With over 20 years of experience in advanced manufacturing and materials, he possesses expertise in core process technologies such as coating, thin-film deposition, and additive manufacturing, as well as core equipment technologies applied in aircraft engines and the energy sector. He has filed over 80 invention patents, published 39 international academic journal articles, and contributed three chapters to international academic monographs.

**Title:** Thin-Film Photovoltaic Technology Advancements and Industrialization Challenges: Sphalerite, Chalcopyrite, and Perovskite





## Sheng-Zhong Liu

Dalian University of Chemical Physics, CAS

Dr. Frank Shengzhong Liu received his PhD from Northwestern University, USA in 1992. He is an RSC (Royal Society of Chemistry) Fellow. Professor Liu's research focus includes nanomaterials, thin film materials, photovoltaic materials and solar cells. His major outcome in basic research has been published in scientific journals, 80 of them being enlisted in ESI's "most cited paper" and "hot paper" lists. Many of his major inventions and patents have been converted into commercial technology and products. In 2011, he accepted a full-time professorship by Shaanxi Normal University and Dalian Institute of Chemical Physics, CAS in 2012. He is now the director of Shaanxi Engineering Lab for Advanced Energy Technology, Shaanxi Key Laboratory for Advanced Energy Devices and Institute for Advanced Energy Materials, Shaanxi Normal University and Associate Director of Solar Energy Department, Dalian National Laboratory for Clean Energy. He is also an Editorial Board Member for Advanced Science, ACS Sustainable Chemistry & Engineering, J. Energy Chemistry and Scientific Report. He is selected as the top 1% most highly cited author by RSC and Clarivate Analytics. He is also among the "Top 2% Scientists Worldwide 2022".

**Title:** Perovskite – a wonder material for solar cells

## Yi-Xin Zhao

Shanghai Jiao Tong University

Yixin Zhao is a distinguished professor at Shanghai Jiao Tong University. He obtained his PhD degree from Case Western Reserve University in 2010 followed by working as a postdoctoral fellow at Penn State University and National Renewable Energy Laboratory. He joined Shanghai Jiao Tong University at 2013 and his current research interests focus on perovskite solar cells and resource catalysis. He had published >200 peer reviewed paper in journals including Science, Nature Sustainability and JACS with >20000 citations and continuously enlisted in 2018-2023 Clarivate highly cited researcher.

**Title:** Low dimensional perovskite and surface termination to passivate and stabilize perovskite photovoltaics.





### Qing Zhao

Peking University

Qing Zhao is a professor at the School of Physics, Peking University. She is mainly engaged in the ion transport of micro-nano structures and the application of related devices. She has published more than 100 papers in journals such as Nature Photonics, Nature Commun., etc., with more than 9,000 citations (Google Scholar), and an H-factor of 50. 6 papers have been selected as ESI Highly Cited Papers, 23 papers have been cited more than 100 times, 7 Chinese invention patents and 1 international invention have been authorized. Her research work was selected as "2016 Important Achievements in Chinese Optics" and "Outstanding Scientific and Technological Papers of the 6th China Association for Science and Technology", and won the second prize of Natural Science Award of the Ministry of Education (2/7, 2023).

**Title:** Ion transport in micro-nano structures and related device applications

### Ping-Qi Gao

Sun Yat-Sen University

Professor Gao Pingqi completed both an BS and PhD degree from Lanzhou University in 2002 and 2010, respectively. From 2007 to 2011, he worked at the Microelectronics Center of School of Electrical and Electronic Engineering at Nanyang Technological university, Singapore. From 2011 to 2013, he worked at Baoding Fengfan photovoltaic energy company. From 2013 to 2018, he worked at Ningbo Institute of Materials Technology and Engineering as an associate processor and a professor. He is currently a deputy dean of the School of Materials, Sun Yat-sen University. His research activities are focused on sustainable photovoltaic (PV) technologies.

**Title:** Indium-saving transparent electrode towards sustainable development of silicon heterojunction solar cells



### Jun-Liang Yang

Central South University

Prof. Junliang Yang was appointed as a full professor in School of Physics at Central South University In March 2012. His research interests are focused on organic/perovskite solar cells and flexible and printed electronics. He has published over 270 papers in the international journals, such as Chem. Rev., Adv. Mater., ACIE, etc., granted 32 patents, and co-founded 2 companies. The published papers are cited over 11000 times and H-index is 59. He is the Fellow of the Royal Society of Chemistry, and selected as the "Top 100000 Scientists in the World" (2021, 2022, 2023) and "World's Top 2% Scientist" (2020, 2021, 2022 and 2023). He has been awarded to be the National Top Young Talents, the Excellent Talents of the Ministry of education, and the Leading Talents of Science and Technology in Hunan Province.

**Title:** Printing Organic and Perovskite Solar Cells and their Modules



### Wei-Min Li

Shenzhen Institute of Advanced Technology CAS

Weimin Li received his Ph.D. degree in electrical and computer engineering from National University of Singapore in 2017. After pursuing his Ph.D. degree, he joined Shenzhen Institute of Advanced Technology, Chinese Academy of Sciences. His research interests include CIGS thin-film solar cells, perovskite/CIGS tandem solar cells.

**Title:** Over 20%-efficiency flexible and bending durable CIGS solar cell on stainless steel substrate through diffusion barrier insertion

### Zai-Xing Yang

Shandong University

Zai-xing Yang is a full professor of School of Physics at Shandong University, China. His research interest mainly focuses on the controlled fabrication of low-dimensional semiconductors for electronic and optoelectronic device applications, including field-effect-transistors, CMOS invertors, photodetectors, and photovoltaic devices. He has published 96 SCI papers so far, including Nat. Commun., PNAS, Nano Lett., ACS Nano, Adv. Funct. Mater. and so on.

**Title:** Low-dimensional antimonide and optoelectronic devices



### Ying Li

Beijing Institute of Technology

Li Ying is an associate professor and doctoral supervisor at the School of Integrated Circuits and Electronics, Beijing Institute of Technology. Her main research focus is the preparation of all-inorganic halide materials and the corresponding research on optoelectronic devices. She has made many original scientific achievements in the fields of visual sensing, polarization detection, and optoelectronic synapses. In the past five years, more than 40 high-level academic papers have been published in international journals, 6 national patents have been granted, and many research results have been selected as highly cited papers by the Essential Science Indicators (ESI). She has also served as a guest editor for the Electronics journal.

**Title:** Study on Bionic Visual Sensors Based on Lead-free Perovskite Materials

## Topic 4: Photocatalysis, thermoelectrics, and energy storage



### Yuan-Hua Lin

Tsinghua University

Lin Yuanhua, Dean, has been working as a research assistant, associate researcher, and professor at the School of Materials Science and Technology, Tsinghua University since August 2001. Research field: 1 Targeting high-end electronic oxide inorganic dielectric materials and devices. 2. Oxide high-temperature thermoelectric materials and devices for energy conversion have published over 300 SCI indexed papers, including more than 100 in journals such as Science, Nat. Mater., Nat. Energy, Nat. Communn., Phys. Rev. Lett., Adv. Mater, etc. SCI papers have been cited over 30000 times.

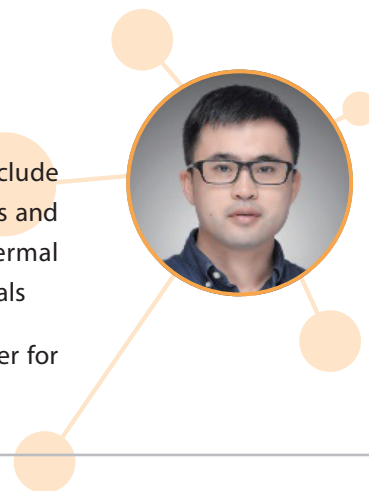
**Title:** High performance dielectric capacitors

### Ping Wei

Wuhan University of Technology

Ping Wei, professor of Wuhan University of Technology. His research interests include research and development of thermoelectromagnetic energy conversion materials and device manufacturing technologies, bi-directional temperature control and thermal management technologies, and electron microscope analysis of new energy materials

**Title:** Optimal design and performance evaluation of stable interfacial barrier layer for Bi<sub>2</sub>Te<sub>3</sub>-Based thermoelectric devices



### Yuan Deng

BeiHang University

Deng Yuan is currently Professor in School of Materials Science and Engineering, Beihang University, China, leading the group of Advanced Functional Materials and Devices. He is also the Director of key laboratory of intelligent sensing materials and chip integration technology of Zhejiang Province, Hangzhou Innovation Institute of Beihang University. He was selected as leading talents in science and technology innovation under the National Special Support Program. He has authored and co-authored more than 200 papers. His main research interests include the design and fabrication of advanced functional materials and device, in particular thermoelectric films and device for energy management and conversion.

**Title:** Multifield-Induced Fabrication Techniques for Bi<sub>2</sub>Te<sub>3</sub>-Based Thermoelectric Thick Films and Microdevices for Innovative Applications



### Li-Wen Sang

Fudan University

Liwen Sang is now the professor of Institute of optoelectronics, Fudan University. She received her Ph.D degree from Peking University, then joined NIMS, Japan as the postdoctoral fellow. In 2014, she was promoted to the permanent position in NIMS as the Independent Scientist. In 2022, She was awarded the MEXT Young Scientist Award from Ministry of Education, Culture, Sports, Science and Technology (MEXT), which is the best award for young scientists in Japan. In 2012 and 2019, she was awarded the JST-PRESTO researcher from Japan Science and Technology Agency (JST). She has published more than 140 peer reviewed papers with the citation of more than 3880 and H index of 32. Her current research interest is interface engineering in III-V nitride semiconductors for optical, electronic and mechanical devices.

**Title:** Homoepitaxial growth of p-GaN for pMOS capacitors

### Chen-Guang Fu

Zhejiang University

Dr. Chenguang Fu is currently a ZJU 100 Young Professor at the School of Materials Science and Engineering, Zhejiang University. His research interest is focused on the discovery and development of new materials for heat-to-electricity energy conversion, especially half-Heusler compounds and topological materials. He has published more than 100 papers (total citations over 10000, H-index of 49) in the field of thermoelectrics and energy materials. He is the recipient of the 2024 Young Investigator Award of the International Thermoelectric Society. He is an academic editor of The Innovation and The Innovation Materials.

**Title:** Topological Heusler magnets for transverse thermoelectric



### Tian-Ran Wei

Shanghai Jiao Tong University

Tian-Ran Wei is a professor at the School of Materials Science and Engineering, Shanghai Jiao Tong University (SJTU). He obtained his BS degree from Shandong University in 2012 and PhD from Tsinghua University in 2017. He was a visiting student at Northwestern University in 2015. He worked at Shanghai Institute of Ceramics, Chinese Academy of Sciences before joining SJTU in 2018. His current research focuses on ductile inorganic nonmetallic materials for flexible and hetero-shaped applications in e.g., thermoelectric energy conversion and sensors. As the first or corresponding authors, he has published more than 30 papers in e.g., Science, Nat. Commun., Adv. Mater., and J. Am. Chem. Soc. He was granted the national science fund for excellent young scholars.

**Title:** Superior plasticity and thermoelectric performance of  $\text{Ag}_2\text{S-Ag}_2\text{Se-Ag}_2\text{Te}$  multinary materials



### Qian Zhang

Harbin Institute of Technology, Shenzhen

She has been selected for the "Youth Project" of the Changjiang Scholars program of the Ministry of Education, approved for the "Guangdong Province Outstanding Youth Project", and the "Shenzhen Outstanding Youth Project". A total of more than 170 SCI papers have been published in journals such as Nature, Nature Energy etc. Serve as the deputy director of the Ministry of Industry and Information Technology's Key Laboratory of Printing Electronics and the deputy editor-in-chief of the journal "Materials Today Physics".

**Title:** High performance  $Mg_3(Bi,Sb)_2$ -based thermoelectric generators

### Pan Xiong

Nanjing University of Science & Technology

Pan Xiong is a Professor at the Nanjing University of Science and Technology, China. He received his PhD degree in Materials Science and Engineering from the same university in 2015. He was a visiting PhD student at the University of Texas at Austin followed by working as a JSPS postdoctoral researcher at the National Institute for Materials Science (NIMS), Japan and then a research associate at the University of Technology Sydney, Australia. He has been selected as a national high-level Overseas Young talent, winner of Jiangsu Province Outstanding Youth Fund, and Jiangsu Distinguished Professor, etc. His main research interests are two-dimensional material design and high efficiency energy conversion technology research, with more than 60 SCI papers published in Nat. Commun., Adv. Mater., Angew.chem.in.ed. and other high-quality

**Title:** Confined Ion Transport in Two-Dimensional Materials and High-Efficiency Energy Utilization



### Li-Ming Yang

Huazhong University of Science and Technology

Li-Ming Yang, professor of Huazhong University of Science and Technology, research interests include artificial intelligence, machine learning, high-throughput screening, theoretical and computational chemistry, computational materials science, multi-scale material simulation, and computational condensed matter physics; At present, the research group focuses on the rational design and screening/function-oriented material design of two-dimensional materials and porous framework materials such as MOFs/COFs, high-throughput screening of photoelectrocatalytic catalysts based on machine learning algorithm, revealing the micro-reaction process, exploring new reaction mechanism, and revealing the structure-activity relationship at the level of atomic and molecular.

**Title:** The electronic structure, magnetism, and its strain modulation on  $A_3BX_2$  compounds





### Jia Li

Tsinghua Shenzhen International Graduate School

Jia Li obtained his PhD degrees from Tsinghua University in 2009. Then he was a Postdoctoral Research Fellow in Fritz-Haber Institute of MPG in Berlin, Germany from 2009 to 2010. In 2011, he joined the Tsinghua Shenzhen International Graduate School, Tsinghua University. His research focuses on theoretical simulation and device design of low-dimensional materials, especially in the energy field. He has published more than 130 peer-reviewed journal articles with a total citation count of more than 11000 and an H-index of 57. In recognition of his achievements, he was awarded the first prize of Science and Technology Award by Chinese Materials Research Society (2/5, 2022) and the Early Career Award of Computational Materials Science by the Computational Materials Science Branch of the Chinese Materials Research Society (2019). He also serves as a member of the Computational Materials Science Committee of the Chinese Materials Research Society.

**Title:** Molecular Understanding of the Critical Role of Solid-Liquid Interface on Electrocatalysis

### Jia-Zhen Wu

Southern University of Science and Technology

Dr. Jiazhen Wu is now an associate professor in Department of Materials and Engineering at Southern University of Science and Technology. Dr. Wu's main research interests include exploration of novel catalyst materials and crystal growth for efficient ammonia synthesis, CO<sub>2</sub> reduction and water splitting. He is also interested in interdisciplinary researches between physical properties and heterogeneous catalysis. He has published papers in Nature Catalysis, Science Advances, Advanced Materials, etc. He obtained many fundings from NSFC and many other science foundations, including Science Fund for Outstanding Young people.



**Title:** Ru/Si 2D superlattice for alkaline hydrogen evolution reaction



### Jian-Ping Xiao

Dalian University of Chemical Physics, CAS

Prof. Dr. Jianping Xiao worked as a postdoc fellow with Prof. Xinhe Bao at Dalian Institute of Chemical Physics, CAS in 2013. After 2019, Prof. Xiao moved back to Dalian Institute of Chemical Physics, Chinese Academy of Sciences and been appointed as professor and the group leader in the group of Computation and Data Driven Catalysis. Recently his main research interests are developing methods for establishing reaction phase diagram to understand the evolution of activity, selectivity, and mechanism, also rationally design catalyst by artificial intelligence and machine learning techniques.

**Title:** Computational Catalyst Design Based on Energetic Descriptors and Reaction Phase Diagram Analysis Accelerated by Machine Learning



### Si-Qi Shi

Shanghai University

Siqi Shi is a Professor and PhD supervision at School of Materials Science and Engineering, Shanghai University. His current research focuses on the calculation and design of electrochemical energy storage materials, material databases, and machine learning, committed to promoting the research and development of artificial intelligence enabling materials. In 2001, he firstly applied the first principles calculation to investigate lithium-ion battery materials in China. He has published more than 180 research papers and a monograph called "Computation、 Modeling and Simulation in Electrochemical Energy Storage". He also created an electrochemical energy storage material calculation and data platform with independent intellectual property rights. He is in charge of 12 projects supported by the NSFC or the National Key Research and Development Plan.

**Title:** Design and Discovery of Novel Battery Materials

### Hua-Bin Zhang

KAUST Catalysis Center

Dr. Huabin Zhang graduated from Chinese Academy of Science. In 2021, he moved to KAUST as assistant professor. He has been awarded as One-Hundred-Talents in Chinese Academy of Science and National overseas high-level young talents (China). He mainly focuses on the development single atom catalyst for photo/electro-catalysis, including water splitting and CO<sub>2</sub> reduction. He has published over 150 SCI papers with total citation times of more than 17000 and H-index of 65. Over 30 papers are highly cited in Web of Science, and more than 50 papers have been cited over 100 times. Based on these works, Dr. Zhang has been rated/honored as a "Highly Cited Researcher" by Web of Science for consecutive 4 years from 2020 to 2023.

**Title:** Stories about single atom catalysis





### Li-Dong Zhao

BeiHang University

Li-Dong Zhao, professor of BeiHang University, Since joining Beihang in 2014, it has won the national young talents, Beijing Teachers' morality pioneer, young scientists of the International Society of Thermoelectricity, national leading talents, and the 2019-2023 Science Exploration Award and he Liang He Li Science and Technology Innovation Award. Main research interests: the development of thermoelectric materials with wide temperature range and high efficiency by using anisotropic decoupling of heat transfer and electric transfer. More than 300 important papers have been published in the journals of Nature and Science, and have been cited more than 30,000 times

**Title:** Advanced thermoelectric cooling materials

### Wan-Jian Yin

Soochow University

Wan-Jian Yin , professor of Suzhou University, his main research fields are theory and computation of solar cell materials, high-throughput computation and machine learning of materials design, and theory and computation of graphene growth mechanism. Review articles in international journals of physics, Chemistry and materials

**Title:** Expanding Multinary Oxide Perovskites for High-Performance Catalysts by Symbolic Regression



## Topic 5: Light emitting materials and light manipulation



### Ai-Wei Tang

Beijing Jiaotong University

Aiwei Tang received his Ph.D degree in optics from Beijing Jiaotong University, China, in 2009. Then he moved to the Institute of Semiconductors, CAS as a postdoctoral fellow. In 2011, he joined Beijing Jiaotong University, and now he is a full professor at the School of Physical Science and Engineering, Beijing Jiaotong University. His recent research interests are focused on synthesis, functionalization, and optical properties of Cd-free semiconductor nanomaterials and their applications in light-emitting diodes and photocatalytic hydrogen evolution

**Title:** Tunable Luminescence of Narrow-Bandwidth I-III-VI Type Semiconductor Nanocrystals for QLEDs



### Jian-Xin Tang

Macau University of Science and Technology

Jianxin Tang was appointed professor at the Institute of Nano Functional & Soft Materials (FUNSOM), Soochow University. In 2021, he was appointed professor at Macao Institute of Materials Science and Engineering (MIMSE), Macau University of Science and Technology. He was the selected member for Ten Thousand Talent Program Innovation Leader of China, and Youth Chang Jiang Scholars of Ministry of Education of China, and was awarded as NSFC Excellent Young Scholars. His current research areas/interests span device physics and surface science on organic and perovskite light-emitting diodes technology for flat panel display and solid-state lighting, and organic/perovskite photovoltaic cells for renewable energy.

**Title:** Synergetic Interface Engineering on Blue Perovskite Light-Emitting Diodes

### Rong-Jun Xie

Xiamen University

Rong-Jun Xie obtained his PhD in Inorganic Non-metallic Materials at Shanghai Institute of Ceramics, CAS in 1998, and joined National Institute for Materials Science (NIMS) as a Senior Researcher in 2003, and was promoted to Principal Researcher in 2007 and to Chief Research in 2017. In 2018, he moved to Xiamen University as a full professor at College of Materials. Xie's research interests include (i) phosphors for lighting and displays; (ii) mechanoluminescent materials for sensing technologies; and (iii) quantum dots for emissive displays. He has contributed to 300+ published papers and 100+ invited talks, and held 50+ patents.

**Title:** Luminescent materials for advanced displays



### Guo-Fa Cai

Henan University

Guofa Cai, Professor and doctoral advisor, has been awarded as the Outstanding Youth Foundation Scholar of the National Natural Science Foundation, distinguished Professor of Henan Province of China, Young Scientist Medal of International Association of Advanced Materials (IAAM) and Young Leader of the Society for Information Display (SID). Currently working at Henan University, School of Nanoscience and Materials Engineering. As the first or corresponding author, the applicant has published 50 research articles in academic journals over the past few years, such as Sci. Adv., Nano Energy, etc. These publications have attracted more than 7000 citations, of which 9 papers are identified as the ESI highly cited papers. In addition, Cai has presided over 3 National Natural Science Foundation of China and participated in 2 research projects in Singapore, and 7 invention patents have been authorized.

**Title:** Electrochromic Materials and Multifunctional Large-size Device



### Yang Chai

The Hong Kong Polytechnic University

Prof. Yang Chai is the Associate Dean of the Faculty of Science, the Director of Joint Research Center of Microelectronics of the Hong Kong Polytechnic University, the Vice President of the Physical Society of Hong Kong, a member of The Hong Kong Young Academy of Sciences, an IEEE Distinguished Lecturer since 2016, the Vice Chair of IEEE EDS region 10, the Chair of IEEE EDS Nanotechnology Committee, and was the Chair of IEEE ED/SSC Hong Kong Chapter (2017-2019). His current research interest mainly focuses on emerging electronic devices.

**Title:** Bioinspired in-sensor computing for artificial vision

### Liang Li

Soochow University

Liang Li, Professor, Soochow University, Suzhou, China. Research directions are photoelectronic conversion devices including photodetectors and solar cells. Winner of the China National Outstanding Youth Funding. Director of the Jiangsu Provincial Key Laboratory of Thin Film Materials. Fellow of the Royal Society of Chemistry (RSC). Published over 300 SCI papers with a citation of 23000 times and H-factor of 81. Authorized 17 invention patents and edited 1 English book. Served as Editors and Editorial Board Members of several international journals.

**Title:** Perovskite Optoelectronic Devices



### Hui Huang

University of Chinese Academy of Sciences

Hui Huang is a full professor at University of Chinese Academy of Sciences. His research focused on the synthesis and applications of conjugated polymers. He has published over 140 papers in peer-reviewed journals including Nat. Mater., Nat. Chem. etc. He has received several prestigious awards, such as CCS-BASF Young Innovators Award.

**Title:** Precise and Scalable Synthesis of Conjugated Polymers





### Hua Li

Shanghai Institute of Microsystem and Information Technology, CAS

Hua Li, Ph.D., Professor of Shanghai Institute of Microsystem and Information Technology (SIMIT), CAS. His research interests include high performance terahertz semiconductor lasers and frequency combs. He has published more than 90 peer-reviewed papers, delivered more than 30 invited talks at international conferences, and obtained more than 22 licensed China invention patents and 1 licensed international PCT patent. He is the recipient of NSFC for Distinguished Young Scholars, NSFC for Excellent Young Scholars, Shanghai Outstanding Academic Leaders, Shanghai Youth Top Talent Support Program, etc.

**Title:** GaAs/AlGaAs semiconductor laser based terahertz frequency combs

### Shao-Teng Wu

Institute of Semiconductors, CAS

Wu Shaoteng, a Researcher at the Institute of Semiconductors, CAS, engaging in research on Group IV heterogeneous integration and optoelectronics. Successively, achievements were realized, including 8-inch GeOI and GeSnOI wafers, the highest detection rate Ge and SiGeSn infrared detectors, germanium-based LED emitters on 12-inch silicon substrates, and prototype devices of germanium-based vertical cavity surface emitting lasers (VCSELs). Starting from 2022, he joined the research group of Researcher Li Shushen and Researcher Luo Junwei at the Institute of Semiconductors. Over the past five years, he has published over 19 SCI papers in the field of photonics. Additionally, there are 10 patent applications/authorizations, including one PCT patent.

**Title:** Research on infrared SiGeSn LED on 12 inches silicon



### Yi-Zheng Jin

Zhejiang University

Dr. Yizheng Jin is the professor of Chemistry at Zhejiang University, China. His research interests encompass material chemistry, device engineering and device physics of solution-processed optoelectronics. His research has resulted in over 60 journal papers in peer-reviewed journals, including Nature, Nature Photonics, Nature Communications, Science Advances and Advanced Materials. Prof. Jin received several awards, including Changjiang Scholar, National Natural Science Funds for Excellent Young Scholar, Chinese Chemical Society Award for Outstanding Young Chemist and Top 10 scientific advances of 2014 in China.

**Title:** Device physics and material chemistry of quantum-dot light-emitting diodes



### Zhi-Feng Shi

Zhengzhou University

Zhifeng Shi is a professor in School of Physics, Zhengzhou University. He received his Ph.D. degree in Microelectronics and Solid-State Electronics at Jilin University in 2015. His research interests relate to the controllable synthesis and photophysics of semiconductor optoelectronic materials and their applications in functional devices. He has published over 100 peer-reviewed papers with more than 8000 citations. He was awarded the Youth Science and Technology Award of Henan Province and was selected into the National Young Talents Program.

**Title:** Lead-free halide perovskites luminescent materials and devices

### Ting Wang

Institute of Physics, CAS

Ting Wang started his academic career by taking Associate Professor position in the Nanoscale Physics and Devices Laboratory at Institute of Physics with commissioning the first III-V/IV hybrid Molecular Beam Epitaxy reactor for silicon photonics in China. His current research interest focuses on the silicon photonic heterogeneous integration by using Molecular Beam Epitaxy, including the development of novel optoelectronic devices including on-chip integrated lasers, detectors, and modulators. Wang is a pioneer of silicon based III-V lasers, acknowledged as one of the initial inventors of InAs quantum-dot laser on Si for monolithic silicon photonic integration. Wang has published over 120 papers and one book in the field of silicon photonics and semiconductor lasers, while holding several patents on integrated silicon photonics.

**Title:** III-V Quantum Dot Comb Laser on Silicon for Integrated Optical I/O



### Xing-Jun Wang

Peking University

Xingjun Wang, Second Class Professor, Doctoral Supervisor, Vice Dean of the College of Electronics, Peking University, Deputy Director of the State Key Laboratory of Regional Optical Fiber Communication Networks and New Optical Communication Systems, Member of the Discipline Evaluation Group of the State Council, Selected as Distinguished Professor for the Ministry of Education's Major Talent Program, Chief of the Key R&D Program of the Ministry of Science and Technology, and Leader of the Key Projects of the NSFC (2 times). In the past five years, he has published more than 60 papers as the first/ corresponding author in high-level journals such as Nature, Nature Photonics, etc.

**Title:** Silicon photonics and system



### Jian-Wei Wang

Peking University

Dr. Jianwei Wang is an Professor in the Physics department at Peking University. He obtained his PhD from the University of Bristol in 2016. His research group focuses on Quantum Information Science and Technologies with Integrated Photonics. Their work centers around on-chip generation, processing, and detection of complex entangled states of light, as well as integrated photonic quantum computing, quantum networking, and quantum simulation. Dr. Wang has a prolific publication record, with peer-reviewed papers in prestigious journals such as Science (3), Nature Physics (5), Nature Photonics (5), etc.. He has been awarded the National Science Fund for Distinguished Young Scholars (2023), Daheng Wang Award (2023), C.N. Yang Award (2022), and Yutai Rao Fundamental Optics Award (2019).

**Title:** Large-scale integrated quantum photonics

### Xue Bai

Jilin University

Xue Bai is a Professor at State Key Laboratory of Integrated Optoelectronics, College of Electronic Science and Engineering, Jilin University, China. She received her PhD degree in condensed matter physics from Changchun Institute of Optics. Fine Mechanics and Physics, Chinese Academy of Science in 2008. Her research interests focus on lanthanide-based nanomaterials and optoelectronic devices. She has published more than 180 SCI index papers with more than 10200 citations in the international journals such as Nature Comm., Nano Lett., and Angew .Chem. Int. Ed. etc. The current h-index value is 52 according to ISI search report. In 2023, she was awarded the National Science Fund for Distinguished Young Scholars.

**Title:** Lanthanide based materials and optoelectronic devices



### Jing-Xuan Wei

University of Electronic Science and Technology of China

Prof. Jingxuan Wei received his B.S. degree from the Department of Physics at Nanjing University China in 2013, his Ph.D degree from the Department of Electrical and Computer Engineering at National University of Singapore in 2021. In November 2022, he joined the School of Optoelectronic Science and Engineering at the University of Electronic Science and Technology of China (UESTC) as a professor. His research interests include integrated photonics, micro/nano-photonics, and optical sensors.

**Title:** Novel Polarization-sensitive Photodetectors Based on Photonic-Electronic Nanostructures





### Chang-Xi Zheng

Westlake University

Dr. Changxi Zheng earned his undergraduate degree in Material Physics from Lanzhou University, Master degree in Material Physics and Chemistry from Sun Yat-sen University, and Ph.D. in Condensed Matter Physics from Monash University, Australia. He is currently an Assistant Professor at Westlake University. Dr. Zheng's research is centered on the development and application of cutting-edge imaging techniques based on low-energy electron microscopy and photoemission electron microscopy.

**Title:** Imaging deep ultraviolet photon-matter interaction using low-temperature quantum electron microscopy

## Topic 6: Complex wide-band-gap materials

### Jian-Dong Ye

Nanjing University

Jian-Dong Ye, Professor of Nanjing University. he was supported by the National Outstanding Youth Fund and the Outstanding Youth Fund of Jiangsu Province in 2013. In recent years, he is mainly engaged in the research of oxide semiconductor optoelectronic materials and information functional devices. To preside over and complete 3 projects of National Natural Science Fund and 3 projects of provincial and ministerial level. A total of 108 academic papers published, including 89 SCI papers, with cited more than 1400 times, H Factor 23. Three papers cited more than 100 times.

**Title:** An avalanche-and-surge robust NiO/Ga<sub>2</sub>O<sub>3</sub> p-n heterojunction power diode



### Xiao Yu

Hangzhou Institute of Technology, Xidian University

Prof. Xiao YU is currently a professor of the Hangzhou Institute of Technology, Xidian University, China. His research interest focusses on novel semiconductor device technologies and their reliability, including fabrication and characterization, the reliability mechanism, the modeling and simulation of novel device and array of non-volatile memory with new channel material. He has published over 80 papers in highly-recognized journals in the industry such as IEEE Transaction on Electron Devices (TED) and IEEE Electron Devices Letter (EDL) and at international conferences including top-level conferences such as International Electron Devices Meeting (IEDM) and VLSI, for over 900 citations. He was granted the Roger A. Haken Best Student Paper Award at IEDM 2015 and EDS Japan chapter Award by IEEE.

**Title:** Impact of Oxygen Vacancy on Ferroelectric Characteristics and Reliability of Hf<sub>0.5</sub>Zr<sub>0.5</sub>O<sub>2</sub> (HZO) Thin Films



### Wen-Bin Li

Westlake University

Wenbin Li is an Assistant Professor of Materials Science and Engineering at Westlake University. He received his bachelor's, master's, and doctoral degrees in Materials Science and Engineering from Zhejiang University, the University of Pennsylvania, and MIT, respectively, and was a Marie Curie Fellow at the University of Oxford. His research focuses on the computational modeling and design of advanced electronic materials, with a particular emphasis on electron-phonon coupling and related properties.

**Title:** Origin of the Unusually High Electrical Conductivity of the Delafossite Metal PdCoO<sub>2</sub>

### Yu-Ning Wu

East China Normal University

Prof. Yu-Ning Wu received his BS in Physics from University of Science and Technology of China in 2006 and PhD in Physics from University of Florida in 2012. Currently he works in Department of Electronics at East China Normal University. His research focuses on the defect physics of semiconductors, including the defect properties and the related carrier dynamics.

**Title:** Simulations of the irradiation damage of wide-bandgap semiconductors



### Xue-Fen Cai

Shenzhen University

Xuefen Cai is currently an assistant professor in the College of Physics and Optoelectronic Engineering at Shenzhen University. She obtained her Ph.D. in physics in 2021 from the Beijing Computational Science Research Center under the supervision of Prof. Su-Huai Wei. Then she did postdoctoral study at the Institute of Semiconductors, Chinese Academy of Sciences, from 2021 to 2023. Her research focuses on the crystal phases, electronic structures, defect and doping physics of both common and complex semiconductors. She has published about 30 SCI papers in academic journals such as Physical Review B, Physical Review Applied, and Applied Physics Letters. She is hosting the grants from the Young Program of the National Natural Science Foundation of China.

**Title:** Bismuth-alloyed Ga<sub>2</sub>O<sub>3</sub> as a novel p-type transparent conducting oxide



### Hong-Lei Wu

Shenzhen University

Honglei Wu, professor and Ph.D. supervisor at Shenzhen University, distinguished scholar, and Deputy Director of the State Key Laboratory of Radio Frequency Heterogeneous Integration. He developed an aluminum nitride single crystal growth apparatus with complete intellectual property rights, producing 4-inch crack-free AlN crystals and, for the first time internationally, colorless inch-sized AlN crystals. He also developed AlN deep ultraviolet photodetectors with a detection wavelength of less than 200 nm and achieved AlN light-emitting devices covering the visible to ultraviolet spectrum through energy level adjustment. He has led 14 research projects, including those funded by the NSFC, the Ministry of Science and Technology's Key R&D Programs, and the Guangdong Provincial Key Research and Development Programs.

**Title:** Impact of different energy level of aluminum nitride on photodetectors

### Peng Zhang

Shenzhen University

Peng Zhang received his doctoral degree from Xiamen University, Xiamen, China, in 2014 and became a postdoctoral researcher in Korea Advanced Institute of Science and Technology (KAIST) in 2014 and Beijing Computational Science Research Center (CSRC) in 2016. He is currently an assistant professor in the college of physics and optoelectronic engineering of Shenzhen University, Shenzhen, China. His research interests include the computational materials science, optoelectronic materials, energy conservation and storage materials, and semiconductors.

**Title:** Theoretical exploration of electrified materials with exotic physical properties



### Jin-Song Xia

Huazhong University of Science and Technology

Jinsong Xia, Prof. PhD, Huazhong University of Science and Technology. He received the B. S. degree from USTC in 1999, and Ph.D. from Chinese Academy of Science in 2004. In 2010, he joined WNLO-HUST. He is recipient of the National High Level Talent Program. His research interests include thin-film lithium niobate photonic devices, metasurface, and nano-fabrication. He has published more than 150+ journal papers and 60+ invited conference talks.

**Title:** Photonic Devices based on Thin-Film Lithium Niobate





### Ya-Dong Xu

Northwestern Polytechnical University

Yadong XU received his PhD in School of Materials Science & Engineering, Northwestern Polytechnical University in 2010 and is currently a Professor in State Key Laboratory of Solidification Processing and Key Laboratory of Radiation Detection Materials and Devices, NPU, China. Dr. XU has received many prestigious awards including "Second-class of National Technological Invention", P.R. China, 2013, and "First-class of Scientific and Technical Awards", Shaanxi Province, 2019 and 2012. "The Ministry of education of Yangtze River scholar Professor (Young)", "Youth outstanding talent support program" in Shaanxi, China, (2020), Excellent Talents project in Shaanxi Province, China, 2016, etc. His research interests cover development of new semiconductor materials for X/γ-ray detectors. Dr XU has published more than 150 SCI papers and documented 25 patents.

**Title:** In Pursuit of high resolution CsPbBr<sub>3</sub> Gamma-ray Detectors by Optimization of Contact and Configuration

### Yan-Jun Fang

Zhejiang University

Dr. Yanjun Fang is a professor of the National Key Laboratory of Silicon and Advanced Semiconductor Materials at Zhejiang University. In 2018, he joined the School of Materials Science and Engineering at Zhejiang University. His primary research focuses on the optoelectronic properties of halide perovskite materials and their applications in photodetectors. His work has been cited over 19,000 times in SCI journals, with an H-index of 48. In 2018, he was selected for the National High-Level Overseas Talent Recruitment Program, and in 2021, he received the Zhejiang Provincial Outstanding Youth Fund. From 2020 to 2023, he was consecutively listed as a Clarivate Highly Cited Researcher.

**Title:** Suppression of Ion Migration in Halide Perovskites for Sensitivity and Stable X-ray Detectors



### Rong Wang

Zhejiang University

Dr. Rong Wang received her Ph.D. degree at Zhejiang University in 2014. She is a professor of Hangzhou Innovation Center of Zhejiang University. Her research mainly focuses on defects in 4H silicon carbide (4H-SiC), providing new clue for high-quality single-crystal growth, processing and homoepitaxy of 4H-SiC. Over the past five years, she has published more than 40 SCI papers as the first author or corresponding author. She holds 26 granted China National Invention Patents and two granted U.S. Invention Patents. Six of the patents have been transferred or licensed, and two of the key technological achievements have been industrialized.

**Title:** Tailoring the kinetic and electronic properties of dislocations in 4H-SiC by doping





### Hong-Liang Zhang

Xiamen University

Hong-Liang Zhang, Professor of Xiamen University, his research interests include epitaxial growth of thin films, synthesis of nanomaterials, optical, electrical, magnetic and catalytic properties, and their applications in new electronic devices and clean energy. So far in Phys. Rev. Lett. Nature commun. Jack. Am. Chem. Soc. Adv. Mater. Phys. Rev. B publications published more than 130 papers.

**Title:** The electronic structure and band alignment  $(Al_xGa_{1-x})_2O_3/Ga_2O_3$  heterojunctions

### Liang Wu

Hangzhou Dianzi University

As a National Distinguished Expert, Prof. Liang WU received his Ph.D., master from University of Louvain, Tsinghua University. Before joining Hangzhou Dianzi University, he was a full professor at Shanghai University, and also held various R&D and management positions at Intel, FEMAGSoft SA (Belgium), and GCL Energy Holding Limited, respectively. He was also the founder of Ultratrend Technologies Co. Ltd.. Prof. Liang Wu has more than 20 years of research and development experience on various crystal growth processes and material engineering for semiconductor, solar and LED applications, including crystal growth equipment & hotzone design, modeling & optimization, defect engineering and material characterization. His team developed world-first 60 mm crack-free bulk AlN single crystalline wafer with leading DUV transparency in 2019, and 3-inch bulk AlN crystals at the end of 2022. He has been granted more than 60 patents and authored one book published in Germany.



**Title:** Progress and device prospects on bulk AlN crystal growth by PVT method

### Jing-Xiu Yang

Jilin Jianzhu University



Yang Jingxiu, Associate Professor, School of Materials Science and Engineering and Key Laboratory of Comprehensive Energy Saving in Cold Regions, Ministry of Education., Jilin Jianzhu University.

Ph.D. at Dalian Institute of Chemical Physics, Chinese Academy of Sciences (2010-2016); Joint Ph.D. Program supported by RIKEN IPA Project in Japan (2013-2014); Postdoctoral Fellow, Beijing Computational Science Research Center (2016-2019). She has published over 40 SCI papers in high-impact international journals such as Nat. Commun., J. Am. Chem. Soc., Phys. Rev. B, J. Phys. Chem. Lett., with a total citation frequency of over 4300. In 2021, awarded the "Most Influential Paper of 2021" by the Chinese Physical Society.

**Title:** Manipulation of Band Structure and Defect Properties in Semiconductor Materials

## Topic 7: Spintronic, multiferroic, and other magnetic compounds



### Maciej Sawicki

Institute of Physics, Polish Academy of Sciences, Warsaw, Poland

Prof. Maciej Sawicki has spent most of his scientific career at the Institute of Physics, Polish Academy of Sciences in Warsaw. He currently heads the Laboratory of Cryogenic and Spintronic Research and leads the Group of Magnetism of Spintronic Materials. His undergraduate background in solid state physics led him to pursue interests in magnetic interactions in semiconductors. He built a fully automated SQUID magnetometer from scratch, gaining a unique perspective and understanding of this experimental technique. He spearheaded the inaugural demonstration of magnetic anisotropy control in a ferromagnetic material through purely electrical means. He currently holds a second visiting professorship at Tohoku University in Japan. He continues to pursue his primary research interest while also exploring other current topics in solid state physics, where antiferromagnetic spintronics is emerging as a dominant field.

**Title:** Towards Electric-Field Manipulation of Magnetization in Insulating Dilute Ferromagnets

### Nguyen Duy KHANH

Dr. Nguyen Duy Khanh is currently a Research Associate in the Department of Applied Physics at The University of Tokyo. He earned both his Ph.D. and M.Sc. degrees from the Department of Physics at Tohoku University, Japan. Following doctoral studies, he conducted research at RIKEN and The University of Tokyo. His research is centered on exploring emergent phenomena in quantum materials, with a particular emphasis on systems featuring non-trivial topological spin and electronic structures, such as understanding and manipulating magnetic skyrmions and other non-coplanar magnetic orders. Parts of his studies have been published in peer-reviewed journals, including Nature Nanotechnology, Nature Materials, and Nature Communications ...

**Title:** Topological transport behavior in intercalated van der Waals antiferromagnets





### Yong-Bing Xu

Nanjing University

Yongbing Xu, postdoctoral fellow at Cambridge University, Director of the Nanjing University Spintronics International Joint Research Centre at the University of York, director of the National Key Laboratory for Nanjing University Chip and Technology, and a national specialist, chief Scientist of the National Major R & D program (973). Professor Xu specializes in advanced electronic materials and devices, Spintronics, spin memory (MRAM) chips and ultrafast materials science. He is one of the initiators of STT effect (STT-mram) and spin chip material (SpinFET) in zero magnetic field. In 2000, he was awarded the EPSRC Fellowship Award by the National Engineering and Physical Sciences Research Department and was the only one selected by Cambridge University.

**Title:** Manipulation of spin ordering in 2D magnets

### Chun-Gang Duan

East China Normal University

Prof. Chun-Gang Duan earned his Ph.D. degree in theoretical physics from Institute of Physics, Beijing, Chinese Academy of Sciences, China in 1998. Then he worked in University of Nebraska, USA from 1998 to 2007. In 2008, he joined East China Normal University as full professor. He is now the director of key lab of polar materials and devices, Ministry of Education, China. He published more than 300 papers in peer-reviewed journals with more than 16000 citations. His group is currently working on multiferroics, valleytronics, energy conversion and neuromorphic computing materials.

**Title:** Ternary and multinary ferrovalley materials



### Jin-Xing Zhang

Beijing Normal University

Professor Jinxing Zhang has joined department of physics at Beijing Normal University as a full professor since the spring of 2012. The ultimate goal in Jinxing's group is the artificial control of symmetries in strongly correlated oxides for emergent quantum phenomena and functionalities, e.g. magnetoelectric phase transition, water-printing of ferroelectric polarization, topological spin textures and efficient spin-wave propagation. Recently, he has taken great efforts on exploring the potential applications of those fundamental discoveries on Beyond-CMOS devices. In 2022, he was supported by NSFC for Distinguished Young Scholars.

**Title:** Artificial Symmetry Design for Magnetoelectric Phase Transition



### Jin-Bo Yang

Peking University

Jinbo Yang, Professor, Ph.D, Peking University. He has long been engaged in the research of magnetism and the structure and properties of novel magnetic functional materials. As the principal investigator, he has led more than ten projects, including the National Key R&D Program (as the chief scientist), the NSFC's key projects/special projects. He has obtained more than ten national invention patents and published over 400 papers in international renowned journals with citations exceeding 9000 times. He has received awards such as the Second Prize of the National Natural Science Award, the National Hundred Outstanding Doctoral Dissertations Award, the Second Prize of Beijing Natural Science twice and the 2021 International Outstanding Achievement Award in Research on Permanent Magnet Materials.

**Title:** Development of Iron-rich Rare-earth permanent magnetic materials

### Hong-Jun Xiang

Fudan University

Prof. Xiang's research focuses on computational condensed matter physics, with significant contributions in the establishment of models for multiferroics and the development of computational methods. Prof. Xiang has developed the material simulation package PASP, which can be used to analyze the structural, electronic, magnetic, and thermodynamic and kinetic properties of complex magnetic and ferroelectric systems. As first author or corresponding author, he has published over 100 research papers, including 25 Physical Review Letters, ect.. In 2018, he received the International Center for Theoretical Physics (ICTP) Prize from Italy, and in 2021, he was elected as a Fellow of the American Physical Society (APS). In 2023, he was awarded the Huang Kun Physics Prize.

**Title:** Property analysis and simulation package for materials (PASP) and its applications to magnetic and ferroelectric materials



### Shuai Dong

Southeast University

Prof. Shuai Dong is the chair of school of physics, Southeast University. He obtained Bachelor and Phd degrees from Nanjing University, and once studied/worked in University of Tennessee at Knoxville/Oak Ridge National Laboratory for three years. He obtained the Funds for Distinguished/Excellent Young Scholars from NSFC and Changjiang Youth Scholar from MOE. He once served as an associate editor for NPJ Quantum Materials, and now is a divisional associate editor for PRL.

**Title:** Alterferroicity





### Pu Yu

Tsinghua University

Pu Yu, Professor of Physics at Tsinghua University. Prof. Yu obtained the PhD from the Department of Physics at the University of California, Berkeley in 2011. He joined the faculty at Physics of Tsinghua University in 2012 as a tenure-track assistant professor, and then promoted to associate professor in 2017 and full professor with tenure in 2018. His research interests span from condensed matter physics, materials science to solid-state chemistry. His favorite research platform is the correlated oxides, and he has been employing state-of-art growth techniques to design/synthesize novel systems at atomic scale and exploring novel strategies to manipulate the electronic states through ionic evolution.

**Title:** A correlated ferromagnetic polar metal by design

### You-Wen Long

Institute of Physics, CAS

Youwen Long is now a professor at the Institute of Physics, CAS. He focuses on high-pressure synthesis, ambient- and high-pressure physical properties, structure-property relationships, and structure and electronic states under external stimuli for new quantum materials with strongly electronic correlation, especially for multiferroic materials, high-temperature half metals and ferromagnetic insulators and semiconductors. He published more than 130 peer-reviewed papers including in Nature, Phys. Rev. Lett. etc. More than 20 papers were selected as journal cover, editors' suggestion, and/or research highlights.

**Title:** Charge and spin states of  $\text{PbFeO}_3$  and  $\text{PbCoO}_3$  prepared under high pressure



### Chang-Qing Jin

Institute of Physics, CAS

Changqing JIN is major in research on Quantum Emergent Materials & Phenomena at Extreme Conditions. He was awarded the National Prize for Natural Science in 2016, the first class Prize of Beijing Natural Science, the first class Prize of Chinese Materials Research Society in 2018 & 2023, YE QiSun Prize of Chinese Physics Society in 2015. He is Chair of the 26th International Conference on High Pressure Science & Technology, Commission, Chair of International Union of Crystallography (IUCr) on Crystallography of Materials, vice President of Chinese Crystallography Society. He jointly published 400+ papers including Nature, Nature Physics, Nature Communications. He is one of highly cited Chinese researchers recognized by Elsevier. He was authorized 36 patents on new materials. He was awarded Distinguished Young Scholar in 1997, the PI of Creative Research Team of NSFC in 2019. For more details pls visit team Web: <http://uhp.iphy.ac.cn>

**Title:** New Spintronic Materials: Design , Synthesis & Characterizations



### Ning Tang

Peking University

Ning Tang is a professor at School of Physics, Peking University. He received a Ph.D. degree in 2007 from School of Physics, Peking University. His current research mainly focuses on wide band gap semiconductor spintronics.

**Title:** Spin properties of the two-dimensional electron gas in GaN-based heterostructures

### Gang Xiang

Sichuan University

Gang Xiang is a full professor of physics at Sichuan University, where he also serves as the Vice Dean of the College of Physics. His research interests involves design and synthesis of semiconductors and magnetic materials and study of spintronic phenomena in these materials. His research is published in over 100 articles and has over 2400 citations (Google Scholar). He was selected as a New Century Excellent Talent by the Ministry of Education and a High-level Talent in Sichuan Province. His other honors include Sichuan Youth Science and Technology Award and the Tang Lixin Award for Teaching Excellence from Sichuan University.

**Title:** Transition Metal-doped Gallium Oxide Magnetic Semiconductor Thin Films: Fabrication, Characterizations and Potential Application in Magnetic Memristors



### Zhi-Min Liao

Peking University

Zhi-Min Liao, a Boya Distinguished Professor at Peking University, obtained a Ph.D. from the School of Physics at Peking University in 2007, then joined the faculty at Peking University. During 2010-2011, he conducted visiting research at Trinity College Dublin in Ireland. In recent years, he has made research advancements in the field of topological quantum transport properties and novel device effects, receiving honours such as the National Science Fund for Distinguished Young Scholars and the First Prize of Beijing Natural Science Award.

**Title:** Control over Berry curvature dipole and orbital magnetic moments



### Jian Zhou

Xi'an Jiaotong University

Jian Zhou, Professor at School of Materials Science and Engineering, Xi'an Jiaotong University. His current research interests mainly focuses on first-principles calculations of nonlinear optics of condensed matter materials, photoinduced material structures, and topological phase transitions. So far, he has co-authored over 100 papers in PNAS, PRL, JACS, Nano Letters, etc. These papers have been cited ~ 7,000 times, with an h-index of 36, and was selected as "Elsevier Chinese Highly Cited Scholar" and "World's Top 2% Scientists". These works are sponsored by grants from the Chinese Young-Talent Program and National Natural Science Foundation of China.

**Title:** Neel vector tuning hidden bulk photocurrent generation in Mn-based ternary antiferromagnets

### Tian-Xiang Nan

Tsinghua University

Tianxiang Nan's research interest is on Beyond-CMOS technology including microsystems and spintronics. He was named to MIT Technology Review's 35 Innovators Under 35 in China. He has published over 60 peer-reviewed articles. He is currently an Associate Professor in School of Integrated Circuits at Tsinghua University. Prior to joining Tsinghua University, he was a Post-Doctoral Researcher with the University of Wisconsin-Madison from 2015 to 2018, and with the Cornell University, from 2018 to 2019.

**Title:** Control of magnon spin transport in antiferromagnetic and multiferroic materials



### Yu-Rong Yang

Nanjing University

Yurong Yang is an professor of College of Engineering and Applied Science, Nanjing University. He was a post-doctoral in University of Arkansas from 2011-2013, and then became a research professor in University of Arkansas until 2018, when he joined Nanjing University as a professor in College of Engineering and Applied Science. He is experienced in developing/using first-principles based methods to explain the complex phenomena in oxide-based materials, predict and design new functional materials with distinguished properties. He has authored and co-authored more than 100 journal articles.

**Title:** External effects of ferroelectrics from first principles



### Chang-Song Xu

Fudan University

Changsong Xu joined the Department of Physics at Fudan University as an Associate Professor in 2021. In 2022, he was awarded a national youth program, and in 2023, he was selected as a Xiaomi Young Scholar. His research focuses on computational condensed matter physics, primarily using and developing density functional theory and first-principles-based effective Hamiltonian methods to study novel interactions and physical properties in ferroic systems, such as ferromagnetic, ferroelectric, and multiferroic systems. His recent research topics include magnetic topological defects, quantum spin liquids, magnetoelectric coupling and mutual control, and two-dimensional materials.

**Title:** Fractional Quantum Ferroelectricity

### Zhi-Qi Liu

BeiHang University

Zhiqi Liu obtained his B.S. degree from the Lanzhou University in 2009 and Ph.D. degree from the National University of Singapore in 2013. Afterwards, he performed postdoc research at the Oak Ridge National Laboratory, University of California, Berkeley, and Los Alamos National Laboratory. He is now a faculty professor and serves as the Head of Department of Materials Physics at the School of Materials Science and Engineering of Beihang University. His research interests include magnetic materials, strongly correlated oxide electronics, multiferroic heterostructures, and topological electron systems.

**Title:** High-temperature ferromagnetism in ternary oxide  $\text{La}_2\text{CoO}_{4\pm x}$  thin films and its electrochemical applications



### Da-Hai Wei

Institute of Semiconductors, CAS

Prof. Wei is Team leader and doctoral advisor at the Institute of Semiconductors, CAS. Prof. Wei's research focuses on the physics and devices of semiconductor spintronics. His work involves the magnetic semiconductors, and spin-related transport phenomena such as the spin Hall effect and spin-orbit torque. He has published over 60 papers in journals including Nature Communications and Physical Review Letters. Prof. Wei has received several honors, including the Humboldt Fellowship in Germany, and the Young Scientist Award from the Asia Pacific Magnetism Society. He is also the principal investigator of a youth team under the Chinese Academy of Sciences' stable support program for basic research and was the project leader of a youth project of National Key Research and Development Program of China.

**Title:** Progresses of room temperature magnetic semiconductors based on Antimonides and Germanide

## Topic 8: Miscellaneous



### Hang-Hui Chen

NYU Shanghai

Dr. Hanghui Chen is an associate professor of physics at NYU Shanghai and a global network associate professor of physics at New York University. He obtained his Ph.D. degree in Physics from Yale University. Before joining NYU Shanghai's faculty, Dr. Chen held a postdoc position in the Department of Physics at Columbia University. Dr. Chen's research area is at the intersection of condensed matter physics and materials science. He uses state-of-the-art first-principles calculations to study electronic, magnetic, structural, and superconducting properties of quantum materials, particularly emphasizing complex oxides and oxide heterostructures.

**Title:** A first-principles study of nickelate superconductors

### Liang Qiao

University of Electronic Science and Technology of

Liang Qiao is currently a professor of Physics, University of Electronic Science and Technology of China. He obtained his B.S. and PhD degree at Beihang University. After graduation, he worked as a postdoc fellow at Pacific Northwest National Lab (2009-2011) and Oak Ridge National Lab (2011-2014), then as a Lecturer at The University of Manchester (2015-2017). His research interest includes thin-film epitaxy, correlated oxides and quantum materials, superconducting and magnetic materials etc. He has published more 200 papers in Nature, Nat. Mater., Nat. Commun., PRL etc..



**Title:** Critical Role of H for Superconductivity in Infinite-layer Nickelates



### Xin Yang

Center for High Pressure Science&Technology

Dr. Xin Yang obtained her Bachelor and Ph.D. degree at Jilin University. Since 2023, she has been working as a postdoctoral researcher at the Center for High Pressure Science & Technology Advanced Research (HPSTAR) in Beijing under the guidance of Prof. Huiyang Gou. Her research focuses primarily on the design of high-temperature superconductors and theoretical research on electrocatalysts of two-dimensional materials.

**Title:** Theoretical Design of High-temperature Superconductivity in Metal Borides



### Zhe-Shuai Lin

Technical Institute of Physics and Chemistry, CAS

Zheshuai Lin is a professor in Technical Institute of Physics and Chemistry (TIPC), Chinese Academy of Sciences (CAS). He obtained his Ph.D. from Fujian Institute of Research on the Structure of Matter, CAS in 2002, and then spent two years as a postdoctoral research assistant at TIPC. From 2004 to 2008 he was a research associate in the Cavendish Laboratory and the Department of Materials Sciences and Metallurgy at the University of Cambridge, UK. In 2008 he returned back to China and held the current academic position. His research into optoelectronic functional crystals employs a variety of modelling techniques spanning analytical and quantum mechanics, as well as experimental exploration.

**Title:** Isotropic Zero Thermal Expansion and Good Optical Transparency in Sodalite Framework Crystals

### Jun-Yi Zhu

The Chinese University of Hong Kong

Prof Jun-Yi Zhu, Ph.D., Professor at the Chinese University of Hong Kong. Her research are Semiconductor defects and doping, Electronic properties of solids, Surface and interface phenomena, Using first principles and molecular dynamics approaches, and Elastic theory modeling.

**Title:** Revised Electron counting models based on six-fold coordination and layers and its application in the phase change in transition metal oxides



### Wei Ji

Renmin University of China

Ji, Wei is a computational physicist, working in the field of surface and interface modelling of low-dimensional materials. His recent research interests include theoretical modelling of electronic, magnetic and optical properties, as well as growth and exfoliation of two-dimensional materials. He currently holds the Wu Yuzhang Chair Professorship of Renmin University of China. He was supported by or awarded with four national innovative projects or professorships in 2014, 2015, 2016 and 2021. He published over 200 papers in scientific journals like Science, Nature Materials, and Nature Nanotechnology, which have received over 14,000 citations (WoS).

**Title:** Coexistence of ferromagnetism and ferroelectricity in van der Waals bilayers



### Yi Du

BeiHang University

Yi Du, Ph.D, Professor at the School of Physics, Beihang University. He has been awarded Australian Research Council "Future Fellowship" and the National High-Level Talent Program. He is currently the Executive Director of the Quantum and Matter Research Centre at Beihang University, Deputy Director of the Beihang-Wollongong Joint Research Centre, and team leader of Surface Physics and Quantum Matter in Beihang University. His research interests focus on the design and development of two-dimensional quantum materials for advanced application. His expertise includes molecular beam epitaxial growth, scanning tunneling microscopy, atomic force microscopy and angle-resolved photoemission spectroscopy. He has published over 200 research articles in the journals, with over 15,000 citations and an h-index of 70.

**Title:** 2D Frustrated Materials with Exotic Electronic Flat Bands

### Song Li

Winger physics Center

Dr. Song Li is now a research assistant professor in Beijing Computational Science Research Center (CSRC). Prior to moving to CSRC, he was a research fellow at Wigner Research Centre for Physics with Prof. Adam Gali. He obtained his Ph.D. degree in City University of Hong Kong with the supervision from Prof. Alice Hu. He works on theoretical and computational semiconductor materials and quantum information science. He is interested in advanced first-principles calculations to characterize the crucial optical and spin properties of promising point defects in quantum technology applications.

**Title:** Quantum Emission from Coupled Spin Pairs in hBN



### Shi Liu

Westlake University

Dr. Shi Liu was then offered a Carnegie Fellowship at the Carnegie Institution for Science in Washington, D.C. He received the American Physical Society's Nicholas Metropolis Award for Computational Physics in 2017 and the SEDD (Sensors and Electronic Devices Directorate) Distinguished Fellowship at the U.S. Army Research Laboratory in 2018. In June 2019, Dr. Liu joined the School of Science at Westlake University. A major focus of his research group now is to comprehend the structure-property relationships of complex oxides such as hafnia using deep-learning-based large-scale modeling. He has published more than 50 papers since joining Westlake University and is the recipient of multiple grants from the National Science Foundation of China and the Ministry of Science and Technology.

**Title:** Understand Ferroelectrics with Universal Force Field



### Bo-Nan Zhu

Beijing Institute of Technology

Bo-Nan Zhu, Professor of Beijing Institute of Technology, focuses on theoretical design and prediction of new energy materials, first-principles and defect engineering of optoelectronic materials, and development of high performance computing software. By the year 2022, we will have national-level young talents. And he is Editor of the Journal of Open Source Software.

**Title:** Exploring earth-abundant Li-ion cathode materials using random structure searching

### Jun Di

Nanjing University of Science & Technology

Di Jun, a professor/doctoral supervisor at Nanjing University of Science and Technology, is a national overseas high-level young talent and a specially appointed professor in Jiangsu Province. He mainly engages in research on two-dimensional material design, energy photocatalytic technology, and carbon dioxide resource utilization. So far, more than 150 SCI papers have been published, including 85 first author/corresponding (co) papers, Cited over 14000 times, with an H-factor of 65. Selected for Elsevier's "China Highly Cited Scholars" list, the top 2% of global scientists list, and the top 100000 global scientists list.



**Title:** 2D atomic layer for photocatalytic CO<sub>2</sub> reduction



### Li-Hui Song

Zhejiang University

Lihui Song, Ph.D., Principal Investigator, and doctoral advisor, is a recipient of the Qiu Shi Sci-Tech Innovation Scholars Program. He works at the Institute of Advanced Semiconductors at the ZJU-Hangzhou Global Scientific and Technological Innovation Center. Dr. Song has led 11 research projects funded by the NSFC, the Zhejiang Provincial Department of Science and Technology, and others. He has published over 60 papers in prestigious SCI journals in the field of semiconductor materials and authored two academic monographs published by European Academic Publishers. He holds 12 patents granted both domestically and internationally, with several patents successfully commercialized on a large scale. He was awarded the "West Lake Pearl Project" Special Support Program for Young Innovative Talents in Hangzhou.

**Title:** Research on the Irradiation Effects of Silicon Carbide



## POSTERS LIST

Poster No.	Poster Title	Author	Institution
P-001	Optical conductivity CdGa <sub>2</sub> S <sub>4</sub> , CdGa <sub>2</sub> Se <sub>4</sub> , CdGa <sub>2</sub> Te <sub>4</sub> and ZnIn <sub>2</sub> Se <sub>4</sub> crystals	Irada Mamedova	Institute of Physics
P-002	Dielectric relaxation in CdGa <sub>2</sub> Se <sub>4</sub> crystals	Irada Mamedova	Institute of Physics
P-003	First-principles study on refractive index of $\beta$ -Ga <sub>2</sub> O <sub>3</sub> in wide spectral range	Masato Ishikawa	Chiba University
P-004	The Influence of AlGa <sub>N</sub> Shell on the Absorption Spectrum of Mg <sub>x</sub> Zn <sub>1-x</sub> O Core-Shell Nanowires	Yaman Tang	Inner Mongolia University
P-005	Tunneling Time of Carrier through AlGa <sub>N</sub> /Ga <sub>N</sub> Double-Barrier	Yan Guo	Inner Mongolia University
P-006	Substrate Ferroelectric Proximity Effects Have a Strong Influence on Charge Carrier Lifetime in Black Phosphorus	Yonghao Zhu	Institute of Semiconductors, CAS
P-007	First-principles calculation of effect of Bi doping on magnetic and optical properties of LaFeO <sub>3-x</sub>	Yuqing Sun	Hebei Normal University
P-008	Modeling of magnetic properties and disorder effects in Mn <sub>2</sub> TiGe Heusler alloy	Evgenii Chernov	M.N. Mikheev Institute of Metal Physics, Ural Branch, Russian Academy of Sciences
P-009	Origin of the Nonmonotonic Pressure Dependence of the Band Gap in the Orthorhombic Perovskite CsPbBr <sub>3</sub>	Zehua Chen	Beijing Computational Science Research Center
P-010	Chemical trend of radiative recombination in III-nitrides	Zheng Liu	Beijing Computational Science Research Center
P-011	Crystal-Crystal Matches method and its application to TiO <sub>2</sub> phases	Qiushi Huang	Beijing Computational Science Research Center
P-012	Manipulation of nonlinear optical responses in layered ferroelectric niobium oxide dihalides	Liangting Ye	Beijing Computational Science Research Center
P-013	Landscape of Thermodynamic Stabilities of A <sub>2</sub> BB'O <sub>6</sub> Compounds	Yateng Wang	University of Science and Technology Beijing
P-014	Ultrastrong Coupling between Polar Distortion and Optical Properties in Ferroelectric MoBr <sub>2</sub> O <sub>2</sub>	Zhaojun Li	University of Science and Technology Beijing
P-015	Trilayer Moiré Superlattices of MoS <sub>2</sub> as a Simulator for the Ionic Hubbard Model on Honeycomb Lattice	Hongzhen Zhong	Beijing Computational Science Research Center
P-016	A posteriori energy correction of formation enthalpies for SCAN density-functional	Shuji Kanayama	Yokohama National University

P-017	CVD Synthesis of Millimeter-Scale BiSb Nanorods and Bandgap Tuning via Structural Arrangement	Biao Zeng	Shanghai Institute of Ceramics,CAS
P-018	Thermal stability and resistance drift of Sb-based phase change thin films	Guoxiang Wang	Ningbo University
P-019	A novel approach for fast-response $\beta$ -Ga <sub>2</sub> O <sub>3</sub> photodetectors by Modulating small polarons	Shujie Jiao	Harbin Institute of Technology
P-020	Strong polarization anisotropy in surface grating silicon	Ayaz Bayramov	Institute of Physics, CAS
P-021	Thermodynamics and Kinetics in Anisotropic Growth of One-Dimensional Mid-Entropy Nanoribbons	Shuxi Wang	Xi'an Jiaotong University
P-022	Bubble Evolution in U <sub>3</sub> Si <sub>2</sub> and its Influence on Thermal Conductivity	Jiaxu Zhou	Inner Mongolia University
P-023	Electronic structure and optical properties of Bi <sub>1.8</sub> X <sub>0.1</sub> In <sub>0.1</sub> Se <sub>3</sub> (X = Mn, Co, Cr), Bi <sub>1.8</sub> In <sub>0.2</sub> Se <sub>3</sub> and Bi <sub>1.7</sub> In <sub>0.3</sub> Se <sub>3</sub>	Danil Beliaev	M.N. Mikheev Institute of Metal Physics of Ural Branch of Russian Academy of Sciences
P-024	Effect of Interlayer Interaction on Fluctuations in Bi <sub>2</sub> Te <sub>3</sub> Crystal's Electron Density Distribution	Samir Gahramanov	Institute of Physics named after H.M. Abdullayev of MSE
P-025	Effects of compositional control of the conduction band minimum on Cu(In,Ga)Se <sub>2</sub> photoelectrodes for CO <sub>2</sub> reduction	Kazuma Okada	Tokyo University of Science
P-026	Impact of structural transition during crystal growth on microstructure and thermoelectric properties in CdSnAs <sub>2</sub>	Shoki Kishida	Kyoto University
P-027	Investigation of the Potential of Cu <sub>2</sub> (Sn, Ge)S <sub>3</sub> Photoelectrodes for Water Splitting	Kanamori Daiki	Tokyo University of Science
P-028	High Defect Tolerance in Heavy-band Thermoelectrics	Qianhui Lou	Zhejiang University
P-029	p-type Dopability in Half-Heusler Thermoelectric Semiconductors	Lirong Hu	Zhejiang University
P-030	Diffusion Behaviors of Lithium Ions at the Cathode/Electrolyte Interface from Global Neural Network Potentials	Yufeng Sun	Fudan University
P-031	Hierarchy of exchange-correlation functionals in computing lattice thermal conductivities of rocksalt and zinc-blende semiconductors	Jiacheng Wei	Key Laboratory of Advanced Materials and Devices for Post-Moore Chips, Ministry of Education, University of Science and Technology Beijing, Beijing 100083, China
P-032	Investigation of the deposition mechanism for SnS thin films using a novel deposition method, "Electrostatic Spray Deposition"	Kohta Hori	Tokyo University of Science
P-033	Fabrication of N-doped p-type SnS thin films by reactive sputtering and sulfurization	Taketo Tsuchiyama	Tokyo University of Science

P-034	Temperature-dependent study of the electrical properties of germanium-doped tin(II) sulfide thin films	Ayaka Kanai	Nagaoka University of Technology
P-035	Cu <sub>2</sub> SnS <sub>3</sub> thin films deposition on Mo-coated substrates by dual-source Fine channel mist CVD method for CTS solar cell fabrication	Hiroataka Maeta	Nagaoka University of Technology
P-036	Influence of sulfurization in controlled Sn-S and S mixed vapors on properties of Cu <sub>2</sub> SnS <sub>3</sub> thin films	Yuki Igarashi	Nagaoka University of Technology
P-037	Linear electrooptic effect in CuInS <sub>2</sub> single crystal.	Ibrahim Qasimoqlu	Institute of Physics named after H.M.Abdullayev of the Ministry of Science and Education of the Republic of Azerbaijan
P-038	Thermal-Driven Point Defect Transformation in Antimony Selenosulfide Photovoltaic Materials	Bo Che	University of Science and Technology of China
P-039	Disordering in a chalcopyrite compound ZnSnP <sub>2</sub> : A Raman spectroscopy study	Yoshitaro Nose	Kyoto University
P-040	Effect of 8-MeV electron irradiation on the electronic properties of indium doped Cu <sub>2</sub> SnS <sub>3</sub> crystals	Aleksei Lobanov	M.N. Mikheev Institute of Metal Physics UB RAS
P-041	Optical conductivity of magnetic semiconductors TlFeS <sub>2</sub> and TlFeSe <sub>2</sub>	Zibakhanum Badalova	Ministry of Science and Education Institute of Physics
P-042	The influence of defects on the temperature of the magnetic phase transition in new magnetic topological insulators MnSb <sub>2</sub> Te <sub>4</sub>	Nadir Abdullayev	Institute of Physics, CAS
P-043	Raman scattering and spin-phonon interaction in magnetic topological insulators MnBi <sub>2</sub> Te <sub>4</sub> and MnSb <sub>2</sub> Te <sub>4</sub>	Nadir Abdullayev	Institute of Physics, CAS
P-044	Features of Raman scattering in new magnetic topological insulators MnSb <sub>2</sub> Te <sub>4</sub>	Khayala Aliguliyeva	Azerbaijan
P-045	Features of Raman scattering in new magnetic topological insulators	Khayala Aliguliyeva	Azerbaijan
P-046	The influence of defects on the temperature of the magnetic phase transition in new magnetic topological insulators	Khayala Aliguliyeva	Azerbaijan
P-047	Switching Intrinsic Magnetic Skyrmions in van der Waals Multiferroic Heterostructures	Yusheng Hou	Sun Yat-Sen University
P-048	Origin of the contrasting magnetic stability of antiferromagnetic CuMnAs and CuMnSb	Gaofeng Teng	Beijing Computational Science Research Center
P-049	Tunneling current-voltage characteristics in semiconductor core-shell structured nanowires with elliptical cross-section	Yulong Lian	School of Physics Science and Technology, Inner Mongolia University
P050	The photoinduced hidden metallic phase of monoclinic VO <sub>2</sub> driven by local nucleation via a self-amplification process	Feng-Wu Guo	Institute of Semiconductors, CAS

# PRESENTATION INSTRUCTIONS

## ORAL PRESENTATION

### Test your presentation files

It is recommended that each speaker come to the Slides Desk to test the document as soon as your arrival, and copy your slides to your meeting room computer at least 30 minutes before the session. For speakers who do not copy the slides to his meeting room, the time for copying your slides to the computer will be included in your presentation time.

Please name your slides file in this format: **Meeting Room Number + Date + Time + Name**

Presentation slides loaded on the provided computers will be completely deleted by the volunteers of your session after your presentation.

If you have music, video or other Multimedia attachments in your slides, please test them earlier in the slides desk before your session(s) to ensure the playing performance.

### Equipment List in Each Meeting Room

The equipment is in different meeting rooms with different sizes of screens, and please prepare your slides according to the following information.

#### Oral Presentation in Purple Crystal Palace

Slides Ratio: 16:9

#### Equipment in the Meeting Room:

- LED screen
- Windows-operating computers (Windows 7 Operating System as well as with Microsoft Office (2010 or above) and Adobe Acrobat Reader (9.0 or above))
- A highlight pointer for LED

#### Oral Presentation in Meeting Room 3, 5, 6, 9

Slides Ratio: 16:9

**Equipment in the Meeting Room:**

- LED screen
- Windows-operating computer (Windows 7 Operating System as well as with Microsoft Office (2010 or above) and Adobe Acrobat Reader (9.0 or above))
- A highlight pointer for LED

**Presentation Time**

Keynote Presentation	30 minutes
Invited Oral Presentation	20 minutes
Oral Presentation (from abstract)	20 minutes

## POSTER PRESENTATION

**Poster Presentation Information**

**Location of Poster Area:** Meeting Room 12 on second floor of Conference Center

**Time for putting up:** From 16:00 on 09 September 2024

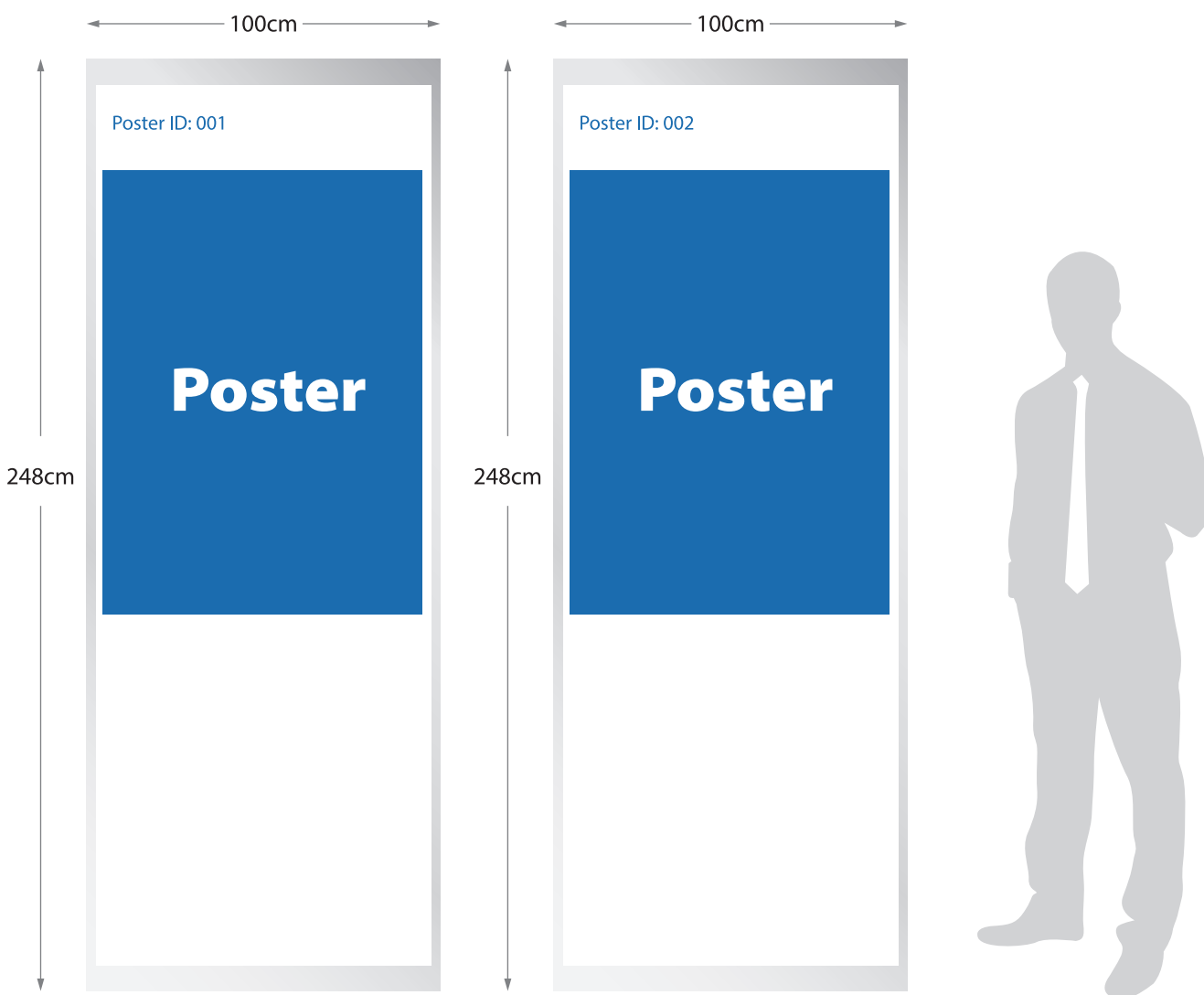
**Poster Session Time:** 15:50-18:00 on 11 September 2024

**Time for takedown:** Before 12:00 on 13 September 2024

**Poster Service Desk:** Meeting Room 12 on second floor of Conference Center

### Tips for Poster presentation

- Since the poster board is 2.5 meters in height x 1 meter in width, in order to give the audience a better performance, please keep your poster in the suggested size 90 cm (35 in width) x 120cm (47 in length)).
- Congress organizers will provide a board for the poster. Each poster board will be marked with the Poster ID at the left corner. Authors will be responsible to do printing and put up/take down the poster. The tape will be provided for poster mounting.
- If you attend the congress in person, during the poster sessions, please stand by your poster to communicate with the audience.
- Kindly note that the poster service desk will not collect the posters not been takedown after 12:00 on 13<sup>th</sup> September 2024.



# 北京龙讯旷腾科技有限公司

材料计算模拟工具软件研发创新领导者

## PWmat

基于密度泛函理论的第一性原理计算 /

**功能丰富：**具备很多特色功能，包括大体系计算、快速杂化泛函HSE计算、溶剂效应及恒电势模拟、含时密度泛函rt-TDDFT、非绝热分子动力学NAMD、电声耦合计算等。

**多种材料体系计算：**包括半导体材料、金属材料、陶瓷材料、纳米材料、二维材料、量子点、团簇、小分子以及表面和界面体系等。

### 主要功能

- 电子结构计算
- 分子动力学模拟
- NAMD非绝热动力学
- 磁性计算
- 声子谱计算
- 局域结构优化及全局搜索
- 过渡态搜索
- rt-TDDFT含时密度泛函
- 溶剂效应+恒电势
- 电声耦合计算

### 计算模块

- 物质结构
- 电子结构及声子计算
- 缺陷性质
- 电化学性质
- 输运性质
- 光、磁、力学和极化性质
- 大体系计算
- 机器学习力场
- 超快动力学过程
- Beyond DFT
- 电子束辐照分解

## QFlow

在线可视化提交任务工具 /

Q-Flow将第一性原理计算图形化，把PWmat的功能模块分解为不同计算组件，用户通过拖拽这些计算组件，连接成为 workflow，即可完成特定性质的计算。

## 解决方案

满足不同应用场景客户的计算需求 /

## PWMLFF

机器学习力场 (PWmat Machine Learning Force Field) /

机器学习力场借助已有的第一性原理计算结果，拟合单个原子的能量，可在不进行第一性原理计算的情况下获得体系能量。对于平衡态附近的体系，机器学习力场有望大幅加速分子动力学计算，提高在有限计算资源内可模拟的体系的大小以及模拟的时长。

## QStudio

在线建模工具 /

Q-Studio是基于jsmol开发的在线建模工具，用户无需安装任何软件，只需打开浏览器就可以使用Q-Studio。

### Mstation

一体化解决方案

单机双路服务器包含4块GPU卡且预装PWmat代码以及PWmat的运行环境和其他开放源代码，开箱即用，可完全满足小规模团队的计算需求。

### Mcluster

由多台GPU服务器通过Infiniband高速互联而成，具有共享文件系统及作业调度系统，可直接使用PWmat计算5,000原子体系的第一性原理计算，也可使用LS3DF进行1,000,000原子大型体系计算。

### Mcloud

SaaS平台解决方案

Mcloud是由龙讯旷腾自建高性能集群和云桌面组成的超算云平台，云平台集成了PWmat及Lammps等计算软件，提供SaaS材料模拟计算服务。

- **功能强大：**一键完成建模+计算
- **简单易用：**web注册登录即可使用
- **高性价比：**零建设成本，按需付费
- **资源丰富：**360块GPU卡，包括1080Ti、3080Ti和3090以及P100，具有高可用性，减少排队时间。



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