The 33rd International Conference on Defects in Semiconductors (ICDS-33)

Sep. 14-19, 2025

Yifu Building of Science and Technology

Fudan University, Shanghai, China

School of Physics, Eastern Institute of Technology, Ningbo
Institute of Computational Physical Sciences, and Key Laboratory of Computational
Physical Sciences (Ministry of Education), Fudan University
Institute of Semiconductors, Chinese Academy of Sciences

Sep. 14 (Sunday)

9:00-22:00 **Registration**

Tutorial 1 (Lecture Hall, 1st Floor)

Chair: Benjamin Hourahine

10:00-11:30 First-principles study on defects in semiconductors

Anderson Janotti, University of Delaware

Tutorial 2 (Lecture Hall, 1st Floor)

Chair: Shiyou Chen

14:00-15:30 First principles calculations for inorganic transition metal

compounds and defects therein

Hannes Raebiger, Yokohama National University

15:00-17:00 Modeling defects in Semiconductors

Benjamin Hourahine, The University of Strathclyde

Sep. 15 (Monday)

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8:10-8:20 **Opening Ceremony** (Lecture Hall, 1st Floor)

Xin-Gao Gong, Fudan University

Junwei Luo, Institute of Semiconductors, Chinese Academy of Sciences

Session 1: Plenary talks (Lecture Hall, 1st Floor)

Chair: Deren Yang

8:20-9:00 Fluorescent quantum-coherent materials from point defects in semiconductors

Adam Gali, HUN-REN Wigner Research Centre for Physics

9:00-9:40 Understanding and Engineering Defect Properties for Quantum

Information Science

Gregory Fuchs, Cornell University

9:40-10:00 **Coffee Break**

Session 2-1: Invited talks & Contributed talks (Lecture Hall, 1st Floor)

Chair: Adam Gali

10:00-10:30 **Hexagonal diamond: a promising platform for quantum**

applications

Chong-Xin Shan, Zhenzhou University

10:30-11:00 Towards an accurate prediction of the qubit decoherence in 3D and

2D materials: integration of density functional theory and quantum spin dynamics

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Hosung Seo, Sungkyunkwan University

11:00-11:20 Theory of spin-orbit-phonon processes governing the anisotropic

relaxation of SiV and other G4V centers in diamond

Gergo Thiering, HUN-REN Wigner Research Centre for Physics

11:20-11:40 Identifying high performance spectrally-stable quantum defects in

diamond

Yihuang Xiong, Dartmouth College

11:40-12:00 Theoretical investigation of high-energy states of NV and NV⁰ with

wavefunction-based methods

Ádóm Ganyecz, HUN-REN Wigner Research Centre for Physics

Session 2-2:	
	Invited talks & Contributed talks (Multi-function Hall, 2 nd Floor)
	Chair: Bing Huang
10:00-10:30	Unravelling Defect Physics in GaN Heteroepitaxy: From Point Defects to Dislocation Climb
	Xuelin Yang, Peking University
10:30-11:00	Defects in III-nitride semiconductor materials grown on Si
	Qian Sun , Suzhou Institute of Nano-Tech and Nano-Bionics, Chinese Academy of Sciences
11:00-11:30	Unique Deep-Level Defects in Low-dimensional Antimony Selenosulfide Semiconducting Materials
	Tao Chen, University of Science and Technology of China
11:30-11:50	Band-Offset Compensation Strategy for Asymmetric Doping in Wide-Bandgap Semiconductors
	Xiaobao Ma , Changchun Institute of Optics, Fine Mechanics and Physics, Chinese Academy of Sciences
12:00-13:30	Lunch
Session 3-1:	Invited talks (Lecture Hall, 1st Floor)
	Chair: Yeliang Wang
13:30-14:00	Erbium-Hyperdoped Silicon Nanocrystals
	Xiaodong Pi, Zhejiang University
14:00-14:30	Molecular hydrogen dissociation in silicon
	Ben Hourahine, The University of Strathclyde
14:30-15:00	Electrical activity and modulation of oxygen-related defects in
	photovoltaic silicon
	photovoltaic silicon Xuegong Yu, Zhejiang University
15:00-15:30	Xuegong Yu, Zhejiang University
15:00-15:30	Xuegong Yu, Zhejiang University Molecular Hydrogen in Semiconductors: The Sleeping Beauty of
	Xuegong Yu, Zhejiang University Molecular Hydrogen in Semiconductors: The Sleeping Beauty of Defect Engineering
	Xuegong Yu, Zhejiang University Molecular Hydrogen in Semiconductors: The Sleeping Beauty of Defect Engineering Eduard Lavrov, TUD Dresden University of Technology
	Xuegong Yu, Zhejiang University Molecular Hydrogen in Semiconductors: The Sleeping Beauty of Defect Engineering Eduard Lavrov, TUD Dresden University of Technology Invited talks & Contributed talks (Multi-function Hall, 2 nd Floor)

Tao Wang, Peking University
Various defects in AlGaN alloys
Igor Prozheev, University of Helsinki
The Behavior of oxygen in AlN: From Localized Phonons to Radiative Recombination
Erfei Zhang, Peking University
On the origin of the electrically active defects E1 and E3 in GaN and dilute AlxGa1-xN films grown on Ammono-GaN substrates
Piotr Kruszewski, Institute of High Pressure Physics PAS
Coffee Break
Invited talks & Contributed talks (Lecture Hall, 1st Floor)
Chair: Xiaodong Pi
Defect and strain induced energy level modulation and spin polarization in novel 2D materials
Yeliang Wang, Beijing Institute of Technology
Growth Mechanism of III-Nitride Semiconductors on Two- dimensional Substrates
Bing Huang, Beijing Computational Science Research Center
In situ Synchrotron X-ray Characterization of the Nucleation and Growth of AlN Epitaxial Films on Sapphire (0001)
Guangxu Ju, Peking University
Overcoming asymmetric carriers injection in III-nitride LEDs through defect engineering
Yuxin Yang , Changchun Institute of Optics, Fine Mechanics and Physics, Chinese Academy of Sciences
Climb or Glide? ——A Novel Understanding of the Atomistic Dynamic Paths of Threading Edge Dislocations in GaN
Han Yang, Peking University
Invited talks & Contributed talks (Multi-function Hall, 2 nd Floor)
Chair: Eduard Lavrov
Electroluminescence of NV Color Centers in Diamond p-i-n Diodes mediated by Charge-state Dynamics
Yuning Wu, East China Normal University

16:20-16:40	Theoretical investigation of the spin decoherence of carbon-related defects in hexagonal boron nitride	
	Hyeonsu Kim, Sungkyunkwan University	
16:40-17:00	Magnetic-field dependent V_{B}^{-} spin decoherence in hexagonal boron nitrides: A first-principles study	
	Jaewook Lee, Sungkyunkwan University	
17:00-17:20	Stark Shift from Quantum Defects in Hexagonal Boron Nitride	
	Song Li, Beijing Computational Science Research Center	
17:20-17:40	Strain-induced coherence enhancement of solid-state spin defects at zero magnetic field	
	Huijin Park, Sungkyunkwan University	
17:40-18:00	Decoherence dynamics of quantum spins in transition metal dichalcogenides	
	Taejoon Park, Sungkyunkwan University	

18:00-20:00 **Dinner**

Sep.	16	(Tuesday)
Sep.	10 ((I uesuay

Plenary talks (Lecture Hall, 1st Floor) **Session 5:**

Chair: Gregory Fuchs

Bulk GaN growth and defect characterization 8:20-9:00

> Ke Xu, Suzhou Institute of Nano-Tech and Nano-Bionics, Chinese Academy of Sciences

The role of hydrogen in persistent photoconductivity and 9:00-9:40

photochromism

Matthew McCluskey, Washington State University

9:40-10:00 **Coffee Break**

Session 6-1: Invited talks (Lecture Hall, 1st Floor)

Chair: Ke Xu

10:00-10:30 Tailoring Defects in Semiconductors: from Highly Mismatched **Alloys to Polytype Heterostructures**

Rachel Goldman, University of Michigan

10:30-11:00 Unconventional approaches to realize perfect semiconductor

superlattices and heterostructures

Yong Zhang, The University of North Carolina at Charlotte

11:00-11:30 Long carrier lifetime InAs/InAsSb type-II superlattices without Garelated defects for HOT MWIR infrared imaging

Zhi-Chuan Niu, Institute of Semiconductors, Chinese Academy of Sciences

11:30-12:00 Disorder-Assisted Epitaxy of Polymorph Heterostructures

Andrej Kuznetsov, University of Oslo

Session 6-2: Invited talks & Contributed talks (Multi-function Hall, 2nd Floor)

Chair: Jiandong Ye

10:00-10:30 Study on Defects and Thermal Stability in CVD-Grown Si-based Ge

and GeSn Semiconductors

Chi Xu, Institute of Semiconductors, Chinese Academy of Sciences

10:30-10:50 Deep level traps in as-grown epilayers of (010) β-Ga₂O₃ grown by

metal organic chemical vapor deposition on native Sn-doped

substrates

Christopher Dawe, University of Manchester

10:50-11:10	Stabilization of unrelaxed Ga vacancies and ionized acceptors in $\beta\text{-}Ga_2O_3$ through Al-alloying and Si-doping
	Iuliia Zhelezova, Helsinki Accelerator Laboratory
11:10-11:30	Electronic Structure and Doping Properties in Ga ₂ O ₃ -Based Alloys
	Xuefen Cai, Shenzhen University
11:30-11:50	Machine Learning Model for Defect Dynamics in Complex Ga ₂ O ₃ Polymorphs
	Junlei Zhao, Southern University of Science and Technology
12:00-13:30	Lunch
Session 7-1:	Invited talks & Contributed talks (Lecture Hall, 1 st Floor)
	Chair: Hannes Raebiger
13:30-14:00	Performance limiting inhomogeneities of defect states in Ga_2O_3 diodes
	Jiandong Ye, Nanjing University
14:00-14:30	Atom-level mechanisms of solid-to-solid phase transformations in gallium oxide under ion irradiation in the broad range of energies
	Flyura Djurabekova, University of Helsinki
14:30-14:50	The electric field influence on EC-0.18 eV electron trap level in (100)-oriented $\beta\text{-}Ga_2O_3$ crystals grown by the Czochralski method
	Piotr Kruszewski, Institute of High Pressure Physics PAS
14:50-15:10	Observation of Conductive Interstitial Ga Line Defects in $\beta\text{-}Ga_2O_3$
	Debo Hu, National Center for Nanoscience and Technology
15:10-15:30	Gaussian band trap as compensation defect in hetero-epitaxial $\beta\text{-}$ Ga_2O_3 measured by photo-induced current transient spectroscopy
	Rujun Sun, Xidian University
Session 7-2:	Invited talks & Contributed talks (Multi-function Hall, 2 nd Floor)
	Chair: Lei Liu
13:30-14:00	Absorption lines of F centers in MgO and CaO through time-dependent hybrid-functional theory calculations
	Mathilde Franckel, École Polytechnique Fédérale de Lausanne
14:00-14:30	Epitaxy of highly uniform GaN wafers on 2D materials: effect of surface defects manipulation
	Xinqiang Wang, Peking University

14:30-14:50	Why are point-like emitters in Aluminum Nitride so bright?
	Anthony Bennett, Cardiff University
14:50-15:10	Wavefunction theory: a robust tool for color center characterization
	Zsolt Benedek, Eotvos Lorand University
15:10-15:30	First-principles calculations of optical spectra for luminescent centers based on one-dimensional configuration coordinate model
	Harutaka Saito, Osaka University
15:40-15:50	Coffee Break
Session 8-1:	Invited talks (Lecture Hall, 1st Floor)
	Chair: Mathilde Franckel
15:50-16:20	Single Bond Resolved Vibrational Characterization of the Semiconductor Defects Below Surface
	Lei Liu , Changchun Institute of Optics, Fine Mechanics and Physics, Chinese Academy of Sciences
16:20-16:50	Current Status of Semiconductor Intracenter Photonics
	Yasufumi Fujiwara, Ritsumeikan University/Osaka University
Session 8-2:	Invited talks (Multi-function Hall, 2 nd Floor)
	Chair: Yong Zhang
15:50-16:20	Electron Trapping and Luminescence Mechanisms in Rare-Earth Doped Materials
	Khang Hoang, North Dakota State University
16:20-16:50	Deep-Level Defect Characterization and Property Modulation in Two-Dimensional Semiconductors
	Penghong Ci , Institute of Semiconductors, Chinese Academy of Sciences
16:50-18:00	Poster presentation (Entrance Hall, 1st Floor)

18:00-20:00 Dinner & IAC/ISC meeting

Session 9:	Plenary talks (Lecture Hall, 1st Floor)
	Chair: Filip Tuomisto
8:20-9:00	Defect Theory in the Age of Artificial Intelligence
	Aron Walsh, Imperial College London
9:00-9:40	Revisiting the Formulation of Charged Defects in Solids
	Shengbai Zhang
9:40-10:00	Coffee Break
Session 10-1:	Invited talks (Lecture Hall, 1st Floor)
	Chair: Aron Walsh
10:00-10:30	Acceptor Doping and Hole Compensation in CdTe
	Anderson Janotti, University of Delaware
10:30-11:00	Modulation Doping and Polarization-Defect Coupling for 2D Materials Electronics
	Xian-Bin Li, Jilin University
11:00-11:30	Doping and defect physics in low-dimensional semiconductors
	Huixiong Deng , Institute of Semiconductors, Chinese Academy of Sciences
11:30-12:00	First-principles calculations of shallow impurities in semiconductors
	Jun Kang, Beijing Computational Science Research Center
Session 10-2:	Contributed talks (Multi-function Hall, 2 nd Floor)
	Chair: Yu Kumagai
10:00-10:20	Ab initio modeling of doping in hexagonal-diamond silicon
	Marc Túnica, Université Paris-Saclay, CNRS
10:20-10:40	PINN-Based Elastic Field Mapping Around Silicon Nano- inclusions from Atomistic simulation
	Yi Cui, Nagoya University
10:40-11:00	Efficient Generation of Spin Photocurrent by Defect-Mediated Resonant Excitation
	Shixiong Zhang Hubei Normal University

Sep. 17 (Wednesday)

11:00-11:20	Interplay Between Intrinsic Structural Defects and Optoelectronic Properties in Semi-Heusler Gapped Metals
	Muhammad Rizwan Khan, Shenzhen University
11:20-11:40	First-Principles Characterization of the Native Defect Landscape Across Half-Heusler Chemistries
	Angela Pak, University of Illinois at Urbana-Champaign
11:40-12:00	Multidimensional Defect Identification of Semiconductors in Nonequilibrium
	Jun Liu , Key Laboratory of Materials Physics, Institute of Solid State Physics, HFIPS, Chinese Academy of Sciences
12:00-13:30	Lunch
Session 11-1:	Invited talks (Lecture Hall, 1st Floor)
	Chair: Huixiong Deng
13:30-14:00	Prediction of Defect Formation Energies by Machine Learning
	Yu Kumagai, Tohoku University
14:00-14:30	Computational Strategies for Modelling Defects in Semiconductors
	Seán Kavanagh, Harvard University
14:30-15:00	Leveraging defects and interfaces based on low-dimensional materials for memristor applications
	Wennie Wang, University of Texas at Austin
15:00-15:30	Electronic transitions at defects: from theory to applications
	Menglin Huang, Fudan University
Session 11-2:	Contributed talks (Multi-function Hall, 2 nd Floor)
	Chair: Anderson Janotti
13:30-13:50	Giant Flexoelectricity in Bent Semiconductor Thinfilm
	Dongbo Zhang, Beijing Normal University
13:50-14:10	Computational Prediction of an n-type Transparent Conducting Oxide F-doped Sb_2O_5
	Ke Li, University College London
14:10-14:30	Mechanistic Control of Small Interstitial Clusters for Room- Temperature, Post-Synthesis Defect Engineering of Oxides
	Grace McKnight, University of Illinois

14:30-14:50	p-Type (Ultra-) Wide Bandgap NiO-based Semiconductors: Band/Defect Engineering and Their Applications in Bipolar Devices
	Chao Ping Liu, Shantou University
14:50-15:10	P/N-Type Doping in ZnO within Two-Dimensional Limit
	Dong Han, Northeastern University
15:10-15:30	$\label{eq:continuous} Effects \ of \ native \ defects \ in \ ZnO \ electron \ transport \ layers \ on \ stability \ of \ organic \ solar \ cells$
	Chun Yuen Ho, University of Southern Denmark
15:30-15:50	Coffee Break
Session 12-1:	Invited talks (Lecture Hall, 1 st Floor)
	Chair: Shengbai Zhang
15:50-16:20	First-Principles Theory for Excited-States Kinetics and Optical Readout of Quantum Defects
	Erik Perez, University of Wisconsin-Madison
16:20-16:50	Chemical trend of defect-assisted nonradiative carrier recombination in halide perovskites
	Xie Zhang, Northwestern Polytechnical University
16:50-17:20	Defect Theory under Steady Illuminations and Applications
	Ji-Hui Yang, Fudan University
Session 12-2:	Contributed talks (Multi-function Hall, 2 nd Floor)
	Chair: Xianbin Li
15:50-16:10	Impact of Defect-Mediated Recombination on the Performance of Emerging Photovoltaics
	Xinwei Wang, Imperial College London
16:10-16:30	Interaction-induced magnetoconductivity and the Hall effect in disordered massive – massless fermion mixtures
	Yuping Huang , Guangdong Technion – Israel Institute of Technology
16:30-16:50	Theoretical Study of the Magnetic Mechanism of a Pca21 C_4N_3 Monolayer and the Regulation of Its Magnetism by Gas Adsorption
	Dongqiu Zhao, Anyang Normal University
16:50-17:10	Enhanced Gas Sensing Performance of Pd-Doped Janus ZrSSe Monolayer for Early Detection of Lithium-ion Battery Thermal Runaway: A DFT Study
	Guanxiang Yang, North China Electric Power University
18:00-21:00	Banquet

Sep.	18	(Thursday)
Sep.	10	(Illui Suay)

Session 13: Plenary talks (Lecture Hall, 1st Floor)

Chair: Yasufumi Fujiwara

 $8:20-9:00 \qquad \textbf{Building a "defective"} \qquad \textbf{materials genome: high-throughput}$

computational materials design including point defects

Geoffroy Hautier, Rice University

9:00-9:40 Large electronic structure calculations of semiconductor defects

and devices

Lin-Wang Wang, Institute of Semiconductor, Chinese Academy of

Sciences

9:40-10:00 **Coffee Break**

Session 14-1: Invited talks (Lecture Hall, 1st Floor)

Chair: Geoffroy Hautier

10:00-10:30 (Vacancy) defect identification in (compound) semiconductors and

their alloys with positron annihilation spectroscopy

Filip Tuomisto, University of Helsinki

10:30-11:00 **Defect of Kesterite: Synthesis Design Perspectives**

Xiaojin Hao, School of Photovoltaic and Renewable Energy Engineering UNSW

11:00-11:30 Facile Reconstruction of Extended Defects in Antimony Selenide

Keith McKenna, University of York

11:30-12:00 Investigation of basic defects in silicon, acting as spin-to-photon

interfaces

Peter Deák, Beijing Computational Science Research Center

Session 14-2: Invited talks & Contributed talks (Multi-function Hall, 2nd Floor)

Chair: Ji-Hui Yang

10:00-10:30 Nondestructive Visualization of SiC Single-crystal Defects and the

Evolution Mechanism of Typical Defects

Jun Yin, Xiamen University

10:30-10:50 **Defect control in ultra-thick 4H-SiC homoepitaxial layers**

Rong Wang, Zhejiang University

10:50-11:10 Review of the defects in silicon carbide and its influence on the reliability of power devices

Peng Dong, Microsystem and Terahertz Research Center, Institute of Electronic Engineering, China Academy of Engineering Physics

11:10-11:30 **Pre-Filled vs. Pre-Emptied: Distinct Interface State Responses in 4H-SiC VDMOSFETs via Carrier Occupancy Modulation**

Zilan Wang, Dalian University of Technology

11:30-11:50 Key Interface Factors in Total Ionizing Dose Effect of 4H-SiC MOS Devices

Chenfeng Ji, Key Laboratory of Materials Physics, Institute of Solid State Physics, HFIPS, Chinese Academy of Sciences

12:00-13:30 Lunch

Session 15-1: Invited talks (Lecture Hall, 1st Floor)

Chair: Jeffrey McCallum

13:30-14:00 Recent Advances in Understanding the Interface States and Band Tail States in Advanced CMOS Devices at Cryogenic Temperature Runsheng Wang, Peking University

14:00-14:30 Optical spectroscopy of interfacial point defects via electrically stimulated recombination in fully processed silicon carbide power MOSFETs

Dominic Waldhoer, Institute for Microelectronics at TU Wien

14:30-15:00 First-principles study of the random telegraph noise in 2D field-effect transistors

Yong-Hoon Kim, Korea Advanced Institute of Science and Technology

15:00-15:30 Multiscale Ab initio Reliability Simulator (MARS) based on defect database in amorphous SiO₂/HfO₂ interface

Yue-Yang Liu, Institute of Semiconductors, Chinese Academy of Sciences

Session 15-2: Contributed talks (Multi-function Hall, 2nd Floor)

Chair: Xiaojin Hao

13:30-13:50 Impact of Phosphorus Diffusion Pre-gettering on the Electrical Properties of Oxygen Precipitate in n-Type Czochralski Silicon for Heterojunction Solar Cells

Ruokai Wu, Zhejiang University

13:50-14:10	Origin of hole density pinning in group-V doped CdTe
	Baoying Dou, Henan University
14:10-14:30	Data-driven Discovery of Novel High -performance Quaternary Chalcogenide Photovoltaics
	Mohammad Ubaid, Indian Institute of Technology Kanpur
14:30-14:50	Investigation of Defect Evolution in High-Bandgap Kesterite Solar Cells via Advanced Characterisation and First-Principles Insights
	Jialiang Huang, University of New South Wales
14:50-15:10	Defect Engineering in Perovskites for Photovoltaic Applications
	Jian Xu, Beijing Institute of Technology
15:10-15:30	Mitigating Face - Sharing Octahedral Impurity Phases for Efficient Perovskite Photovoltaics
	Yong Wang, Zhejiang University
15:30-15:50	Coffee Break
Session 16-1:	Invited talks & Contributed talks (Lecture Hall, 1st Floor)
	Chair: Yong-Hyun Kim
15:50-16:20	First-principles Study of Defects in Statically Unstable Solids
	Yi-Yang Sun, Shanghai Institute of Ceramics, Chinese Academy of Sciences
16:20-16:50	Multiscale Modeling of Radiation Effects in Semiconductor Devices
	Yonggang Li , Key Laboratory of Materials Physics, Institute of Solid State Physics, HFIPS, Chinese Academy of Sciences
16:50-17:10	Paramagnetic Intrinsic Defects in Calcium Oxide: A First-Principles Study
	YongHyun Kwon, Sungkyunkwan University
17:10-17:30	Improvement of photoluminescence from GaAsPN/GaP alloys by electron irradiation and rapid thermal annealing
	Emil Mihai Pavelescu, IMT Bucharest
Session 16-2:	Contributed talks (Multi-function Hall, 2 nd Floor)
	Chair: Keith McKenna
15:50-16:10	Universal polaron formations in chemically-doped MoS_2 revealed from first principles
	Soungmin Bae, Tohoku University
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16:10-16:30	Study of native and irradiation-induced deep-level defects in transition metal dichalcogenides MX_2 (M = Mo,W; X = S, Se, Te)
	Łukasz Gelczuk, Wrocław University of Science and Technology
16:30-16:50	Persistent photoconductivity and charge carrier absorption in Sb_2Se_3
	Frank Herklotz, Dresden University of Technology
16:50-17:10	Atomically precise Defect Engineering of Semiconductors via Scanning Probe Microscopy
	Hanyan Fang, Nanjing University
17:10-17:30	Microscopic Understanding, Engineering, and Utilization of Defect Behavior in Wide-Bandgap Semiconductors
	Zhiming Shi, Changchun Institute of Optics, Fine Mechanics and Physics (CIOMP), Chinese Academy of Sciences

18:00-20:00 **Dinner**

Sep. 19 (Friday)

Session 17: Plenary talks (Lecture Hall, 1st Floor)

Chair: Matthew McCluskey

8:20-9:00 **Defect Spectroscopy of Ion Implanted Silicon for Quantum**

Technologies

Jeffrey McCallum, University of Melbourne

9:00-9:40 Carbon-based Gap States and Mobility Degradation at SiC/SiO₂

Interfaces

John Robertson, Cambridge University

9:40-10:00 **Coffee Break**

Session 18: Invited talks (Lecture Hall, 1st Floor)

Chair: John Robertson

10:00-10:30 Theory of Static Electricity: Triboelectric Series, Static Adhesion,

and Granular Charging

Yong-Hyun Kim, Korea Advanced Institute of Science and Technology

10:30-11:00 The role played by impurities in 2D Dirac semiconductors near the

critical temperature of the superconducting transition

Ivan Savenko, Guangdong Technion Israel Institute of Technology

11:00-11:30 **Defect Modulation in AlScN Ferroelectric Materials**

Xiaojuan Sun, Changchun Institute of Optics, Fine Mechanics and

Physics, Chinese Academy of Sciences

Closing Session

11:30-11:40 **Closing Remarks**

11:40-13:30 **Lunch**

Poster presentation

P1. Si/SiO₂ MOSFET reliability physics: From four-state model to all-state model

Xinjing Guo, Fudan University

P2. Dynamic phase transformation in Ga₂O₃

Ru He, University of Helsinki

P3. Bridging the Gap Between Hybrid and GGA functionals for Nitrogen and Vacancy Related Defects in Diamond

Samuel Frost, University of Warwick

P4. Exploring the Sb(V) Oxides: Intrinsic Defect Properties and Extrinsic Doping of ASb₂O₆ (A=Mg, Cd)

Ke Li, University College London

P5. Generalized A(n)BC Recombination Model in Semiconductors with Multi-Level Defects

Shanshan Wang, Fudan University

P6. Hole localization in Li-doped antiferromagnetic MnO

Yunfeng Zhu, Yokohama National University

P7. Machine Learning Hamiltonian Enables Scalable and Accurate Defect Calculations: Vacancies in Amorphous SiO₂

Zhenxing Dai, Fudan University

P8. Insights into the Origin of Electron Trapping in Sn(IV) Oxides and Sulfides from First-Principles Calculations

Teruya Nagafuji, Institute of Science Tokyo

P9. Transition metal-hydrogen complexes in SnO₂

Frank Herklotz, Dresden University of Technology

P10. Automating recognition and identification of dislocations in electron channeling images acquired in the scanning electron microscope

Ben Hourahine, The University of Strathclyde

P11. Characterization of deep-level defects in n- and p-type dilute BxGa1-xAs alloys grown at low temperature and their evolution upon annealing

Łukasz Gelczuk, Wrocław University of Science and Technology

P12. First principles study on electronic structure and thermoelectric properties of GaN materials doped with C and Mg atoms

Boyang Huang, Shihezi University

P13. Defect Phonon Renormalization during Nonradiative Multiphonon Transitions in Semiconductors

Junjie Zhou, Fudan University

P14. "One defect, one potential" strategy for accurate machine learning prediction of defect phonons

Junjie Zhou, Fudan University

P15. Independent determination of carrier densities and analysis of different recombination channels in GaAs through Raman scattering of LO phonon-plasmon coupled mode

Fan Zhang, Songshan Lake Materials Laboratory, Dongguan

P16. Nanoscale arsenic doping in silicon by self-assembled molecular monolayers

Xuejiao Gao, North China Electric Power University

P17. Characterizing non-equilibrium doping effects in Aluminum nitride under multiple fabrication conditions

Kai Liu, Shenzhen Technology University

P18. Comprehensive research of the hydrogenated intrinsic vacancies of β -Ga₂O₃ by first principles

Tao Wang, Xi'an Jiaotong University

P19. Investigation of point defects in semiconductors via positron annihilation spectroscopy

Xingzhong Cao, Institute of High Energy Physics, CAS

P20. Effects of Nitrogen doping on defect behaviour in Czochralski silicon: An ab initio investigation

Hao Hu (Yu Pei), Shanghai Advanced Silicon Technology

P21. Scalable Defect Modeling in Amorphous HfO₂: From Small to ultra-Large Supercells with GNN Interatomic Potentials

Shuqi Tang, Fudan University

P22. Probing Interface Phonons and Defects in Correlated Oxide Heterostructures via Sum-Frequency Spectroscopy

Tongying Liu, Fudan University

P23. Atomistic mechanisms of radiation-induced defects in β-Ga₂O₃: Insights from molecular dynamics simulations

Huan He, Xi'an Jiaotong University

P24. Study and analysis of radiation effects in single-photon avalanche diodes

Zixuan Wang, Hunan Normal University

P25. Effects of Gamma Irradiation on ESD Performance of High-Voltage SCR with double-snapback characteristic

Yujie Liu, Hunan Normal University

P26. Resolidified Chalcogen Precursors for High-Quality 2D Semiconductor Growth

Di Yang, Tsinghua Shenzhen International Graduate School

P27. Reassessing Dynamic Jahn Teller effect in diamond NV- center based on saddle point excited state theory

Lei Sun, Peking University

P28. Exclusive Generation of Single-atom Sulfur for Ultrahigh Quality Monolayer MoS₂ Growth

Yunhao Zhang, Tsinghua Shenzhen International Graduate School

P29. Influence of Surface Treatments on the Ohmic Contact Performance on the N-Face of Iron-Doped Semi-Insulating Freestanding GaN

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

P30. Study of the Growth Mechanism and Defects of GaN Films by Remote Epitaxy

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