

Symposia – G02

Advanced Materials by Computational Design and Simulation

Oct 15 (Sunday), 2023

Conference Room: 5702, 7# floor

8:40-10:40 Session I

Chair: Xiaoming Zhang

8:40-9:20 (G02-01)

First-principles study of unusual material properties of Cu-based compounds (Keynote)

Suhuai Wei, Beijing Computational Science Research Center, China

9:20-9:40 (G02-02)

Dilute Element Compounds and Application in Energy Storage Materials (Invited)

Yiyang Sun, Shanghai Institute of Ceramics, Chinese Academy of Sciences, China

9:40-10:00 (G02-03)

Thermoelectric properties of pyrite-type dichalcogenides (Invited)

Yongsheng Zhang, Qufu Normal University, China

10:00-10:20 (G02-04)

Molecular Understanding of the Critical Role of Alkali Metal Cations in CO₂ Electroreduction on Copper Surface (Invited)

Jia Li, Tsinghua Shenzhen International Graduate School, China

10:20-10:40 (G02-05)

Stacking bilayer ferroelectricity and ferrovalley (Invited)

Changsong Xu, Fudan University, China

10:40-10:55 Coffee Break

10:55-12:35 Session II

Chair: Yiyang Sun

10:55-11:35 (G02-06)

Excitonic Condensation in a Quantum Semiconductor of Superatomic Graphene with Yin-Yang Flat Bands (Keynote)

Feng Liu, University of Utah, USA

11:35-11:55 (G02-07)

Various topological phases in layered van de Waals materials (Invited)

Zhenhua Qiao, University of Science and Technology, China

11:55-12:15 (G02-08)

Large family Kagome materials for topology and correlation in low-dimension (Invited)

Jiatao Sun, Beijing Institute of Technology, China

12:15-12:35 (G02-09)

Topological Superconductivity Based on

Antisymmetric Spin-Orbit Coupling (Invited)

Xiaoming Zhang, Ocean University of China, China

12:35-13:45 Lunch

13:45-15:45 Session III

Chair: Xunhua Zhao

13:45-14:25 (G02-10)

Accelerating the Discovery and Design of Novel Materials by ALKEMIE (Keynote)

Zhimei Sun, Beihang University, China

14:25-14:45 (G02-11)

Paving a Data-centric Highway for Materials Science (Invited)

Miao Liu, Institute of Physics, Chinese academy of sciences, China

14:45-15:05 (G02-12)

Defect Stability of Metals: Model Construction and Application (Invited)

Wang Gao, Jilin university, China

15:05-15:25 (G02-13)

Multiscale Modeling of Radiation Effects in Semiconductor Devices (Invited)

Yonggang Li, Hefei Institutes of Physical Science, Chinese Academy of Sciences, China

15:25-15:45 (G02-14)

New understanding of effects of shock loading on irradiated grain boundaries by molecular dynamics method (Invited)

Ning Gao, Shandong University, China

15:45-16:00 Coffee break

16:00-17:52 Session IV

Chair: Miao Liu

16:00-16:20 (G02-15)

Molecular Simulations on Wettability and Evolution of Surface Nanobubbles (Invited)

Hui Li, Beijing University of Chemical Technology, China

16:20-16:40 (G02-16)

Simulating dynamics of electrochemical interfaces under realistic conditions

Xunhua Zhao, Southeast University, China

16:40-17:00 (G02-17)

Microstructure evolution and thermal-mechanical properties in tungsten: mesoscale approach simulations (Invited)

Linyun Liang, Beihang University, China

17:00-17:20 (G02-18)
Enhancing XYG3-type Doubly Hybrid Approximations Through the Self-Interaction Correction and Deep-Learning Methods (Invited)
Sheng Bi, Zhejiang Lab, China

17:20-17:40 (G02-19)
Anisotropy and flexibility engineering of graphene by heterojunctions (Invited)
Lizhao Liu, Dalian University of Technology, China

17:40-17:52 (G02-20)
The stability of interstitials in high-entropy alloys: the determining role of chemical environments and magnetic moments (Oral)
Zhiling Luo, Jilin University, China

17:52-18:04 (G02-21)
A Rule of Solute Segregation at Grain Boundaries (Oral)
Xin Li, Jilin University, China

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Oct 16 (Monday), 2023

8:45-10:40 Session I

Chair: Wei Jiang

8:45-9:25 (G02-01)
Atomistic modeling of single and double moire patterned graphene and hexagonal boron nitride multilayer systems (Keynote)
Jeil Jung, University of Seoul, South Korea

9:25-9:45 (G02-02)
Insights into exotic quantum materials via first-principles hyperfine coupling calculations (Invited)
Zheng Liu, Tsinghua University, China

9:45-10:05 (G02-03)
Spin crystalline group in magnetic materials (Invited)
Qihang Liu, Southern University of Science and Technology, China

10:05-10:25 (G02-04)
Improving graph neural network models for catalysis systems (Invited)
Xiaolong Zou, Tsinghua Shenzhen International Graduate School, China

10:25-10:40 (G02-05)
Topology Conservation Theorem, Quantum Instability and Violation of Subperiodic Symmetry of Complex Low-Dimensional Lattices (Oral)
Pavel Avramov, Kyungpook National University, South Korea

10:40-10:55 Coffee Break

10:55-12:07 Session II

Chair: Zheng Liu

10:55-11:15 (G02-06)
Emergent phenomena of oxide thin films and heterostructures (Invited)
Hanghui Chen, NYU Shanghai and New York University, China

11:15-11:35 (G02-07)
Nonlinear electric spin generation (Invited)
Shengyuan Yang, University of Macau, Macau SAR, China

11:35-11:55 (G02-08)
Enhancement of Intrinsic Spin Hall Effect in Chiral Topological Semimetals (Invited)
Wei Jiang, Beijing Institute of Technology, China

11:55-12:07 (G02-09)
Distinct Current Induced Spin Polarization in One-Dimensional Chiral Nanowires (Oral)
Guoxiang Zhi, Tianmushan Laboratory, China

12:07-14:00 Lunch

14:00-15:40 Session III

Chair: Weiwei Sun

14:00-14:20 (G02-10)
Emerging Ferroelectricity and Negative Piezoelectricity in two-dimensional single-element materials (Invited)
Yunhao Lu, Zhejiang University, China

14:20-14:40 (G02-11)
Covalent-Like Bondings and Abnormal Formation of Ferroelectric Structures in Binary Ionic Salts (Invited)
Menghao Wu, Huazhong University of Science and Technology, China

14:40-15:00 (G02-12)
Structural evolution and novel application of low-dimensional surface, defects, and supported clusters (Invited)
Junfeng Gao, Dalian University of Technology, China

15:00-15:20 (G02-13)
Large enhancement of Curie temperature in Fe_3GeTe_2 by Fe intercalation in the van der Waals gap (Invited)
Cong Wang, Renmin University of China, China

15:20-15:45 Coffee break

15:45-17:17 Session IV

Chair: Junfeng Gao

15:45-16:05 (G02-14)
Emergent quantum states in two-dimensional charge density wave materials (Invited)
Chen Si, Beihang University, China

16:05-16:25 (G02-15)

From MXene to anti-MXene: hydrogen enhanced superconducting behavior and exotic magnetic interaction (Invited)

Weiwei Sun, Southeast University, China

16:25-16:45 (G02-16)

Designing of anode materials for alkali metal-ion batteries through DFT calculations and machine learning methods (Invited)

Haiyuan Chen, University of Electronic Science and Technology of China, China

16:45-17:05 (G02-17)

TBA (Invited)

Inspur group, China

17:05-17:17 (G02-18)

Quantifying the effects of nanoparticles on the printability of AlSi10Mg manufactured by laser powder bed fusion (Oral)

Liping Guo, Shanghai Jiao Tong University, China