

Program of the Workshop

Venue: Lecture Hall 552, Physics Building, Haiyun Campus, Xiamen University

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| October 20 | Registration |
| October 21 | |
| Welcome & Opening Remarks 8:30~8:50 | Chair: Prof. Xingao Gong (Fudan University) Prof. Rong Zhang (President, Xiamen University) Prof. Zhenyu Zhang (USTC) |
| Session I | Fundamentals |
| | Chair: Prof. Zijing Lin (USTC) |
| 8:50~9:25 | How Energy is Dissipated in Nanomechanical Non-equilibrium: Classical and Quantum Friction at Large Temperature, Speed, or Pressure Erio Tosatti (International School for Advanced Studies (SISSA), Italy) |
| 9:25~10:00 | Non-Abelian Properties of Jackiw-Rebbi Zero Modes Xincheng Xie (Peking University, China) |
| 10:00~10:25 | Photo Time & Coffee Break |
| Session II | Emergent Phenomena in 2D Materials |
| | Chair: Prof. Zi-Zhong Zhu (Xiamen University) |
| 10:25~11:00 | Exploring New Territories of the 2D Materials World Steven G. Louie (University of California at Berkeley, USA) |
| 11:00~11:35 | Semiconductors in the 2D Limit: from Topological Insulator to Excitonic Insulator Shengbai Zhang (Rensselaer Polytechnic Institute, USA) |
| 11:35~12:10 | Study of Interlayer Magnetism in Bilayer CrX ₃ Shiwei Wu (Fudan University, China) |
| 12:10~14:00 | Lunch |
| Session III | Carbon-Based Low-D Materials |
| | Chair: Prof. Zhenhua Qiao (USTC) |
| 14:00~14:35 | Single Crystal Graphene and AB-stacked Graphene, and Synthesis & Properties of Diamane Rodney Ruoff (IBS Center for Multidimensional Carbon Materials, UNIST, Korea) |
| 14:35~15:10 | Diamond: From Jewellery to Semiconductor Material Chongxin Shan (Zhengzhou University, China) |
| 15:10~15:45 | Computational Design of Functional Nanostructures Shixuan Du (Institute of Physics, CAS, China) |



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| 15:45~16:05 | Coffee Break |
| Session IV | Energy Conversion Systems & Processes Chair: Prof. Jisoon Ihm (Pohang University of Science and Technology, Korea) |
| 16:05~16:40 | Water on Rutile TiO ₂ (110) and Anatase TiO ₂ (001) Surfaces Bing Wang (USTC, China) |
| 16:40~17:15 | Simulation of Spin Chains using Room Temperature Polariton Condensates Zhanghai Chen (Xiamen University, China) |
| 17:15~17:50 | <i>Ab Initio</i> Investigations on the Excited Carrier Dynamics in Condensed Matter Systems Jin Zhao (USTC, China) |
| 18:00~ | Banquet |
| October 22 | |
| Session V | Predictive Discoveries of Low-D Materials Chair: Prof. Yu Jia (Zhengzhou University) |
| 8:30~9:05 | Universal Linear Scaling of Topological Phase Transition in Band Theory Feng Liu (University of Utah, USA) |
| 9:05~9:40 | Computationally-aided Materials Discovery Caizhuang Wang (Iowa State University, USA) |
| 9:40~10:00 | Coffee Break |
| Session VI | Predictions & Processes in Energy Materials Chair: Prof. Tai Min (Xi'an Jiaotong University) |
| 10:00~10:35 | Determining Spectrum-structure Relations with Machine Learning Techniques Yi Luo (USTC, China) |
| 10:35~11:10 | Anharmonic Effects in Heat and Charge Transport Christian Carbogno (Fritz Haber Institute of the Max Planck Society, Germany) |
| 11:10~11:45 | Cs Corrected Transmission Electron Microscopy for Thermoelectric Materials Jiaqing He (Southern University of Science and Technology, China) |
| 12:00~14:00 | Lunch |
| 13:00~14:00 | Poster Setup |
| Session VII | Exotic Properties of Novel Functional Materials Chair: Prof. Jianxin Zhong (Xiangtan University) |
| 14:00~14:35 | Classical Wave Counterparts of Topological Materials Che Ting Chan (Hong Kong University of Science and Technology, Hong |



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| | Kong) |
| 14:35~15:10 | Phononic Semimetals and the Surface States Zhengyou Liu (Wuhan University, China) |
| 15:10~15:45 | Topics of Two-Dimensional Materials and Their Heterostructures Mei-Yin Chou (Institute of Atomic and Molecular Sciences, Academia Sinica, Taiwan & Georgia Institute of Technology, USA) |
| 15:45~18:10 | Poster Session (with Light Refreshments) |
| 18:30~ | Dinner Receptions |
| October 23 | |
| Session VIII | Nanoplasmonics for Energy Chair: Prof. Changgan Zeng (USTC) |
| 8:30~9:05 | Some Thoughts on Plasmonic Chemistry and Spectroscopy Zhongqun Tian (Xiamen University, China) |
| 9:05~9:40 | Plasmon-enhanced Single-molecule Optical Spectroscopy Zhenchao Dong (USTC, China) |
| 9:40~10:15 | Signatures of Quantum Effects in the Absorption and Emission of Plasmon-exciton Hybrid Systems Xiaoguang Li (Shenzhen University, China) |
| 10:15~10:35 | Coffee Break |
| Session IX | Solar Energy Conversion Chair: Prof. Qunxiang Li (USTC) |
| 10:35~11:10 | Band Structure Engineering and Doping Control of Wide-Band-Gap Materials for Optoelectronic Applications Suhuai Wei (Beijing Computational Science Research Center, China) |
| 11:10~11:45 | High-efficiency CZTSSe Solar Cells through Design of Grading Active Layer Sixin Wu (Henan University, China) |
| Best Poster Awards & Concluding Remarks 11:45~12:15 | Prof. Xingao Gong (Fudan University) Prof. Steven G. Louie (UC Berkeley) Prof. Shouzhu Zhang (formerly at National Natural Science Foundation) |
| 12:15~ | Lunch & Departure |