

## Program of the 8<sup>th</sup> International Workshop on Quantum Energy

Venue: 5F, Nanya Hall (南亚厅), Howard Johnson Tropical Garden Plaza Kunming

<b>October 16</b>	<b>Registration</b>
<b>October 17</b>	
<b>Welcome &amp; Opening Remarks</b> 8:40~9:00	Chair: Prof. Shumei Hao (Yunnan University) Prof. Li Zhang (Vice President, Yunnan University) Prof. Xingao Gong (Director, Key Laboratory of Computational Physical Sciences of MOE, Fudan University)
<b>Session I</b>	<b>Fundamentals &amp; Methodologies</b> Chair: Prof. Xingao Gong (Fudan University)
9:00~9:35	New <i>Ab Initio</i> Many-body Approaches to Excited-State Phenomena for Quantum Energy Steven G. Louie (University of California at Berkeley, USA)
9:35~10:10	Materials Informatics and Machine Learning for Material Discovery Hong Guo (McGill University, Canada)
10:10~10:35	<b>Photo Time &amp; Coffee Break</b>
<b>Session II</b>	<b>Topological Quantum Materials</b> Chair: Prof. Zhong Fang (Institute of Physics, CAS)
10:35~11:10	Quantum Spin Hall Effect and Spin Bott Index in a Quasicrystal Lattice Feng Liu (University of Utah, USA)
11:10~11:45	Catalogue of Topological Electronic Materials Chen Fang (Institute of Physics, CAS, China)
11:45~12:20	ARPES Investigation on Electronic Correlation Effects in Topological Quantum States Nan Xu (Wuhan University, China)
12:20~14:00	<b>Lunch</b>
<b>Session III</b>	<b>Growth and Properties of 2D Materials</b> Chair: Prof. Jianxin Zhong (Xiangtan University)
14:00~14:35	Metal Growth on and under Graphene: Controlling Morphology and Intercalation Michael Tringides (Iowa State University, USA)
14:35~15:10	Exploring Two-Dimensional Porous Polymeric Materials via Molecular Assembly for Photocatalytic Water Splitting Xiaojun Wu (USTC, China)

15:10~15:45	First-Principles Study of Two-Dimensional Layered Electrides Jinho Choi (Soochow University, China)
15:45~16:05	<b>Coffee Break</b>
<b>Session IV</b>	<b>Energy Conversion Processes</b> <b>Chair: Prof. Chongxin Shan (Zhengzhou University)</b>
16:05~16:40	Imaging Hydrogen Dynamics at Water Oxide Interface Bing Wang (UTSC, China)
16:40~17:15	A New Strategy for Hydrogen Doping into Energy Materials Jun Jiang (USTC, China)
17:15~17:50	Perspectives of Future Green Energy Systems Xuesen Wang (National University of Singapore, Singapore)
18:00~	<b>Banquet</b>
<b>October 18</b>	
<b>Session V</b>	<b>Nanoplasmonics for Energy</b> <b>Chair: Prof. Hongxing Xu (Wuhan University)</b>
8:40~9:15	Plasmonics for Sustainability and Societal Impact Naomi J. Halas (Rice University, USA)
9:15~9:50	Exploring Single-Molecule Optoelectronics with Scanning Tunneling Microscope Induced Luminescence Technique Yang Zhang (USTC, China)
9:50~10:10	<b>Coffee Break</b>
<b>Session VI</b>	<b>Optoelectronics</b> <b>Chair: Prof. Zhenchao Dong (USTC)</b>
10:10~10:45	Plasmon-Induced Hot Carrier Generation and Applications Peter Nordlander (Rice University, USA)
10:45~11:20	Implications of Electronic Dimensionality of Optoelectronic Materials Yanfa Yan (University of Toledo, USA)
11:20~11:55	Non-Blinking Quantum-Dot-Based Light-Emitting Diodes Huaibin Shen (Henan University, China)
12:00~14:00	<b>Lunch</b>
13:00~14:00	<b>Poster Setup</b>
<b>Session VII</b>	<b>Excited-State and Nonequilibrium Phenomena</b> <b>Chair: Prof. Yang Wang (Pittsburgh Supercomputing Center, USA)</b>
14:00~14:35	Fluctuations, Entropy and Rare Events Michele Parrinello (ETH Zürich, Switzerland)
14:35~15:10	Excitonic Insulators in Direct-Gap Solids Shengbai Zhang (Rensselaer Polytechnic Institute, USA)

15:10~15:30	<b>Coffee Break</b>
<b>Session VIII</b>	<b>Nanoscale Transport Phenomena</b> Chair: Prof. Shengjun Yuan (Wuhan University)
15:30~16:05	Non von Neumann Spintronic Devices Jian Shen (Fudan University, China)
16:05~16:40	Predicting New Transition Metal Oxides for Photovoltaics and Spintronics Guang-Yu Guo (National Taiwan University, Taiwan)
16:40~18:10	<b>Poster Session (with Light Refreshments)</b>
18:30~	<b>Dinner Receptions</b>
<b>October 19</b>	
<b>Session IX</b>	<b>Novel Materials Discoveries by Design</b> Chair: Prof. Qunxiang Li (USTC)
8:40~9:15	Computational Studies of Thermoelectric Materials Mei-Yin Chou (Institute of Atomic and Molecular Sciences, Academia Sinica, Taiwan & Georgia Institute of Technology, USA)
9:15~9:50	Search for Rare-earth Free Permanent Magnets Caizhuang Wang (Iowa State University, USA)
9:50~10:05	<b>Coffee Break</b>
<b>Session X</b>	<b>Solar Cells</b> Chair: Prof. Yu Jia (Zhengzhou University)
10:05~10:40	Theoretical Investigation of Stable Halide Perovskite for Solar Cell Applications Suhui Wei (Beijing Computational Science Research Center, China)
10:40~11:15	Interface in the Device of the Organic Solar Cells Zhu Liu (Yunnan University, China)
11:15~11:50	Towards the Optimization of Solar Cell Materials: Theoretical Design and Defect Engineering Jihui Yang (Fudan University, China)
<b>Best Poster Award Ceremony</b> 11:50~12:00	Prof. Steven G. Louie (UC Berkeley, USA) Prof. Michele Parrinello (ETH Zürich, Switzerland) Prof. Shouzhu Zhang (NSFC, China)
<b>Concluding Remarks</b> 12:00~12:10	Prof. Hongxing Xu (Wuhan University) Prof. Zhenyu Zhang (USTC)
12:10~	<b>Lunch &amp; Departure</b>