SCIENTIFIC PROGRAM

Thursday, 24 October, 2013

3:00 – 8:00 PM Registration
6:00 – 8:00 PM Reception

Friday, 25 October, 2013

8:30 – 8:35 AM Introductory Remarks
8:35 – 8:50 AM Welcome Address

Session A: Clusters and Nanoparticles
Chairman: Xingao Gong, *Fudan University, China*

8:50 – 9:20 AM "Atomic Clusters: What Can They Teach Us about Materials for Sustainable Energy?"
Puru Jena, *Virginia Commonwealth University, USA*

9:20 – 9:40 AM "Enhanced Photon Conversion and Absorption in Nanostructured Solar Cells"
Yalin Lu, *University of Science and Technology of China, China*

9:40 – 10:00 AM "The Smallest Member of the Thiolated Gold Nanoclusters"
De-En Jiang, *Oak Ridge National Laboratory, USA*

10:00 – 10:20 AM "Size-Dependent Structural Characteristics and Phonon Thermal Transport in Silicon Nanoclusters"
Hai-Peng Li, *China University of Mining and Technology, China*

10:20 – 10:40 AM TEA BREAK

Session B: Materials Design I
Chairman: Yalin Lu, *University of Science and Technology of China*

10:40 – 11:10 AM "Higher Level of *Ab Initio* Computer Simulation for Materials Design: How to Perform Theoretical Design of Materials"
Yoshiyuki Kawazoe, *Tohoku University, Japan*

11:10 – 11:30 AM "Manipulate Electronic and Spin States in Zigzag Graphene Nanoribbons"
Zhi Zeng, *Institute of Solid State Physics, Chinese Academy of Sciences, China*

11:30 – 11:50 AM "MXene: Computational Studies on Electronic Properties, Surface Functionalizations, and Applications to Energy Storage"
Zhen Zhou, *Nankai* University, *China*

11:50 – 12:10 PM "Thermoelectric Properties of Bi-based Nanomaterials"
Huijun Liu, *Wuhan University, China*

12:10 – 12:30 PM "Modulating Electrons and Phonons in Two-Dimensional Silicon Nanostructures"
R.Q. Zhang, *City University of Hong Kong, China*

12:30 – 1:30 PM **LUNCH**

Session C: Hydrogen Storage I
Chairman: Dalin Sun, *Fudan University, China*

2:00 – 2:30 PM "The Physical Potential and Limitations of Hydrogen Storage"
Andreas Züttel, *EMPA Swiss Federal Laboratories for Materials Testing and Research, Hydrogen & Energy, Switzerland*

2:30 – 2:50 PM "Hydrogen Storage Over Chemicals Containing Protic and Hydride Hydrogens: Materials Design and Catalytic Modification"
P. Chen, *Dalian Institute of Chemical Physics, Chinese Academy of Sciences, China*

2:50 – 3:10 PM "Modeling on Adsorption Properties in Novel Hydrogen Storage Materials"
H. Mizuseki, *Korea Institute of Science and Technology (KIST), Republic of Korea*

3:10 – 3:30 PM "Theoretical Study of Hydrogen Storage in Low-Dimensional Materials"
Qiang Sun, *Zhengzhou University, China*

3:30 – 3:50 PM "First-Principles Design of Nanomaterials for Hydrogen Generation and Storage"
Jijun Zhao, *Dalian University of Technology, China*

3:50 – 4:10 PM **TEA BREAK**

Session D: Hydrogen Storage II
Chairperson: Zhi Zeng, *Institute of Solid State Physics, CAS, China*

4:10 – 4:40 PM "Computer Simulation of Adsorption and Storage of Gases in Nanoporous Carbons"

Julio A. Alonso, *University of Valladolid, Spain*

4:40 – 5:00 PM "Recent Research Progress on Hydrogen Storage in Porous Materials in Korea"
Jisoon Ihm, *Seoul National University, Republic of Korea*

5:00 – 5:20 PM "Cluster-Based Nanostructures for Hydrogen Storage and Heterogeneous Catalysis"
Qingfeng Ge, *Southern Illinois University, USA*

5:20 – 5:40 PM "Hierarchical One-Dimensional Nanostructure for Advanced Energy Storage"
Liqiang Mai, *Wuhan University of Technology, China*

7:00 – 9:30 PM BANQUET

Saturday, 26 October, 2013

Session E: Monolayer Materials
Chairman: Zhigang Shuai, *Tsinghua University, China*

8:30 – 9:00 AM "Interface Effect on Thermal Conduction of Nanomaterials and Its Manipulation"
Xingao Gong, *Fudan University, China*

9:00 – 9:20 AM "Is Graphene Chemical Vapor Deposition (CVD) Growth Epitaxial?"
Feng Ding, *Hong Kong Polytechnic University, China*

9:20 – 9:40 AM "Double-Chain Substructures in Nanoribbon $B_nH_2^{0/-/2-}$ Clusters (n = 6–22) and Cage-Like D_{2d} B_{40} Fullerene"
Si-Dian Li, *Shanxi University, China*

9:40 – 10:00 AM "Recent Progress in Understanding Water"
Chang Q Sun, *Nanyang Technological University, Singapore*

10:00 – 10:20 AM TEA BREAK

Session F: Modeling Methods
Chairman: Si-Dian Li, *Shanxi University, China*

10:20 – 10:50 AM "Defects with Energy-Relevant Functionality in 2D Materials--Graphene, h-BN, Metal-Disulfides"
Boris I. Yakobson, *Rice University, USA*

10:50 – 11:10 AM "Modeling of Organic Energy Materials: Charge Mobility and Thermoelectrics"
Zhigang Shuai, *Tsinghua University, China*

11:10 – 11:30 AM "Antiferromagnetic Topological Insulator for Spintronics"
Xiao Hu, *National Institute for Materials Science (NIMS), Japan*

11:30 – 11:50 AM "Stochastic Surface Walking Method and Beyond"
Zhi-Pan Liu, *Fudan University, China*

11:50 – 12:10 PM "Inverse Design of Si Nanomaterials for Optoelectronic Applications"
Jun-Wei Luo, *National Renewable Energy Laboratory, USA*

12:10 – 12:30 PM "Toward Multiscale Modeling of Small Molecule Organic Solar Cells"
Chun-Wei Pao, *Research Center for Applied Sciences, Academia Sinica, Taiwan*

12:30 – 1:30 PM **LUNCH**

Session G: Battery Materials
Chairman: Jun Li, *Ningbo Institute of Material Technology and Engineering, China*

2:00 – 2:30 PM "Li Transport in Battery Electrodes"
John S. Tse, *University of Saskatchewan, Canada*

2:30 – 2:50 PM "Atomic and Nano-scale Design of Electrode Materials for Lithium Rechargeable Batteries"
Kisuk Kang, *Seoul National University, Republic of Korea*

2:50 – 3:10 PM "Nanoparticles for Lithium-Sulfur Batteries"
Liwei Chen, *Suzhou Institute of Nanotech and Nanobionics, Chinese Academy of Sciences, China*

3:10 – 3:30 PM "Nanoporous Metal-based Electrode Materials for High-Performance Electrochemical Energy Storage and Biosensing"
Qing Jiang, *Jilin University, China*

3:30 – 3:50 PM "The Design of Advanced Functional Materials from *Ab Initio* Calculations"
Li-Min Liu, *Beijing Computational Science Research Center, China*

3:50 – 4:10 PM **TEA BREAK**

Session H: Materials for Energy
Chairman: Zhen Zhou, *Nankai University, China*

4:10 – 4:40 PM "Energy Harvesting with Hierarchical 1D, 2D, and 3D Nanostructures"
Young Hee Lee, *Sungkyunkwan University, Republic of Korea*

4:40 – 5:00 PM "Advanced Carbon-based Nanotubes/Nanocages for Energy Conversion and Storage: Synthesis, Performance and Mechanism"
Zheng Hu, *Nanjing University, China*

5:00 – 5:20 PM "Flexible Nanogenerators"
Yong Qin, *Lanzhou University, China*

5:20 – 5:40 PM "Growth and Atomic-Scale Characterizations of Graphene and Graphene-h-BN Hybrid on Metal Substrates"
Yanfeng Zhang, *Peking University, China*

5:40 – 6:00 PM "Design of Metal Organic Frameworks for Efficient Gas Adsorption by Multi-scale Simulation"
Sang Soo Han, *Korea Institute of Science and Technology (KIST), Republic of Korea*

6:00 – 8:00 PM DINNER

8:00 – 9:30 PM POSTER SESSION

Sunday, 27 October, 2013

Session I: Catalysis I
Chairman: Zhi-Pan Liu, *Fudan University, China*

8:30 – 9:00 AM "Engineering Clusters/Graphene for Catalytic Applications: First-Principles Studies"
Yuan Ping Feng, *National University of Singapore, Singapore*

9:00 – 9:20 AM "Kinetic Theory for Sintering of Supported Metal Particles from First-Principles"
Wei-Xue Li, *Dalian Institute of Chemical Physics, Chinese Academy of Sciences, China*

9:20 – 9:40 AM "Rational Computation Design of Novel Materials for Energy Storage and Conversion"
Jun Li, *Ningbo Institute of Material Technology and Engineering, Chinese Academy of Sciences, China*

9:40 –10:00 AM "Searching of Carbon Based Pt Replacement Catalysts for Oxygen Reduction Reaction"
Lixin Zhang, *Nankai University, China*

10:00 – 10:20 AM "The Recent Advances of Gold Nanocatalysts in CO Oxidation"
Yi Gao, *Shanghai Institute of Applied Physics, Chinese Academy of Sciences, China*

10:20 – 10:40 AM **TEA BREAK**

Session J: Catalysis II
Chairman: Gang Chen, *Jinan University, China*

10:40 – 11:00 AM "A First-Principles Investigation on the Interaction Between Ultrafast Laser and Nano-Materials"
Hong Zhang, *Sichuan University, China*

11:00 – 11:20 AM "The Mechanism of Catalytic Cutting of Carbon Nanotubes and Graphene into Graphene Ribbons"
Jinlan Wang, *Southeast University, China*

11:20 – 11:40 AM "Structural, Electrical and Catalytic Properties of Platinum Nanotubes"
Bikash C. Gupta, *Visva-Bharati, India*

11:40 – 12:00 AM "Quantum Simulation of Low-Temperature Metallic Liquid Hydrogen"
Xin-Zheng Li, *Peking University, China*

12:00 – 12:10 PM **CLOSING REMARKS**

12:10 – 1:30 PM **LUNCH**