

The Sixth General Meeting of ACCMS-VO
(Asian Consortium on Computational Materials Science - Virtual Organization)

February 10-12, 2012

Institute for Materials Research, Tohoku University, Sendai, Japan
Hotel Matsushima Taikanso, Japan

SCIENTIFIC PROGRAM (February 9, 6pm Version, If you have any questions, contact kawalab@imr.edu)

I-*: Invited (30 min., presentation + discussion)

O-*: Oral (15 min., presentation + discussion)

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10th (Friday) (Institute for Materials Research, Tohoku University, Sendai)

9:00-18:00 Registration Desk (Institute for Materials Research)

10:00-10:05 Opening Remarks: Y. Kawazoe

Announcement: H. Mizuseki

10:05-10:10 Greetings from the Director of IMR, M. Niinomi

10:10-12:10 (Chair: Gour P. Das)

I-1: Sukit Limpijumnong, "First Principles Study of Al Doped ZnO"

I-2: Michael Ronald Philpott, "Chymera Magnetic States of Graphene Nanodots"

I-3: Kombiah Iyakutti, "Investigation of Effect of Unequal Effective Mass Fermions in Graphene"

I-4: Jian-Tao Wang, "Mechanism for Direct Conversion of Graphite to Diamond"

12:10-13:00 Lunch (Box Lunch)

13:00-15:00 (Chair: Sukit Limpijumnong)

I-5: Gour P. Das, "Graphene-like Materials and Their Functionalization: Advent of a New Family"

I-6: Umesh Waghmare, "Theory of Defects in Graphene and Related Nano-materials"

I-7: Vijay Kumar, "From Silicon Fullerenes to Bulk Metallic Glasses - My Golden Time with IMR"

I-8: Kaoru Ohno, "All-electron Mixed Basis Approach for Accurate First Principles Calculations"

15:00-15:30 Coffee Break

15:30-17:15 (Chair: Michael Ronald Philpott)

I-9: Marcel Sluiter, "Multinary Cluster Expansions for Dilute Al-Mg-Si and Al-Mg-Li Alloys"

I-10: Yuan Ping Feng, "Spin-dependent Transport of GMR and TMR Devices"

O-1: Andrey Lyalin, "Catalytic Activity of Graphene and h-BN Based Nanomaterials for Oxygen Reduction Reaction"

O-2: Abhishek Singh, "Interfaces in Graphitic Materials"

O-3: Hongming Weng, "Chern Semimetal and Quantized Anomalous Hall Effect in HgCr_2Se_4 "

17:30-19:00 Poster Session (Chair: H. Mizuseki)

18:30-19:30 Registration Desk (Westin Hotel, 2F)

19:30- Banquet

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11th (Saturday) (Institute for Materials Research, Tohoku University, Sendai)

9:00-10:30 (Chair: Umesh Waghmare)

I-11: Katsumi Tanigaki, "Charge Transfer to Organic Semiconductors on the Au Electrodes Modified by Self-assembled Monolayers : Comparison between Experiment and Theory"

I-12: Momoji Kubo, "Tight-Binding Quantum Chemical Molecular Dynamics Simulation on Tribochemical Reaction Dynamics of Diamond-Like Carbon"

O-4: Tamio Ikeshoji, "Charged Interfaces by First Principles Molecular Dynamics Simulations"

O-5: Sang Uck Lee, "Li Mobility in Spinel LiMn_2O_4 "

10:30-11:00 Coffee Break

11:00-12:30 (Chair: Marcel Sluiter)

I-13: Kohzo Ito, "New Entropic Elasticity of Topological Network: Slide-Ring Materials"

I-14: Masanori Tachikawa, "First-principles Calculations for Positron-attached Molecules"

O-6: Nurbosyn Zhanpeisov, "Modified Carbon K4 and IRMOF Structures: A Theoretical DFT Study"

O-7: Tomoo Yamamura, "MP2 Calculation of Co(II) Complexes with Second Coordination Sphere - for an Elucidation of Entropy Contribution in Actinide Complexes"

12:30-13:30 Lunch (Box Lunch), Group Photo, Poster Award

13:30-15:00 (Chair: Vijay Kumar)

I-15: Akira Terasaki, "Advanced Spectroscopic Studies of Size-Selected Free Metal Clusters"

O-8: Masahiko Ichihashi, "Catalytic Methanol Formation by CO_2 Hydrogenation on Metal Cluster Ions"

O-9: Makoto Tagami, "New Growth Mechanism of Cubic Rh Clusters Composed of 8-12 Atoms Found by the Method of Euclidean Designs"

O-10: Mineo Saito, "Hydrogen Chemisorbed on Graphenes and Carbon Nanotubes"

O-11: Tsutomu Ohtsuki, "Half-life Measurement of ^7Be in Several Materials"

15:00-15:30 Coffee Break

15:30-16:45 (Chair: Kaoru Ohno)

O-12: Yasuteru Shigeta, "*pKa* Estimation of Artificial DNA Bases and Amino Acids"

O-13: Hisato Yasumatsu, "Controlling Catalytic Functions of Charge-Polarized Nano-Space"

O-14: Nobuhiko Sarukura, "Development of Luminescent Materials in Vacuum Ultraviolet Region"

O-15: Ryoji Sakurada, "Structural Stability of Beta-Form Belite Doped by Sr Atom"

O-16: Koji Akai, "Study of Electronic Structure and Thermoelectric Properties on Cu-doped Ba-Ga-Sn Clathrates"

17:00 Busses leave

19:00- Dinner (Hotel Matsushima Taikanso) - Restaurant TENKAI

20:00-24:00 "Free Discussion" Room 701

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12th (Sunday) (Hotel Matsushima Taikanso) FUJI

07:00-09:00 Breakfast (Lounge Restaurant La Celese)

09:00-10:30 (Chair: Kwang-Ryeol Lee)

I-16: Vladimir R. Belosludov, "Equation of State and Effect of Self-preservation of Hydrogen Hydrate"

I-17: Jer-Lai Kuo, "Water on GaN Surfaces"

I-18: Fabio Pichierri, "Theory of van der Waals Forces"

10:30-10:45 Coffee Break

10:45-12:00 (Chair: Kombiah Iyakutti)

I-19: Kwang-Ryeol Lee, "Reactive MD Simulation of Si NW Oxidation"

O-17: Abhijit Chatterjee, "A Tight Binding Study to Monitor Gas Sensing in CNT"

O-18: Gang Chen, "Enhanced H_2 Splitting by Surface Step on Transition-metal-doped Al(111) Surfaces"

O-19: Toshiaki Iitaka, "Proton Dynamics in Icy Satellites"

12:00-13:30 Lunch (Lunch at Restaurant Shiosai)

13:30-15:00 (Chair: Vladimir R. Belosludov)

I-20: Bing-Joe Hwang, "A Combined Computational/Experimental Study on Pt-based Bimetallic Alloys for H_2O_2 Oxidation Reaction"

I-21: Leslie Victor Woodcock, "High Performance Computing in the Theory of Liquids"

O-20: Raebiger Hannes, "Polarons in Diluted Magnetic Semiconductors"

O-21: Zhong Zeng, "Convection Control by Rotating Magnetic Field in Floating Zone Model"

15:00-15:30 Coffee Break

15:30-17:45 (Chair: Jer-Lai Kuo)

I-22: Jisoon Ihm, "Scattering of Electronic Waves at Various Graphene Edges"

O-22: Ying Chen, "First Principles Study on Formation and Stability of fcc-NdO_x at Nd/Nd-Fe-B Sintered Magnets Surface"

O-23: Sergey Vladimirovich Seriy, "Modern Molecular Dynamic Computing on GPU with NVidia CUDA and ATI OpenCL Technologies in Atomic Simulation Environment"

O-24: Talgat Inerbaev, "First-Principles Study of Oxygen and Water Adsorption on Perfect and Defect Indium Oxide and Tin-Doped Indium Oxide (111) Surfaces"

O-25: Mohammad Saeed Bahramy, "A Novel Topological State Emerging in the Giant Bulk Rashba Semiconductor BiTeI under Pressure"

O-26: Hitoshi Nejo, "A Consequence of Detecting the Near-field Emission from an Individual Single Molecule"

O-27: John F Maguire, "Cyber-enabled Discovery"

O-28: Hiroshi Ogawa, "Computational Study on Site Occupation and Diffusion of Hydrogen in Mo-substituted Vanadium Monohydride"

17:45-17:50 Closing Remarks: Y. Kawazoe

Announcement for Next Meeting: TBA

18:00 Busses leave (To JR Sendai Station & IMR)