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

November 23-25, 2012
Institute for Materials Research, Tohoku University, Sendai, Japan
Hotel Matsushima Taikanso, Japan

SCIENTIFIC PROGRAM (November 22, 9pm Version, If you have any questions, contact mizulab@imr.tohoku.ac.jp)
K-*: Keynote (30 min., presentation + discussion)
I-*: Invited (30 min., presentation + discussion) or (20 min., presentation + discussion)
O-*: Oral (15 min., presentation + discussion)

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23rd (Friday) (Institute for Materials Research, Tohoku University, Sendai)
9:00-18:00 Registration Desk (Institute for Materials Research)
9:45-10:00 Opening Remarks: Y. Kawazoe
Announcement: H. Mizuseki
10:00-10:05 Greetings from the Director of IMR, M. Niinomi
10:05-15:55 (Chair: G. P. Das)
I-1: Yuan Ping Feng, "Long-Range Ferromagnetic Ordering in Metal-Organic Frameworks with Antiferromagnetic Dimeric-Cu(II) Building Units"
I-2: Ryo Ohmura, "Crystallographic Structures and Thermodynamic Stability of Clathrate Hydrates"
I-3: V. R. Belosludov, "Study of van der Waals Dispersion Coefficients within the All-Electron Mixed-Basis Approach"
I-4(20min.): O. S. Subbotin, "Simulation of Phase Composition and Formation Conditions of Methane and Carbon Dioxide Binary Hydrates"

11:55-13:00 Lunch (Box Lunch)

13:00-15:00 (Chair: Umesh V Waghmare)
I-5: Puru Jena, "Beyond The Periodic Table: Role of Clusters"
I-6: K. Iyakutti, "First Principles Study of Hydrogen Storage in Bulk and Nano MgH_2"
I-7: Jer-Lai Kuo, "First-Principles Studies of the Structural and Electronic Properties of $Zn_{1-x}(LiGa)_{0.5x}O$"
I-8: Tetsuo Mohri, "An Image Restoration Procedure Applied to Phase Field Microstructure"

15:00-15:30 Coffee Break

15:30-17:30 (Chair: Puru Jena)
I-9: G. P. Das, "Electronic and Transport Properties Across Epitaxial Heterojunctions: Some Case Studies"
I-10: Umesh V Waghmare, "First-Principles Investigation of 2-D Electron Gas at the Interface of Insulating Perovskite Oxides"

O-1: V. J. Surya, “First Principles Study on Adsorption of Boron-Nitrogen Atoms in SWCNTs”

O-2: Tamio Ikeshoji, “Charge Transfer Reaction at Solid-Liquid and Solid-Solid Interfaces by First Principles Molecular Dynamics Simulations”

O-3: Ryoji Sahara, “Introduction of TOMBO”

O-4: Hiroshi Mizuseki, “Introduction of the New Supercomputer in IMR”

17:30-20:00 Poster Session (Chair: H. Mizuseki)
18:00-18:30 Visit to IMR Supercomputing Center to see the new supercomputer with 300TFLOPS

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24th (Saturday) (Institute for Materials Research, Tohoku University, Sendai)

9:00-10:35 (Chair: Jer-Lai Kuo)

I-11: Masanori Tachikawa, “Multi Component Molecular Theory for Hydrogen Bonded Systems and Positronic Compounds”

I-12(20min.): Abhishek K. Singh, “Stress Induced Tuning of Band Gap in Bilayer Transition Metal Dichalcogenides”

O-5: Kenta Hongo, “A Quantum Monte Carlo Study of DNA Stacking”

O-6: Nurbosyn U. Zhanpeisov, “New Material Design by Cluster Approach: A Theoretical DFT Study”

O-7: Abhijit Chatterjee, “A Molecular Dynamics Study to Ratioanle the Charge Discharge Behavior within Li Battery Cells”

10:20-11:00 Coffee Break

11:00-12:00 (Chair: Tetsuo Mohri)

K-1: Shinji Tsuneyuki, “Atomistic Modeling of Materials Based on First-Principles Calculation”

I-13: S. Limpijumnong, “The 1100 cm^{-1} Mode in Oxygen-Doped CdTe”

12:00-13:30 Lunch (Box Lunch), Group Photo, Poster Award

13:30-15:00 (Chair: S. Limpijumnong)

I-14: Kwang-Ryeol Lee, “Multi-Scale Simulation of Interfacial Roughness Effects in Silicon Nanowires”

I-15(20min.): Sang Uck Lee, “Charge Transfer Behaviors on the Organic Crystal Structures: OLED & OPV”

O-8: Craig A. J. Fisher, “Surface Structures of Lithium Ion Battery Cathode Materials $LiCoO_2$, $LiFePO_4$, and Li_2MnSiO_4”

O-9: S. K. Tleukenov, “Propagation of Coupled Waves of Different Nature in Anisotropic Continuous Media: Universal Method for Theoretical Description”

15:00-15:30 Coffee Break

15:30-17:00 (Chair: Kwang-Ryeol Lee)

I-16: Kaoru Ohno, "Linear-Dispersive and Flat Bands in Band Structures of One-Dimensional Peanut-Shaped Fullerene Polymers"

O-11: J. Onoe, "Electron Conductivities of One-Dimensional Uneven Peanut-Shaped C_{60} Polymer Film"

O-12: Makoto Tagami, "Some Applications of Spherical Designs"

O-13: Nobuhiko Sarukura, "Various Approach Toward VUV Lasers"

O-14: Masahiko Ichihashi, "CO Oxidation on Composition-Selected Cerium Oxide Cluster Ions"

17:00 Busses leave

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

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25th (Sunday) (Hotel Matsushima Taikanso) FUJI

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

Check Out: by 10:00

09:00-10:15 (Chair: Yuan Ping Feng)

I-17: Motoko Kotani, "Mathematical Challenge at AIMR"

I-18: Momoji Kubo, "Tight-Binding Quantum Chemical Molecular Dynamics Simulation on Chemical Vapor Deposition and Etching Processes"

O-15: P. Murugan, "Structural Stability and Electronic Properties of MoS_{2+x} Nano-platelets"

10:15-10:45 Coffee Break

10:45-12:00 (Chair: Kaoru Ohno)

I-19: Kohzo Ito, "New Entropic Elasticity of Topological Network: Slide-Ring Materials"

O-16: Fabio Pichierri, "Computational Explorations in Ion Recognition Chemistry"

O-17: Ryoji Sakurada, "Structural Stability of Sr-Doped Belite"

O-18: H. Raebiger, "Quantum Mechanical Description of High and Low Spin States"

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

13:30-14:45 (Chair: V. R. Belosludov)

I-21: C. Majumder, "Nanoclusters on Support : A First Principles Study"

O-20: Madhvendra Nath Tripathi, "First Principles Study of the Effect of Magnetic and Non-Magnetic Dopants on the Opto-Electronic Properties of Indium Tin Oxide"

O-21: T. Inerbaev, "Atomistic Simulation of Charge Transfer at Functionalized Semiconductor Surfaces"

O-22: Yayoi Terada, "Phase Behavior of Polydisperse Lennard-Jones System"

14:45-15:15 Coffee Break

15:15-16:15 (Chair: Abhishek K. Singh)

O-23: Mohammad Saeed Bahramy, "Emergent Quantum Confinement at Topological Insulator Surfaces"

O-24: Hongming Weng, "Dirac-Semimetal, Chern-Semimetal and Topological Phase Transitions in a Quantum Simulator: A_3Bi (A=Na, K, Rb)"

O-25: H. Nejo, "A Photon Intensity Correlation indicating Nonlinear Dynamics"

O-26: Sergey V. Seriy, "Wavelet and Fractal Basis Instead Plane-Wave on *Ab-Initio* Calculations"

16:15-16:30 Closing Remarks: Y. Kawazoe

Announcement for Next Meeting: TBA

17:00 Busses leave (To JR Sendai Station & IMR)