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

December 10-13, 2010  
Institute for Materials Research, Tohoku University, Sendai, Japan  
Hotel Matsushima Taikanso, Japan  

SCIENTIFIC PROGRAM (December 12, 3pm Version, If you have any questions, contact kawalab@imr.edu)  
I-*: Invited (30 min., presentation + discussion)  
O-*: Oral (15 min., presentation + discussion)  
S-*: Special Session (10 min.)  

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10th (Friday) (Institute for Materials Research, Tohoku University, Sendai)  
8:30-18:00 Registration Desk (Institute for Materials Research)  
9:00-9:10 Opening Remarks: Y. Kawazoe  
Announcement: H. Mizuseki  

9:10-10:10 (Chair: H. Chen)  
I-1: Marcel H.F. Sluiter, “Ab initio Predictions of the Various Roles of Substitutional Alloying Elements in Low-alloyed Ferritic Steel”  
I-2: Keivan Esfarjani, “Thermal Conductivity of Bulk Crystals from First-principles”  

10:10-10:30 Coffee Break  

10:30-12:00 (Chair: V. Kumar)  
I-3: Jian-Tao Wang, “Magic Monatomic Linear Chains for Mn Nanowire Self-Assembly on Si(001)”  
I-5: S. Vannarat, “Storm Surge Simulation in the Gulf of Thailand with Finite Volume Coastal Ocean Model”  

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

13:00-14:30 (Chair: F. Pichierri)  
O-2: Yoshifumi Noguchi, “All-electron First-principles GW+Bethe-Salpeter Calculation for Optical Absorption Spectra”
14:30-15:00 Coffee Break

15:00-16:30 (Chair: M. R. Philpott)
I-8 H. M. Weng, “Pressure Induced Superconductivity in Topological Compound Bi$_2$Te$_3$”
O-3: Takuya Orikoshi, “Photocurrent Properties of Organic Photovoltaic Cells Laterally Contacted with Metal Electrodes”
O-4: Fabio Pichierri, “Cage Hydrocarbons as Potential Building Blocks for Nanomaterials”
O-5: Masahiko Ichihashi, “Coadsorption of O$_2$ and CO onto Isolated Copper Cluster Ions”
O-6: H. Nejo, “Correlation of Emission from Individual Excited Molecules Controlled by Near-field Optics”

16:30-17:00 Coffee Break

17:00-18:45 (Chair: K. Ohno)
O-7: Tamio Ikeshoji, “Origin of High Ionic Conductivity of Li ion in LiBH$_4$”
O-8: J. Onoe, “Riemannian Geometrical Effects on the Electronic Properties of One-dimensional Metallic C$_{60}$ Polymers with a Periodic Peanut-shaped Unevenness Structure”
O-9: Hiroki Matsubara, “Molecular Dynamics Simulation of OMCTS Liquid under Nanosize Confinement”
O-11: Ryoji Sakurada, “First-Principles Study on Crystal Structural Properties of Sr-doped Belite”
O-12: Tsuyoshi Akiyama, “Effects on Photoelectric Conversion Properties of Bulk Heterojunction Solar Cells of Localized Strong Electric Field”

19:00-19:30 Visit to IMR Supercomputing Center
19:00-21:00 Poster Session (Chair: H. Mizuseki) & Light Meal

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

9:00-9:10 Greetings from the Director of IMR, M. Niinomi
9:10-10:40 (Chair: Q. Sun)
I-10: Ruth Pachter, Withdrawn
I-17: H. Chen, “Edge States and Electronic Devices in Graphene Nanoribbons”
I-11: Vu Ngoc Tuoc, “Molecular Dynamics Study on Strain Distribution and Mechanical Properties of Si/Ge Heterostructure Nanowire along the [111] Direction”

10:40-11:00 Coffee Break

11:00-12:15 (Chair: B.-J. Hwang)
   O-14: Hisato Yasumatsu, “Cocatalytic Effects of Pt-Ag Bi-element Clusters Supported on Silicon Surface”
   O-15: Gyubong Kim, “Carbon Monoxide-tolerant Pt nanoparticles in Defective Graphene Substrate”
   O-17: Nobuhiko Sarukura, “Developments in Fluoride Crystals as Vacuum Ultraviolet Light-emitting Devices”

12:15-13:30 Lunch (Box Lunch), Group Photo, Poster Award

13:30-14:40 Special Session “A Decade of ACCMS” (Chair: Y. Kawazoe)
   S-1: G. P. Das (ACCMS-1, India)
   S-2: V. Belosludov (ACCMS-2, Russia)
   S-3: J.-T. Wang (ACCMS-3, China)
   S-4: K. R. Lee (ACCMS-4, Korea)
   S-5: V. N. Tuoc (ACCMS-5, Vietnam)
   S-6: Y. P. Feng (ACCMS-6, Singapore)

14:40-15:10 Coffee Break

15:10-16:55 (Chair: J.-L. Kuo)
   I-12: Kwang-Ryeol Lee, “Molecular Dynamics Simulations of Amorphous Carbon Film Growth”
   I-13: Gang Chen, “Structural and Electronic Properties of Neutral and Charged Ca$_8$C$_{12}$ Metal Carbides”

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12th (Sunday) (Institute for Materials Research, Tohoku University, Sendai)

09:00-10:30 (Chair: A. K. Singh)
   O-20: M. S. Bahramy, “Effect of Doping on Thermoelectric Properties of Layered RZnSbO (R = La, Ce)”
   O-21: Mineo Saito, “Adatom Related Defects in Nanocarbon Materials”
I-16: G. P. Das, “How do 3d Transition Metal Clusters Behave When Encapsulated Inside BN Cages and Nanotubes?”

10:30-11:00 Coffee Break

11:00-12:30 (Chair: Y. P. Feng)
I-18: Michael R. Philpott, “Multi-radical Ground State and Magnetism of Neutral, Charged and Chemically Modified Zigzag Edged Graphene Nanopatches”
I-20: Vijay Kumar, “Band-gap Engineering of Graphene by BN Doping and Effects of Metal Contacts: Ab-initio Calculations”

12:30-13:30 Lunch (Box Lunch)

Workshop on Computational Materials Science on Hydrogen Storage (WCMS-HS) 12th Afternoon - 13th Morning

13:30-14:45 (Chair: M. H. F. Sluiter)

14:45-15:15 Coffee Break

15:15-16:30 (Chair: G. P. Das)
I-22: Shin-ichi Orimo, “Hydrogen Storage and Ionics in Complex Hydrides”
I-23: Yuan Ping Feng, “Stabilizing Metal Atoms and Clusters on Graphene for Catalytic and Hydrogen Storage Applications”
O-25: Phung Thi Viet Bac, “First-principles Investigation of Hydrogen Diffusion into Aluminum Nanoclusters”

17:00 Busses leave
19:00- Dinner (Hotel Matsushima Taikanso) - Restaurant TENKAI
20:00-21:00 “Closed Meeting for FY2011 by Hydro-Star Members” Room 563
22:00-24:00 “Free Discussion” Room 563

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13th (Monday) (Hotel Matsushima Taikanso) FUJI
07:00-09:00 Breakfast (Lounge Restaurant La Celese)
09:00-10:15 (Chair: K. Iyakutti)
I-25: Qiang Sun, “Enhancing Hydrogen Storage with an Applied Electric Field”

10:15-10:45 Coffee Break

10:45-12:00 (Chair: H. Ogawa)
O-28: H. B. Huang, “First-Principles Study of Ammonia Borane and Alkali-Metal Amidoboranes for Hydrogen Storage”
O-29: Aki Yamane, “Alkali Metal Dependence of Hydrogen Desorption from Alkali Metal Hydride and Ammonia”
O-30: Yasuyuki Matsuura, “First-Principles Calculations of Cobalt Hydrides”

12:00-12:10 Closing Remarks: Y. Kawazoe
Announcement for Next Meeting: TBA

12:10-13:30 Lunch (Lunch at Restaurant Shiosai)

14:00 Buses leave (To JR Sendai Station & IMR)