

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](mailto: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-4: Sang Uck Lee, “The Origin of the Strain Energy Minimum in Imogolite Nanotubes”

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)

I-6: Jer-Lai Kuo, “On the Development of A First-Principle Based Multi-model Method to Study Aqueous Systems: from Clusters, Interfaces to Condensed Phases”

I-7: Bing-Joe Hwang, “Combined Experimental and Theoretical Investigation of Nanosized Effects of Pt Catalyst on Methanol Electro-Oxidation Activity and Pt-O and Pt-OH Stability in Oxygen Reduction Reaction”

O-1: Nurbosyn U. Zhanpeisov, “Structure and Chemical Activity of Transition Metal Oxide, Carbon K4 and IRMOF: A Theoretical DFT Study”

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  $\text{Bi}_2\text{Te}_3$ "

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  $\text{O}_2$  and  $\text{CO}$  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  $\text{LiBH}_4$ "

O-8: J. Onoe, "Riemannian Geometrical Effects on the Electronic Properties of One-dimensional Metallic  $\text{C}_{60}$  Polymers with a Periodic Peanut-shaped Unevenness Structure"

O-9: Hiroki Matsubara, "Molecular Dynamics Simulation of OMCTS Liquid under Nanosize Confinement"

O-10: K. Akai, "Calculation of Carrier Transport Properties of Group-III/IV Clathrate Semiconductors based on Electronic Structure Calculation"

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"

O-13: Ying Chen, "Interplay of Defect Cluster and the Stability of Xenon in Uranium Dioxide by DFT"

19:0-19:30 Visit to IMR Supercomputing Center

19:0-21:00 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-9: John Maguire, "Computer Methods in Nanomanufacturing"

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-16: Yasuteru Shigeta, “Structure and Properties of Metal-containing Mismatch DNA Base”

O-17: Nobuhiko Sarukura, “Developments in Fluoride Crystals as Vacuum Ultraviolet Light-emitting Devices”

O-18: Abhijit Chatterjee, “A High-throughput First Principle Calculation for Battery Electrode Materials”

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  $\text{Ca}_8\text{C}_{12}$  Metal Carbides”

I-14: Abhishek K. Singh, “Digging Wells in Graphane to Mine Graphene Roads and Quantum Dots”

O-19: Mina Park, “The First Principles Study of the Chemical Bonds between the Functionalized CNT and Metals”

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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  $\text{RZnSbO}$  (R = La, Ce)”

O-21: Mineo Saito, “Adatom Related Defects in Nanocarbon Materials”

I-15: Umesh V. Waghmare, "Soft Modes, Hyperelasticity, and Crack Instability: Elastodynamic Analysis from First-principles"

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-19: K. Iyakutti, "Investigation of Wigner Crystallization in Graphene"

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)

O-22: Hiroshi Ogawa, "Computational Studies in the Hydro-Star Project"

O-23: Somlak Ittisanronnachai, "Study of Hydrogen Storage through Spillover in Pt-loaded Zeolite-Templated Carbon"

O-24: Kimichi Suzuki, "Nuclear Quantum Effect on Hydrogen Adsorption Site for Zeolite-Templated Carbon (ZTC) using Path Integral Molecular Dynamics"

I-21: Masanori Tachikawa, "Path Integral Simulation for Hydrogen Bonded Systems: Protonic Quantum Nature and H/D Isotope Effect"

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-24: V. R. Belosludov, "Prediction of Structure, Composition and Phase Behavior of Helium Clathrate Hydrates"

I-25: Qiang Sun, "Enhancing Hydrogen Storage with an Applied Electric Field"

O-26: T. Oguchi, "Structural, Electronic and Magnetic Properties of Iron Hydride: A First-Principles Study"

10:15-10:45 Coffee Break

10:45-12:00 (Chair: H. Ogawa)

O-27: T. Shishidou, "First-Principles Study of Nickel Hydrides"

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"

O-31: R. Sahara, "Theoretical Study of Hydrogen Storage Materials using All-electron Mixed-basis Program TOMBO"

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

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

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