

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

January 12-14, 2010

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

SCIENTIFIC PROGRAM (January 11 Version, If you have any questions, contact kawalab@imr.edu)

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

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

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

11:00-13:30 Registration Desk (Institute for Materials Research)

13:30-13:40 Greetings from the Director of IMR, M. Niinomi

Opening Remarks: Y. Kawazoe

Announcement: H. Mizuseki

13:40-15:40 (Chair: Marcel Sluiter)

I-1: Michael R. Philpott "Bonding and magnetism of graphene nano patches and ribbons"

I-2: Hao Chen, "Transport controlled by transverse electric field in graphene nanoribbon with edge-defect junction"

I-3: Jinming Dong, "Ripples of Suspended Graphenes: a Molecular Dynamics Simulation Study"

I-4: Gour Prasad Das, "From Graphene to Graphane to Inorganic Graphane: a density functional investigation"

15:40-16:20 Coffee Break

16:20-17:50 (Chair: Fabio Pichierri)

I-5: Qian Wang, "Electronic and magnetic properties of functionalized BN sheet"

I-6: Withdrawn

I-7: Anirban Bandyopadhyay, "Design and architecture of a 3 D nano brain for standalone intelligent operation"

O-1: Ying Chen, "First principles modeling of oxygen behavior in UO_2 and CeO_2 "

O-7: Nurbosyn U. Zhanpeisov, "Theoretical DFT Study on Structure and Chemical Activity of Small Indium Oxide Clusters"

18:00-21:00 Poster Session (Chair: H. Mizuseki) & Light Meal

18:00-18:30 Visit to IMR Supercomputing Center

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13th (Wednesday) (Institute for Materials Research, Tohoku University, Sendai)

09:00-10:30 (Chair: Rodion Belosludov)

I-8: Vijay Kumar, "Magnetism in rare earth metal doped silicon clusters"

I-9: Duc Nguyen Manh, "First-principles modelling of irradiated ferritic/martensitic steels: Status and future challenges"

O-3: Ken-ichi Saitoh, "Molecular dynamics with strain tensor control for microstructure change in plastic deformation"

O-4: Koichi Ohno, "Large Scale First Principle Exploration of Unknown Chemical Structures and Reaction Pathways"

10:30-10:50 Coffee Break

10:50-12:05 (Chair: Keivan Esfarjani)

I-10: Kwang Ryelo Lee, "Multiscale Study of CNT-Al Composite Materials"

I-11: Marian Radny, "Adsorption induced excitons on the H/Ge(001) Surface"

O-5: A. Chatterjee, "Siting of Active Site in Zeolite to Design Nano-reactors -A QM/MM Study"

12:05-13:00 Lunch (Box Lunch), Group Photo, Poster Award

13:00-14:45 (Chair: Kwang Ryelo Lee)

I-12: P. Murugan, "Adsorption of Fluorinated C₆₀ Molecule on Si(111)-7×7 Surface"

I-13: Kuo Jer-Lai, "A Multi-scale Approach To understand Water at Nano-scale"

I-14: Withdrawn

O-6: Fabio Pichierri, "Design of 1D and 2D Building Blocks for Nanostructured Materials"

O-2: H. Nejo, "A sophisticated electromagnetic interaction between neighboring molecules embedded on carbon nanotubes"

O-8: Shujun Hu, "Exploration on Novel Half Metals based on First-Principles Calculation"

14:45-15:10 Coffee Break

15:10-16:40 (Chair: Kaoru Ohno)

O-9: Akira Terasaki, "Molecular-dynamics simulation of argon-cluster fragmentation upon impulsive excitation"

O-10: Masahiko Ichihashi, "Size Evolution of Structures and Oxidation Activity in Copper Cluster Cations"

O-11: H. Yasumatsu, "Catalytic Properties of Bimetallic Clusters Supported on Solid Surface"

O-12: Tetsuichiro Hayakawa, "Geometric structure of tungsten clusters anchored on graphite surface"

O-13: K. Egashira, "Electronic states of the silver dimer ion: Measurement and analysis of photodissociation spectra"

O-14: Andrey Lyalin, "Adsorption and catalytic activation of O₂ and C₂H₄ on gold clusters"

17:00 Buses leave

19:00- Banquet (Taikanso Hotel, Matsushima) - TENKAI/AMAMI

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14th (Thursday) (Taikanso Hotel, Matsushima) FUJI

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

09:00-10:15 (Chair: Hao Chen)

I-15: S. Limpijumnong, "Local vibration modes as fingerprints of crystal defects"

I-16: Keivan Esfarjani, "Thermal conductance quantization in a T-junction"

O-15: T. Inaoka, "Acoustic and Intersubband Plasmons in Ultra-thin Metallic Wires"

10:15-10:30 Coffee Break

10:30-11:45 (Chair: Gour Prasad Das)

I-17: M.H.F. Sluiter, "Interstitials in tetrahedrally close packed phases: C, N, O, and F in β tungsten"

I-18: Zeng Zhong, "The Effect of Rotating Magnetic Field on Thermocapillary Flow: Comparison of the Infinite and the $\Phi 1$ - $\Phi 2$ Models"

O-16: Withdrawn

O-17: Yasuteru Shigeta, "Theoretical Study on Stability of Artificial DNA bases"

11:45-13:00 Lunch (Box Lunch at Restaurant Shiosai)

13:00-15:00 (Chair: K. Iyakutti)

I-19: Ihm Jisoon, "Hydrogen Storage in Metal-decorated Polymers, MOFs, and CDCs"

I-20: Abhishek K. Singh, "H-Spillover through the catalyst saturation: A first principle study"

I-21: Purusottam Jena, "Superhalogens as building blocks for a new class of salts and sensors"

O-18: Toshiaki Iitaka, "Hydrogen hydrate under high pressure"

O-19: N. Sarukura, "New Results for Fluorides as Vacuum Ultraviolet Laser Material"

15:00-15:30 Coffee Break

15:30-17:15 (Chair: Purusottam Jena)

I-22: K. Iyakutti, "Investigation of hydrogen storage in carbon based nanostructures coated with light weight hydride, BH_3 "

I-23: V. R. Belosludov, "Extended Low-Frequency Vibrations of Hydrogen-Bond Networks of Amorphous Ices"

O-20: Hao Wang, "First-Principles study on Hydrogen atom hopping in $NaAlH_4$ "

O-21: T. Kaneko, "Quantum Dynamics of Hydrogen in $LaNi_5$ "

O-22: Megumi Kayanuma, "Theoretical Study on Hydrogen Adsorption to Graphene-Like Compounds"

17:15-17:20 Closing Remarks: Y. Kawazoe, T. Ikeshoji

17:30 Buses leave (To JR Sendai Station & IMR)