

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

January 26-28, 2008

Institute for Materials Research, Tohoku University, Sendai, Japan

Hotel Taikanso, Matsushima, Japan

**SCIENTIFIC PROGRAM**

**Jan. 26th, 2008 Saturday**

**(Institute for Materials Research, Tohoku University, Sendai)**

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

13:00-13:10 Opening Remarks: Y. Kawazoe, K. Ohno  
Announcement: H. Mizuseki

**Session 1 :** Chair: Hao Chen

13:10-13:40 Inv-1 First-principles investigation of CdS clusters, nanotubes and nanowires doped with transition metal atoms  
S. Ghosh and G.P. Das  
Department of Materials Science, Indian Association for the Cultivation of Science, Jadavpur, Kolkata, INDIA

13:40-14:10 Inv-2 Clusters: A Bridge Across Disciplines  
Purusottam Jena  
Physics Department, Virginia Commonwealth University, Richmond, Virginia, USA

14:10-14:40 Inv-3 Theory of Hydrogen Hydrates with Hexagonal Structure  
V. R. Belosludov, O. S. Subbotin, R.V. Belosludov, H. Mizuseki, Y. Kawazoe  
Nikolaev Institute of Inorganic Chemistry of SB RAS, Novosibirsk, Russia,  
Institute for Materials Research, Tohoku University, Sendai, Japan

14:40-15:00 Coffee Break

**Session 2 :** Chair: G. P. Das

- 15:00-15:30 Inv-4 Ab Initio Kinetic Monte Carlo Simulations of Diffusion and Trapping of C in Steel  
M.H.F. Sluiter  
Dept of MSE, 3ME, TU Delft, Delft, the Netherlands
- 15:30-16:00 Inv-5 Calculations of single-molecule conductance  
Hao Chen  
Physics Department, Fudan University, Shanghai, P.R. of China
- 16:00-16:20 Oral-1 Fluoride-based materials for deep ultraviolet light emitting devices  
Nobuhiko Sarukura and Yoshiyuki Kawazoe  
Institute of Laser Engineering, Osaka University, Osaka, Japan
- 16:20-18:00 Poster Session (Chair: M. Takahashi) & Coffee Break
- 17:30-18:30 Visit to IMR Supercomputing Center

**Jan. 27th, 2008 Sunday**

**(Institute for Materials Research, Tohoku University, Sendai)**

**Session 3 :** Chair: Purusottam Jena

- 08:30-09:00 Inv-6 Novel growth behaviors of transition metal clusters and the effects of doping: A path to designer clusters  
Vijay Kumar  
Dr. Vijay Kumar Foundation, Haryana, India
- 09:00-09:30 Inv-7 QUASI-EIGENMODES, ENERGY TRANSPORT AND FORCES IN PLASMONIC STRUCTURES  
C.T. Chan  
Hong Kong University of Science and Technology, Hong Kong
- 09:30-10:00 Inv-8 Dilute Magnetic Semiconductors by Doping with Non-traditional Elements  
Y. P. Feng, R. Q. Wu, H. Pan, L. Shen, J. B. Yi, J. Ding  
Department of Physics, National University of Singapore, Singapore
- 10:00-10:30 Coffee Break

**Session 4 :** Chair: K. Ohno

- 10:30-10:50 Oral-2 Direct evidence for 1D metal of the peanut-shaped C<sub>60</sub> polymer  
J. Onoe, T. Ito and S. Kimura  
Research Laboratory for Nuclear Reactors, Tokyo Institute of Technology,  
Tokyo, Japan
- 10:50-11:10 Oral-3 High Spin / Low Spin Phase Transitions of Spin-Crossover Complex in  
Emulsion Polymerization of Trifluoroethylmethacrylate using PVA as a  
Protective Colloid  
Atsushi Suzuki, Motoi Iguchi, Takeo Oku, Motoyasu Fujiwara,  
Masahiko Nishijima
- 11:10-11:30 Oral-4 Delta doping technology with two or more dopants in silicon towards  
quantum information processing platform  
Kazushi Miki  
National Institute for Materials Science (NIMS), Tsukuba, Japan,  
Graduate School of Pure and Applied Sciences, University of Tsukuba, Japan
- 11:30-11:50 Oral-5 Nano-simulation of electrode reaction and membrane in a polymer electrolyte  
fuel cell  
Tamio Ikeshoji  
Research Institute for Computational Sciences (RICS), AIST, Tsukuba,  
and CREST, JST
- 11:50-12:30 Lunch (Box Lunch) (Poster panels are available)

**Session 5 :** Chair: Michael R. Philpott

- 12:30-13:00 Inv-9 Ab Initio Molecular Dynamics Studies for Excited Electronic States of  
Small Molecules  
Kunhye Lee, Heesun Ahn, and Kyoung Koo Baeck  
Department of Chemistry and Advanced Materials, Kangnung National  
University, Gangwondo, Korea
- 13:00-13:30 Inv-10 Fundamentals of Impurity at Growth Front: Above, Below, and At the Surface  
E. G. Wang  
Institute of Physics, Chinese Academy of Sciences, Beijing, China

- 13:30-14:00 Inv-11 Bond Counting Rule for Carbon and its Application to the Roughness of Diamond (001)  
Lifang Xu  
Beijing National Laboratory for Condensed Matter Physics, Institute of Physics, Chinese Academy of Sciences, Beijing, China
- 14:00-14:30 Inv-12 Potential energy curves for Nitrogen adsorption and desorption process in (4,0) Single Walled Carbon Nanotube  
K. Iyakutti, M. Rajarajeswari  
School of Physics, Madurai Kamaraj University, Madurai, Tamilnadu, India
- 14:30-15:00 Coffee Break

**Session 6 :** Chair: Enge Wang

- 15:00-15:30 Inv-13 First principle study of Domain Matching Epitaxy growth semiconductor hetero-interface  
Vu Ngoc Tuoc  
Institute of Engineering Physics (IEP), Hanoi University of Technology (HUT), Vietnam
- 15:30-16:00 Inv-14 Molecular Dynamics Study of Ballistic Rearrangement of Surface Atoms during High Energy Ion Bombardment on Au and Pd Surface  
Sang-Pil Kim and Kwang-Ryeol Lee  
Computational Science Center, Future Technology Research Laboratory, Korea Institute of Science and Technology, Seoul, Korea
- 16:00-16:30 Inv-15 Vibrations of graphene nano-ribbons and doped graphene  
Umesh V. Waghmare, Mousumi Upadhyay Kahaly, Srijan K Saha, H. R. Krishnamurthy and A K Sood  
Theoretical Sciences Unit. J Nehru Centre for Advanced Scientific Research, Bangalore, India
- 16:30-17:00 Inv-16 Planar Graphene Molecules with  $D_{6h}$  Symmetry: Zig-zag  $C_{6m}H_{6m}$  ( $m = 1, 2, \dots, 10$ ) and Crenellated  $C_{6(3m-2-3m+1)}H_{6(2m-1)}$  ( $m = 1, 2, \dots, 6$ )  
Michael R Philpott and Yoshiyuki Kawazoe  
Institute for Materials Research, Tohoku University, Sendai, Japan
- 17:30- Move to Matsushima (by Bus)
- 19:00- Banquet (Hotel Taikanso, Matsushima)

**Jan. 28th, 2008 Monday**  
**(Hotel Taikanso, Matsushima)**

**Session 7 :** Chair: Kwang-Ryeol Lee

- 08:30-09:00 Inv-17 Dislocation Driven Problems in Computational Materials Science  
Duc Nguyen-Manh  
Theory and Modelling Department, Culham Science Centre, United Kingdom  
Atomic Energy Authority (UKAEA), UK
- 09:00-09:30 Inv-18 Computational design of polymers and functionalized molecules for  
hydrogen-storage media  
Jisoon Ihm  
Department of Physics and Astronomy, Seoul National University, Korea
- 09:30-10:00 Inv-19 Activation of (BN)<sub>36</sub> Cage by Impurity Doping : First Principle Study  
Sandeep Nigam and Chiranjib Majumder  
Chemistry Division, Bhabha Atomic Research Center, Mumbai, Trombay, India
- 10:00-10:30 Coffee Break

**Session 8 :** Chair: Akira Terasaki

- 10:30-10:50 Oral-6 Dynamic behavior of 5CB molecules coated Pd particles alignments  
observed by atomic force microscope and STEM  
Hitoshi Nejo, Naoto Nishida and Naoki Toshima  
National Institute for Materials Science, Tsukuba, Japan
- 10:50-11:10 Oral-7 Crystal Structural Properties of Beta-Form Dicalcium Silicates based on  
Ab-initio Calculations  
Ryoji Sakurada, Abhishek Kumar Singh, Masami Uzawa and  
Yoshiyuki Kawazoe  
Department of Civil Engineering, Akita National College of Technology,  
Akita, Japan
- 11:10-11:30 Oral-8 First-Principles Study of Metallic Grain Boundaries using Local Energy  
and Stress Densities  
Masanori Kohyama, Wang Ruzhi, Shingo Tanaka, Guang-Hong Lu,  
Tomoyuki Tamura and Shoji Ishibashi
- 11:30-11:50 Oral-9 Effect of Adsorption of gas molecules on the electronic structure of SWCNT  
Abhijit Chatterjee  
Accelrys K.K., Tokyo, Japan

11:50-12:10 Oral-10 Reduction of Dinitrogen at Room Temperature Mediated by Supported Tungsten Nanoclusters  
Junichi Murakami and Wataru Yamaguchi  
Nanotechnology Research Institute, National Institute of Advanced Industrial Science and Technology (AIST), Tsukuba, Japan

12:10-13:00 Lunch (Box Lunch at Lounge Restaurant "La Celese")

**Session 9 :** Chair: Junichi Murakami

13:00-13:20 Oral-11 A Grid-ready Multi-scale Method to Study Order/Disorder Transitions in Ice Physics and Semiconductor Alloys  
Jer-Lai Kuo  
School of Physical and Mathematical Sciences, Nanyang Technological University, Singapore

13:20-13:40 Oral-12 MAGNETO-OPTICAL SPECTRA OF FREE MANGANESE ION MEASURED BY PHOTON-TRAP SPECTROSCOPY  
Akira Terasaki, Takuya Majima, and Tamotsu Kondow  
Cluster Research Laboratory, Toyota Technological Institute in East-Tokyo Laboratory, Genesis Research Institute, Inc., Ichikawa, Japan

13:40-14:00 Oral-13 Ejection of Clusters from Graphite Surface by Impact of Size-Selected  $(\text{CO}_2)_N^+$   
Hisato Yasumatsu, Yasutaka Yamaguchi and Tamotsu Kondow  
Cluster Research Laboratory, Toyota Technological Institute in East-Tokyo Laboratory, Genesis Research Institute, Inc., Ichikawa, Japan

14:00-14:20 Oral-14 Infrared Photodissociation of Molecule-Adsorbed Cobalt Clusters —Vibrational and Electronic Transitions  
Masahiko Ichihashi, Shinichi Hirabayashi, Tamotsu Kondow  
Cluster Research Laboratory, Toyota Technological Institute in East-Tokyo Laboratory, Genesis Research Institute, Inc., Ichikawa, Japan

14:20-14:40 Oral-15 Transport properties of semiconducting group-IV based clathrates  
T. Eto, T. Uemura, K. Kishimoto, K. Koga, K. Akai, H. Takagi, T. Koyanagi, S. Shimamura, M. Matsuura  
MITC, Yamaguchi Univ., Ube, Japan

14:40-15:00 Oral-16 Prediction of Crystal Structure under High Pressure

Toshiaki Iitaka

RIKEN, Japan

15:00-15:30 Coffee Break

**Session 10 :** Chair: Y. Kawazoe

15:30-15:50 Inv-20 First-Principles Studies of Magnetic Properties of ZnO-based DMSs

Qian Wang, Qiang Sun, Puru Jena, and Y. Kawazoe

Department of Physics, Virginia Commonwealth University, Virginia, USA

15:50-16:10 Inv-21 Effects of Strain on the Dissociation Energetics and Kinetics of Sb<sub>4</sub> on Ge(001)

Jian-Tao Wang, C. F. Chen, E. G. Wang, Ding-Sheng Wang, H. Mizuseki, and Y. Kawazoe

Institute of Physics, Chinese Academy of Sciences, Beijing, China

16:10-16:30 Inv-22 Thermocapillary Convection of Liquid Bridge in Magnetic Field

Z. B. Chen and Z. Zeng

Department of Engineering Mechanics, Chongqing University, P.R. China

16:30-16:50 Inv-23 Computational Nanoscience Consortium

Sornthep Vannarat, Supawadee Namuangruk, Noppawan Tanpipat

Large Scale Simulation Research Laboratory (LSR), National Electronics and Computer Technology Center, Thailand

16:50-17:10 Inv-24 Negative Differential resistance in nanojunctions

Keivan Esfarjani and Hossein Cheraghchi

Dept. of Physics, UC Santa Cruz, CA, USA

17:10-17:30 Inv-25 Effect of Co and Al Substitution in LiNiO<sub>2</sub> Cathode Materials

P. Murugan, Vijay Kumar, Junichi Kawamura, and Yoshiyuki Kawazoe

Institute for Materials Research, Tohoku University, Sendai, Japan,

Central Electrochemical Research Institute, Tamil Nadu, India

17:30-17:50 Oral-17 Golden nanomaterials: from clusters to nanoparticles

Fabio Pichierri

Department of Applied Chemistry, Graduate School of Engineering and Global COE Program, Tohoku University, Sendai, Japan

- 17:50-18:10 Oral-18 Interaction of small molecules with a graphite layer: An integrated ONIOM study  
Nurbosyn U. Zhanpeisov  
Department of Chemistry, Graduate School of Science, Tohoku University,  
Sendai, Japan
- 18:10-18:20 Closing Remarks: Y. Kawazoe, K. Ohno
- 18:30 Go Back to JR Sendai Station and IMR, Tohoku University (by Bus)