

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

**東北大学金属材料研究所ワークショップ
【超大規模計算機シミュレーションによる新物質・材料設計方策の探求】**

February 16-18, 2009

Institute for Materials Research, Tohoku University, Sendai, Japan

Hotel Taikanso, Matsushima, Japan

SCIENTIFIC PROGRAM

Feb. 16th, 2009 Monday

(Institute for Materials Research, Tohoku University, Sendai)

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

13:30-13:40 Opening Remarks: Y. Kawazoe, T. Ikeshoji
Announcement: H. Mizuseki

Session 1 : Chair: G. P. Das

13:40-14:10 Inv-1 First Principle Study on ZnO Nano Wire
Vu Ngoc Tuoc
Institute of Engineering Physics (IEP), Hanoi University of Technology (HUT), Hanoi, Vietnam

14:10-14:40 Inv-2 Magnetic Semiconductors Based on Doped InAs and SiC: A First-principles Study
Umesh V. Waghmare
Theoretical Sciences Unit, JNCASR, Bangalore, India

14:40-15:10 Coffee Break

Session 2 : Chair: Umesh V. Waghmare

15:10-15:40 Inv-3 Ab Initio Predictions of Impurity Diffusion in Aluminum
M.H.F. Sluiter and Darko Simonovic
Dept of MSE, 3ME, TU Delft, Delft, the Netherlands

15:40-16:10 Inv-4 Electroluminescence in nanoscale objects
A.S. Trifonov
Skobeltsyn Institute of Nuclear Physics, M.V.Lomonosov Moscow State University, Russia
National Institute for Material Science, Tsukuba, Japan

16:10-16:30 Oral-1 Control of light emission from an individual molecule by restricting the light emitting space
K. Funaba and H. Nejo
National Institute for Materials Science, Tsukuba, Japan

16:30-19:00 Poster Session (Chair: H. Mizuseki) & Coffee Break

17:30-18:30 Visit to IMR Supercomputing Center

Feb. 17th, 2009 Tuesday
(Institute for Materials Research, Tohoku University, Sendai)

Session 3 : Chair: R. V. Belosludov

09:00-09:30 Inv-5 Designing Nanogadget for Nanoelectronic Device by Carbon Nanotubes
Sang Uck Lee, Mohammad Khazaei, Fabio Pichierri, Rodion V. Belosludov, Hiroshi Mizuseki
and Yoshiyuki Kawazoe
Corporate R&D Center, LG Chem, Ltd / Research Park, Daejeon, Korea

09:30-10:00 Inv-6 Si(001) and Ge(001): Same or Different ?
Marian W. Radny
School of Mathematical and Physical Sciences, The University of Newcastle, Callaghan, Australia

10:00-10:30 Inv-7 Highly stable and symmetric boron caged B@Co₁₂@B₈₀ core-shell cluster
Jian-Tao Wang, Changfeng Chen, E.G. Wang, Ding-Sheng Wang, H. Mizuseki, and Y. Kawazoe
Institute of Physics, Chinese Academy of Sciences, Beijing, China

10:30-11:00 Coffee Break

Session 4 : Chair: Vu Ngoc Tuoc

11:00-11:20 Oral-2 Theory of charge self-regulation in solids
Hannes Raebiger
Yokohama National University, Yokohama, Japan

11:20-11:40 Oral-3 1D peanut-shaped nanocarbon as a new curved quantum system
J. Onoe
Research Laboratory for Nuclear Reactors, Tokyo Institute of Technology, Tokyo, Japan

11:40-12:00 Oral-4 First principles analysis on hydrogen hopping in hydrogen storage materials
Akinori Tezuka, Hao Wang, Hiroshi Ogawa and Tamio Ikeshoji
Research Institute for Computational Sciences (RICS), National Institute of Advanced
Industrial Science and Technology (AIST), Tsukuba, Japan

12:00-13:30 Lunch (Box Lunch) (Poster panels are available)

Session 5 : Chair: T. Ikeshoji

- 13:30-14:00 Inv-8 Theory of mixed hydrogen-methane hydrates
V. R. Belosludov
Nikolaev Institute of Inorganic Chemistry of SB RAS, Novosibirsk, Russia
- 14:00-14:30 Inv-9 First-principles Design of Nanostructures for Hydrogen Storage
G. P. Das
Department of Materials Science, Indian Association for the Cultivation of Science, Kolkata, India
- 14:30-15:00 Inv-10 Design of new materials for storing hydrogen in quasi-molecular form
Qiang Sun
Department of Advanced Materials and Nanotechnology, Peking University, Beijing, China,
Center for Applied Physics and Technology, Peking University, Beijing, China
- 15:00-15:30 Coffee Break

Session 6 : Chair: V. R. Belosludov

- 15:30-15:50 Oral-5 Optical Absorption Spectra of Silver Cluster Ions: Molecular vs. Metallic Behaviors
Akira Terasaki, Chiharu Kasai, Takuya Majima, and Tamotsu Kondow
Cluster Research Laboratory, Toyota Technological Institute, in East Tokyo Laboratory,
Genesis Research Institute, Inc., Ichikawa, Japan
- 15:50-16:10 Oral-6 Dehydrogenation of NH₃ on Transition Metal Cluster Ions
Shinichi Hirabayashi, Masahiko Ichihashi, Tamotsu Kondow
Cluster Research Laboratory, Toyota Technological Institute, in East Tokyo Laboratory,
Genesis Research Institute, Inc., Ichikawa, Japan
- 16:10-16:30 Oral-7 Electronic and geometric structures of single platinum clusters on silicon(111) surface
H. Yasumatsu, T. Hayakawa, P. Murugan, Y. Kawazoe and T. Kondow
Cluster Research Laboratory, Toyota Technological Institute, in East Tokyo Laboratory,
Genesis Research Institute, Inc., Ichikawa, Japan
- 16:30-16:50 Oral-8 Size-selected metal clusters on anchored graphite surface
Tetsuichiro Hayakawa, Hisato Yasumatsu, and Tamotsu Kondow
East Tokyo Laboratory, Genesis Research Institute, Inc., Ichikawa, Japan
- 16:50-17:10 Oral-9 Magnetic control of carbon materials by carrier doping
M. Saito, K. Sawada, F. Ishii, S. Okada and T. Kawai
Division of Mathematical and Physical Science, Graduate School of Natural Science
and Technology, Kanazawa University, Kanazawa, Japan
- 17:30- Move to Matsushima (by Bus)
- 19:00- Banquet (Hotel Taikanso, Matsushima)

Feb. 18th, 2009 Wednesday
(Hotel Taikanso, Matsushima)

Session 7 : Chair: Y. Kawazoe

- 09:00-09:20 Oral-10 Active Site Structures on Modified TiO₂(110): An Insight from DFT Study
Nurbosyn U. Zhanpeisov
Department of Chemistry, Graduate School of Science, Tohoku University, Japan
- 09:20-09:40 Oral-11 Birefringence of β -BaB₂O₄ crystal in the terahertz region for parametric device design
Elmer Estacio, Shigeki Saito, Tomoharu Nakazato, Yusuke Furukawa, Nobuhiko Sarukura,
Marilou Cadatal, Minh Hong Pham, Carlito Ponseca, Jr., Hiroshi Mizuseki, and
Yoshiyuki Kawazoe
Institute of Laser Engineering, Osaka University, Osaka, Japan
- 09:40-10:00 Oral-12 Molecular Dynamics Study on Structural Transformation in Ni-based Alloys: Potential
Functions, Martensite and Amorphous Transformations
Ken-ichi Saitoh, Keisuke Kubota and Tomohiro Sato
Department of Mechanical Engineering, Kansai University, Osaka, Japan
- 10:00-10:20 Oral-13 Structural stability of artificial DNA: theoretical study
Y. Shigeta, T. Matsui, H. Miyachi, T. Sato, Y. Nakanishi, Y. Kitagawa, M. Okumura, and K. Hirao
Institute of Picobiology, University of Hyogo, Hyogo, Japan.
- 10:20-10:50 Coffee Break

Session 8 : Chair: K. Ohno

- 10:50-11:20 Inv-11 Anatomy of Nano Sized Hexagonal Graphene Molecules
Michael R Philpott and Yoshiyuki Kawazoe
Institute for Materials Research, Tohoku Univeristy, Sendai, Japan
- 11:20-11:40 Oral-14 Large-scale quantum molecular dynamics simulation of 3-dimensional C60 polymers
Toshiaki Iitaka
RIKEN (The Institute of Physical and Chemical Research), Wako, Japan.
- 11:40-12:00 Oral-15 In Search of Heterofullerenes
Fabio Pichierri
G-COE Laboratory, Department of Applied Chemistry, Graduate School of Engineering,
Tohoku University, Sendai, Japan
- 12:00-12:20 Oral-16 Electronic Structure of the Si(110)-(16 \times 2) surface
Kazushi Miki, Kazuyuki Sakamoto, Martin Setvin, Kenji Mawatari, P.E.J. Eriksson,
and R.I.G. Uhrberg
National Institute for Materials Science, Tsukuba, Japan

12:20-13:30 Lunch (Box Lunch at Lounge Restaurant "Celese")

Session 9 : Chair: Marcel Sluiter

13:30-14:00 Inv-12 A MACROSCOPIC APPROACH OF THE STRAIN RATE DEPENDENT MATERIAL BEHAVIOUR OF 3D-TEXTILE REINFORCED COMPOSITES

Dr.-Ing. habil. Maik Gude, Prof. Dr.-Ing. habil. Werner Hufenbach
Institut für Leichtbau und Kunststofftechnik (ILK), Technische Universität Dresden,
Dresden, Germany

14:00-14:30 Inv-13 First-principles Investigation of the Structural and Electronic Properties of Cu Based Intermetallics
Abhijit Chatterjee

Accelrys, Material Science, Tokyo, Japan

14:30-14:50 Oral-17 Metropolis-Hastings Algorithm for Sampling and Analyzing the Consensus Secondary Structures of Aligned Nucleic Acid Molecules

Akito Taneda

Graduate School of Science and Technology, Hirosaki University, Hirosaki, Japan

14:50-15:10 " *Announcement of ACCMS-5 in Hanoi!* " Vu Ngoc Tuoc

15:10-15:20 Closing Remarks: Y. Kawazoe, T. Ikeshoji

15:30 Go Back to JR Sendai Station and IMR, Tohoku University (by Bus)