

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

February 26-28, 2007

Institute for Materials Research, Tohoku University, Sendai, Japan

SCIENTIFIC PROGRAM

February 26, 2007 Monday

11:00-13:00 Registration

13:00-13:30 Opening Remarks : Y. Kawazoe

Announcement : H. Mizuseki

Session 1 : Chair: M. R. Philpott

13:30-14:00 Inv-1 TWO-STAGE ROTATION MECHANISM FOR GROUP-V PRECURSOR
DISSOCIATION ON Si(001)

Jian-Tao Wang, C.F. Chen, E.G. Wang, Ding-Sheng Wang,

Hiroshi Mizuseki and Yoshiyuki Kawazoe

Institute of Physics, Chinese Academy of Sciences, China

14:00-14:30 Inv-2 RESEARCH ACTIVITIES AND INFRASTRUCTURE FOR
COMPUTATIONAL NANOSCIENCE IN THAILAND

Sornthep Vannarat

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

14:30-14:50 Oral-1 UNIT SELECTIVE OXIDATION OF Si(111)7X7 SURFACE AND
EVOLUTION OF STRAIN DURING THE REACTION

Kazushi Miki and Tetsuya Narushima

National Institute for Materials Science (NIMS), Tsukuba, Japan

14:50-16:30 Poster Session (Chair: M. Takahashi) + Tea/Coffee

15:30-16:30 Visit to IMR Supercomputer Center

16:30-17:30 Move to Matsushima (by Bus)

19:00-21:00 Banquet (Hotel Taikanso, Matsushima)

February 27, 2007 Tuesday

Session 2 : Chair: Y. P. Feng

9:00-9:30 Inv-3 COMPUTATIONAL DESIGN OF THE HYDROGEN-STORAGE
MATERIALS BASED ON METAL-DECORATED POLYMERS
Jisoon Ihm
Department of Physics and Astronomy, Seoul National University, Korea

9:30-10:00 Inv-4 STRUCTURE PHASE TRANSITION IN AMORPHOUS SOLID ICE
UNDER PRESSURE
Vladimir R. Belosludov

Nikolaev Institute of Inorganic Chemistry, Novosibirsk, Russia

10:00-10:30 Inv-5 TOWARDS MOLECULAR ELECTRONICS: SINGLE ADSORBATES
ON SEMICONDUCTOR SURFACES
Marian W. Radny

School of Mathematical and Physical Sciences, The University
of Newcastle, Australia

10:30-11:00 Coffee Break

Session 3 : Chair: M. W. Radny

11:00-11:30 Inv-6 DENSITY FUNCTIONAL THEORY STUDY OF OXYGEN
REDUCTION REACTION (ORR) ON Pt AND Pt-M (M=Fe, Co)
CLUSTERS

Bing-Joe Hwang and Quan-Nan Lin

Department of Chemical Engineering, National Taiwan University
of Science and Technology, Taiwan, R.O.China

11:30-12:00 Inv-7 ELECTRONIC AND MAGNETIC PROPERTIES OF Mn- AND
Cr-DOPED GaN LOW DIMENSIONAL NANOSTRUCTURES
Qian Wang, Qiang Sun, Puru Jena and Yoshiyuki Kawazoe

Department of Physics, Virginia Commonwealth University, Richmond,
Virginia, USA

12:00-13:00 Lunch

Session 4 : Chair: V. Kumar

- 13:00-13:20 Oral-2 FIRST PRINCIPLES T -MATRIX THEORY
Kaoru Ohno, Yoshifumi Noguchi and Soh Ishii
Department of Physics, Graduate School of Engineering, Yokohama
National University, Japan
- 13:20-13:40 Oral-3 DEVELOPMENT A MULTISCALE MOLECULAR MODELING
METHOD TO STUDY POLYMERIC MATERIALS: POLYETHYLENE
OXIDE SYSTEM
Visit Vao-soongnern
School of Chemistry and Laboratory of Computational and Applied
Polymer Science (LCAPS), Institute of Science, Suranaree University
of Technology, Nakhon Ratchasima, Thailand
- 13:40-14:00 Oral-4 THEORETICAL INVESTIGATION OF THE ROLE OF CARBON
IN THE MECHANICAL PROPERTIES IN PEROVSKITE-TYPE
RARE EARTH RHODIUM BORIDES
Ryoji Sahara, Hidenobu Kojima, Toetsu Shishido, Akiko Nomura, Kunio
Kudou, Shigeru Okada, Vijay Kumar, Kazuo Nakajima and Yoshiyuki
Kawazoe
Institute for Materials Research, Tohoku University, Japan
- 14:00-19:00 Group Photo + Excursion (boat will leave at 15:00)
- 19:00-21:00 Dinner (Hotel Taikanso, Matsushima)

February 28, 2007 Wednesday

Session 5 : Chair: V. R. Belosludov

- 9:00-9:30 Inv-8 COMPUTATIONAL SCIENCE AT KOREA INSTITUTE OF SCIENCE
AND TECHNOLOGY USING A 3 TFLOPS SUPERCOMPUTING
FACILITY
Kwang-Ryeol Lee and Kyu-Hwan Lee
Future Technology Research Division, Korea Institute of Science

and Technology, Korea

- 9:30-10:00 Inv-9 NANOCOATINGS: DESIGNING NOVEL MATERIALS
AT THE NANOSCALE
Vijay Kumar
International Frontier Center for Advanced Materials (IFCAM), IMR,
Tohoku University, Japan
- 10:00-10:30 Inv-10 BONDING AND MAGNETISM IN TRANSITION METAL SANDWICH
MOLECULES
Michael R. Philpott and Yoshiyuki Kawazoe
Institute for Materials Research, Tohoku University, Japan

10:30-11:00 Coffee Break

Session 6 : Chair: J. Ihm

- 11:00-11:30 Inv-11 CARBON-INDUCED Si(001)-c(4X4) SURFACE: ATOMIC STRUCTURE
AND DIMER ROTATION
G.W. Peng, Y.Y. Sun, A.C. H. Huan and Y.P. Feng
Department of Physics, National University of Singapore, Singapore
- 11:30-12:00 Inv-12 ELECTRON COUNTING RULES AND STABILITY: FROM CLUSTERS
TO CRYSTALS
Puru Jena
Physics Department, Virginia Commonwealth University, USA

12:00-13:00 Lunch

Session 7 : Chair: K.-R. Lee

- 13:00-13:20 Oral-5 INCREMENTAL CHARGING OF A MOLECULE FLUCTUATED
BY THE SURROUNDING OTHER MOLECULES
Hitoshi Nejo
National Institute for Materials Science, Japan
- 13:20-13:40 Oral-6 GUEST ATOM EFFECTS ON THE ELECTRONIC STRUCTURE
OF SEMICONDUCTING TYPE-I CLATHRATES
K. Akai, K. Koga, H. Takagi and M. Matsuura
MITC, Yamaguchi University, Japan
- 13:40-14:00 Oral-7 REACTIVITY CONTROL OF METAL CLUSTERS BY DOPING

FOREIGN METAL ATOM -REACTION OF COBALT-SILVER
CLUSTER IONS WITH NITROUS OXIDE

Masahiko Ichihashi, Tetsu Hanmura and Tamotsu Kondow

Cluster Research Laboratory, Toyota Technological Institute, in East Tokyo
Laboratory, Genesis Research Institute, Inc., Japan

14:00-14:20 Oral-8

SINGLE-CLUSTER OBSERVATION OF ELECTRONIC AND
GEOMETRIC STRUCTURES OF SIZE-SELECTED PLATINUM
CLUSTERS PREPARED ON SILICON(111)-7X7 SURFACE

Hisato Yasumatsu, Tetsuichiro Hayakawa and Tamotsu Kondow

Cluster Research Laboratory, Toyota Technological Institute, in East Tokyo
Laboratory, Genesis Research Institute, Inc., Japan

14:20-14:40 Oral-9

THEORETICAL DFT STUDY ON STRUCTURE AND CHEMICAL
ACTIVITY OF TRANSITION METAL AND METAL OXIDE
CATALYSTS

Nurbosyn U. Zhanpeisov

Department of Chemistry, Graduate School of Science, Tohoku University,
Sendai, Japan

14:40-15:00 Oral-10

MOLECULAR NANOSTRUCTURES: ARCHITECTURE & DESIGN

Fabio Pichierri

COE Laboratory, Tohoku University, Japan

15:00-15:20 Closing Remarks

16:00 Go back to JR Sendai Station and IMR, Tohoku University