

**First Working Group Meeting on Clusters and Nanomaterials
of Asian Consortium for Computational Materials Science (ACCMS)**

September 7-9, 2006

Institute for Materials Research, Tohoku University, Sendai, Japan

SCIENTIFIC PROGRAM

September 7, 2006 Thu.

11:00-13:00 Registration Desk

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

Announcement : H. Mizuseki

Session 1 : Hydrogen Storage --- Chair: G. P. Das

13:30-14:00 Inv-1 NANO MATERIALS FOR HYDROGEN STORAGE

P. Jena

Virginia Commonwealth University, Richmond, USA

14:00-14:30 Inv-2 PHYSICAL AND CHEMICAL PROPERTIES OF GAS HYDRATES:
THEORETICAL ASPECTS OF ENERGY STORAGE APPLICATION

Vladimir R. Belosludov

Nikolaev Institute of Inorganic Chemistry, SB RAS, Novosibirsk, Russia

Session 2 : Methodology I --- Chair: H. Yasuhara

14:30-15:00 Inv-3 GIANT SAC/SAC-CI METHOD

H. Nakatsuji, T. Miyahara, and R. Fukuda

Graduate School of Engineering, Kyoto University, Kyoto, Japan

15:00-15:30 Inv-4 TIME-DEPENDENT SCHRÖDINGER EQUATION APPROACH AND
TWO-PARTICLE GREEN'S FUNCTION APPROACH FOR THE EXCITED
STATES OF NANOMATERIALS

Kaoru Ohno

Graduate School of Engineering, Yokohama National University,

Yokohama, Japan

15:30-15:45 Oral-1 SHORT-RANGE ELECTRON CORRELATIONS OF ATOMS AND MOLECULES BY FIRST PRINCIPLES T -MATRIX CALCULATIONS
Yoshifumi Noguchi, Soh Ishii, and Kaoru Ohno
Graduate School of Engineering, Yokohama National University,
Yokohama, Japan

15:45-16:05 Coffee Break

Session 3 : Cluster I --- Chair: J. Dong

16:05-16:35 Inv-5 ACTIVATION AND REACTIONS OF N_2 ON SUPPORTED TUNGSTEN NANOCLUSTERS

Junichi Murakami and Wataru Yamaguchi

Nanotechnology Research Institute, AIST, Tsukuba, Japan

16:35-16:50 Oral-2 HIGH MAGNETIZATION AND HIGH ELECTRICAL RESISTIVITY IN DENSE Fe AND Fe ALLOY CLUSTER ASSEMBLED FILMS FOR HIGH FREQUENCY USE

K. Sumiyama, D. L. Peng, H. Yamada, D. Kobayashi, and T. Hihara

Nagoya Institute of Technology, Nagoya, Japan

16:50-17:05 Oral-3 THEORETICAL AND EXPERIMENTAL STUDIES OF METAL/INORGANIC NANO-INTERFACES

Masanori Kohyama, Kazuyuki Okazaki, Shingo Tanaka, Tomoki Akita, and Satoshi Ichikawa

Research Institute for Ubiquitous Energy Devices, National Institute of Advanced Industrial Science and Technology, Osaka, Japan

17:05-17:20 Oral-4 SYNTHESIS AND STRUCTURES OF BORON NITRIDE NANOTUBES

Takeo Oku, Naruhiro Koi, Katsuaki Suganuma, Rodion V. Belosludov, and Yoshiyuki Kawazoe

Institute of Scientific and Industrial Research, Osaka University, Japan

17:20-18:50 Poster Session (90 min.) + Tea/Coffee

18:50-19:20 Visit to IMR Supercomputing Center

September 8, 2006 Fri.

Session 4 : Carbon Nanotube --- Chair: P. Jena

- 8:30-9:00 Inv-6 COMPUTATIONAL APPROACH TO THE DESIGN OF NANOMATERIALS: BASIC THEORY AND INDUSTRIAL APPLICATIONS OF CARBON NANOTUBES
Jisoon Ihm
Seoul National University, Seoul, Korea
- 9:00-9:30 Inv-7 QUANTUM SIZE EFFECT IN FIELD EMISSION AND NANOTUBES
C. T. Chan
Hong Kong University of Science and Technology and NAMI
- 9:30-9:45 Oral-5 DEBUNDLED CARBON NANOTUBES ON A SUBSTRATE FOR THE PHOTO-EMISSION STUDY
Hitoshi Nejo and Takeshi Akasaka
National Institute for Materials Science, Tsukuba, Japan
- 9:45-10:00 Oral-6 GENERATION OF CHARGED NANOPARTICLES AND THEIR DEPOSITION AS THIN FILMS, NANOWIRES OR NANOTUBES DURING CHEMICAL VAPOR DEPOSITION
Chan-Soo KIM and Nong-Moon HWANG
National Research Laboratory (NRL) of Charged Nanoparticles, Seoul National University, Korea

10:00-10:20 Coffee Break

Session 5 : Low Dimensional Systems --- Chair: J. Ihm

- 10:20-10:50 Inv-8 TRANSPORT PROPERTIES OF NANOSCALE SYSTEMS FOR MOLECULAR ELECTRONICS APPLICATION
Hiroshi Mizuseki, Tomoki Uehara, Rodion V. Belosludov, Sang Uck Lee, Amir A. Farajian, and Yoshiyuki Kawazoe
IMR, Tohoku University, Sendai, Japan
- 10:50-11:20 Inv-9 VIBRATIONAL AND OPTICAL PROPERTIES OF GOLD CLUSTERS AND GOLD NANOTUBES
Jinming Dong, W. Fa, J. Zhou, and C. F. Luo
National Lab. of Solid State Microstructures and Dept. of Physics, Nanjing University, Nanjing, P. R. China.

11:20-11:35 Oral-7 ENHANCED GROWTH AND FIELD EMISSION OF CARBON NANOTUBE BY NITROGEN INCORPORATION: THE FIRST PRINCIPLE STUDY
Hyo-Shin Ahn, Seungwu Han, and Kwang-Ryeol Lee
Future Technology Research Division, Korea Institute of Science and Technology, Seoul, Korea

11:35-13:00 Group Photo + Lunch

Session 6 : Methodology II --- Chair: K. Ohno

13:00-13:15 Oral-8 APPLICATION OF THE REACTIVITY INDEX TO PROPOSE INTRA AND INTERMOLECULAR REACTIVITY IN METAL CLUSTER INTERACTION OVER OXIDE SURFACE

Abhijit Chatterjee

Material Science, Accelrys, Tokyo, Japan

13:15-13:30 Oral-9 CORRECT INTERPRETATION OF HUND'S RULE AND CHEMICAL BONDING BASED ON THE VIRIAL THEOREM

Kenta Hongo, Takayuki Oyamada, Youhei Maruyama, Yoshiyuki Kawazoe, and Hiroshi Yasuhara

IMR, Tohoku University, Sendai, Japan

13:30-13:45 Oral-10 QUANTUM-CHEMICAL DESIGN OF COVALENT LINKAGES FOR INTERCONNECTING CARBON NANOTUBES

Fabio Pichierri, Mohammad Khazaei, and Yoshiyuki Kawazoe

COE Laboratory, IMRAM, Tohoku Univ., Sendai, Japan

13:45-14:00 Oral-11 THEORETICAL STUDY ON THE CARBON NANOTUBES WITH MULTI-DICHLOROCARBENE ADDITION

Guo Wang and Yuanhe Huang

Beijing Normal University, Beijing, China

14:30-15:30 Move to Matsushima (by Bus)

Sightseeing

Godaido, Zuiganji-Temple

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

September 9, 2006 Sat.

~10:00 (Go back to IMR, Tohoku Univ. by bus)

Session 7 : Nano Magnetism --- Chair: C. T. Chan

- 10:00-10:30 Inv-10 ROOM TEMPERATURE DOPED FERROMAGNETIC OXIDES:
A CURRENT SCENARIO TOWARDS MAGNETIC p-n JUNCTIONS
K. V. Rao
Royal Institute of Technology, Stockholm, Sweden
- 10:30-11:00 Inv-11 HIGH TEMPERATURE FERROMAGNETISM IN Fe-DOPED ZnO:
A DENSITY FUNCTIONAL INVESTIGATION
D. Karmakar, I. Dasgupta, and G.P. Das
Indian Association for the Cultivation of Science, Jadavpur, Kolkata, India
- 11:00-11:30 Inv-12 ELECTRONIC STRUCTURES OF POLAR OXIDE HETEROINTERFACES
A. Ohtomo, P. Murugan, T. Nishimatsu, Y. Kawazoe, and M. Kawasaki
IMR, Tohoku University, Sendai, Japan. PRESTO, Japan
- 11:30-11:45 Oral-12 RADIOACTIVE DECAY OF ⁷Be SPEED UP BY PLACING INSIDE C₆₀
CAGES
T. Ohtsuki, K. Ohno, and T. Morisato
Laboratory of Nuclear Science, Tohoku University, Mikamine, Taihaku,
Sendai, Japan

11:45-13:00 Lunch

Session 8 : Cluster II --- Chair: K. Sumiyama

- 13:00-13:30 Inv-13 SIZE-DEPENDENT CHARACTERISTICS OF METAL CLUSTERS
T. Kondow
Cluster Research Laboratory of Toyota Technological Institute, Japan
- 13:30-14:00 Inv-14 INTERACTIONS OF ATOMS AND MOLECULES ON Au CLUSTERS
AND Au (111) SURFACES: TUNING THE ELECTRONIC PROPERTIES
FROM FIRST PRINCIPLE CALCULATIONS
C. Majumder
Bhabha Atomic Research Centre, Mumbai, India

- 14:00-14:15 Oral-13 PHOTON-TRAP MAGNETO-OPTICAL SPECTROSCOPY OF MASS-SELECTED TRAPPED IONS
Akira Terasaki, Takuya Majima, and Tamotsu Kondow
 Cluster Research Laboratory, Toyota Technological Institute, Japan
- 14:15-14:30 Oral-14 LOCAL DENSITY OF STATES AND SPATIAL DISTRIBUTION OF VALENCE ELECTRONS OF SINGLE-LAYERED PLATINUM CLUSTERS DEPOSITED ON SILICON (111)-7X7 SURFACE
H. Yasumatsu, T. Hayakawa, and T. Kondow
 Cluster Research Laboratory, Toyota Technological Institute, Japan
- 14:30-14:45 Oral-15 INDUCED MAGNETIZATION IN COBALT/PALLADIUM MULTILAYER THIN FILMS
Susumu Imai, Norio Ota, P. Murugan, and Yoshiyuki Kawazoe
 Hitachi Maxell, Ltd., Ibaraki, Japan
- 14:45-15:00 Oral-16 ATOMIC AND MOLECULAR CLUSTERS IN FUEL CELLS - A FIRST PRINCIPLES MD STUDY -
 Tamio Ikeshoji
 CREST, JST and RICS, AIST, Tsukuba, Japan

15:00-15:20 Coffee Break

Session 9 : Soft Matter --- Chair: T. Ikeshoji

- 15:20-15:35 Oral-17 ETHYLENE DEHYDROGENATION ON Fe_n^+ , Co_n^+ AND Ni_n^+ ($n \leq 30$)
Masahiko Ichihashi, Tetsu Hanmura, and Tamotsu Kondow
 Cluster Research Laboratory, Toyota Technological Institute, Japan
- 15:35-15:50 Oral-18 BAND STRUCTURE AND THERMOELECTRIC PROPERTIES OF NANOCAGE LATTICE SYSTEMS: GROUP-IV BASED CLATHRATES
K. Akai, K. Koga, H. Takagi, and M. Matsuura
 MITC, Yamaguchi University, Ube, Japan
- 15:50-16:05 Oral-19 Q-CONJUGACY CHARACTER TABLES OF SOME CHEMICAL MOLECULES BY WREATH PRODUCT
 Ghorban Ali Moghani
 Iran Color Research Center, (ICRC), Tehran, Iran
- 16:05-16:20 Oral-20 PROTEIN FUNCTION EXPRESSION AND MOLECULAR RECOGNITION IN BIO-SYSTEMS
Carlos A. Del Carpio M., Eichiro Ichiishi, Michihisa Koyama, Momoji Kubo, and Akira Miyamoto
 Graduate School of Engineering, Tohoku University, Sendai, Japan

16:20-16:35 Oral-21 SYNTHESIS AND AB INITIO STUDY OF C_{2v} - $C_{71}H_2$ ANNULENE
Chun-Ru Wang
Institute of Chemistry, Chinese Academy of Sciences, Beijing, China

16:35-17:15 Panel Discussion
C. T. Chan, G. P. Das, J. Dong, J. Ihm, T. Kondow, V. R. Belosludov,
and Y. Kawazoe

17:15-17:30 Closing Remarks