

Highlight of ICC-IMR International Workshop

The 6th General Meeting of Asian Consortium on Computational Materials Science – Virtual Organization (ACCMS-VO)

February. 10-12, 2012, Chairperson Y. KAWAZOE (IMR)

This is the 6th annual meeting of “off the net” of the virtual organization for computational materials scientists mainly in the Asian region, who are working collaboratively daily via international computer network using our supercomputer at the Center for Computational Material Science, Institute for Materials Research, Tohoku University (CCMS, IMR, TU). The ACCMS started in Sendai with only 16 researchers from Japan, China, India, Russia, Thai, Iran, US, and Canada in August 2000. After this meeting, 6 main meetings in India, Russia, China, Korea, Vietnam, and Singapore, 6 VO meetings, and 3 WG meetings in Sendai, Singapore, and Korea were held. Especially VO meetings have been held in Sendai continuously every fiscal year. We have published the Proceedings for all the main meeting including invited talks and some of the oral talks from international journal publishers. The present meeting focuses on designing efficient hydrogen storage materials and new methodologies in computational materials science, using the supercomputer at IMR and other member institutions aiming to use the Computer K in Kobe. About 120 researchers from 13 countries gathered supported by ICC-IMR and other organizations, and not only present their recent research results and exchange ideas but also mixed up to start new collaborations among them. These new international collaborations will be continued on the computer network to establish ACCMS-VO as a research basis of the members. The details of the meeting and activities are open through our ACCMS webpage; please check <http://www-lab.imr.tohoku.ac.jp/~accmsvo6/>.

In order to hold Asian Consortium on Computational Materials Science (ACCMS) general/working group/virtual organization (VO) meetings periodically, and more effectively and smoothly, representatives of the participants from China, India, Japan, Korea, Taiwan, Thailand, Russia, and Singapore had a meeting during ACCMS-VO6 meeting. Then, we decided that IMR of Tohoku University will continue to host ACCMS-VO and the next one will be in autumn of 2012.

The list of invited talks is shown below, which covers the recent important area in computational materials science and technology.

- I-1: Sukit Limpijumng (Suranaree University of Technology), “First Principles Study of Al Doped ZnO”
- I-2: Michael Ronald Philpott (University of California Berkeley), “Chymera Magnetic States of Graphene Nanodots”
- I-3: Kombiah Iyakutti (Noorul Islam University), “Investigation of Effect of Unequal Effective Mass Fermions in Graphene”
- I-4: Jian-Tao Wang (Chinese Academy of Sciences), “Mechanism for Direct Conversion of Graphite to Diamond”
- I-5: Gour P. Das (Indian Association for the Cultivation of Science), “Graphene-like Materials and Their Functionalization: Advent of a New Family”
- I-6: Umesh Waghmare (Jawaharlal Nehru Centre for Advanced Scientific Research), “Theory of Defects in Graphene and Related Nano-materials”
- I-7: Vijay Kumar (Dr. Vijay Kumar Foundation), “From Silicon Fullerenes to Bulk Metallic Glasses - My Golden Time with IMR”
- I-8: Kaoru Ohno (Yokohama National University), “All-electron Mixed Basis Approach for Accurate First Principles Calculations”
- I-9: Marcel Sluiter (Delft University of Technology), “Multinary Cluster Expansions for Dilute Al-Mg-Si and Al-Mg-Li Alloys”
- I-10: Yuan Ping Feng (National University of Singapore), “Spin-dependent Transport of GMR and TMR Devices”
- I-11: Katsumi Tanigaki (Tohoku University), “Charge Transfer to Organic Semiconductors on the Au Electrodes Modified by Self-assembled Monolayers: Comparison between Experiment and Theory”
- I-12: Momoji Kubo (Tohoku University), “Tight-Binding Quantum Chemical Molecular Dynamics Simulation on Tribochemical Reaction Dynamics of Diamond-Like Carbon”
- I-13: Kohzo Ito (University of Tokyo), “New Entropic Elasticity of Topological Network: Slide-Ring Materials”
- I-14: Masanori Tachikawa (Yokohama City University), “First-principles Calculations for Positron-attached Molecules”

I-15: Akira Terasaki (Kyushu University), "Advanced Spectroscopic Studies of Size-Selected Free Metal Clusters"

I-16: Vladimir R. Belosludov (Russian Academy of Science), "Equation of State and Effect of Self-preservation of Hydrogen Hydrate"

I-17: Jer-Lai Kuo (Academia Sinica), "Water on GaN Surfaces"

I-18: Fabio Pichierri (Tohoku University), "Theory of van der Waals Forces"

I-19: Kwang-Ryeol Lee (Korea Institute of Science and Technology), "Reactive MD Simulation of Si NW Oxidation"

I-20: Bing-Joe Hwang (National Taiwan University of Science and Technology), "A Combined Computational/Experimental Study on Pt-based Bimetallic Alloys for H₂O₂ Oxidation Reaction"

I-21: Leslie Victor Woodcock (Kyonggi University), "High Performance Computing in the Theory of Liquids"

I-22: Jisoon Ihm (Seoul National University), "Scattering of Electronic Waves at Various Graphene Edges"

