Highlight of ICC-IMR International Workshop
The 5th General Meeting of Asian Consortium on Computational Materials Science – Virtual Organization (ACCMS-VO)
Dec. 10-13, 2010, Chairperson Y. KAWAZOE (IMR)

This is the 5th 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 audiences celebrate the 10th anniversary of the ACCMS, which started in Sendai with only 16 researchers from Japan, China, India, Russia, Thai, Iran, US, and Canada. In these 10 years 5 main meetings in India, Russia, China, Korea, and Vietnam, 5 VO meetings, and 3 WG meetings in Singapore, Korea, and Sendai, were held. Especially VO meetings have been held in Sendai continuously every 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. This meeting is really international. Although many so-called international conferences in Japan accommodate only several foreign speakers, our meetings always have a number of foreigners and enjoy mixing different cultures here in Sendai to establish good and deep understanding with each other. 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.edu/~accmsvo5/index.html.

The list of invited talks are shown below, which covers the recent important area in computational materials science and technology, and some of them will be published as a book form from Springer-Verlag to celebrate the 10th anniversary of the ACCMS society.

1: Marcel H.F. Sluiter (Delft University of Technology), "*Ab initio* Predictions of the Various Roles of Substitutional Alloying Elements in Low-alloyed Ferritic Steel"

2: Keivan Esfarjani (Massachusetts Institute of Technology), "Thermal Conductivity of Bulk Crystals from First-principles"

3: Jian-Tao Wang (Chinese Academy of Sciences), "Magic Monatomic Linear Chains for Mn Nanowire Self-Assembly on Si(001)"

4: Sang Uck Lee (LG Chem, Ltd / Research Park), "The Origin of the Strain Energy Minimum in Imogolite Nanotubes"

5: S. Vannarat (National Electronics and Computer Technology Center), "Storm Surge Simulation in the Gulf of Thailand with Finite Volume Coastal Ocean Model"

6: Jer-Lai Kuo (Academia Sinica), "On the Development of A First-Principle Based Multi-model Method to Study Aqueous Systems: from Clusters, Interfaces to Condensed Phases"

7: Bing-Joe Hwang (National Taiwan University of Science and Technology), "Combined Experimental and Theoretical Investigation of Nanosized Effects of Pt Catalyst on Methanol Electro-Oxidation Activity and Pt-O and Pt-OH Stability in Oxygen Reduction Reaction"

8 H. M. Weng (Chinese Academy of Sciences), "Pressure Induced Superconductivity in Topological Compound Bi2Te3"

9: John Maguire (The U.S. Air Force Research Laboratory), "Computer Methods in Nanomanufacturing"

10: Vu Ngoc Tuoc (Hanoi University of Science and Technology), “Molecular Dynamics Study on Strain Distribution and Mechanical Properties of Si/Ge Heretostructure Nanowire along the [111] Direction”

11: Kwang-Ryeol Lee (Korea Institute of Science and Technology), “Molecular Dynamics Simulations of Amorphous Carbon Film Growth”

12: Gang Chen (University of Jinan), “Structural and Electronic Properties of Neutral and Charged Ca8C12 Metal Carbides”

13: Abhishek K. Singh (Indian Institute of Science), “Digging Wells in Graphane to Mine Graphene Roads and Quantum Dots”

14: Umesh V. Waghmare (Jawaharlal Nehru Centre for Advanced Scientific Research), “Soft Modes, Hyperelasticity, and Crack Instability: Elastodynamic Analysis from First-principles”

15: G. P. Das (Indian Association for the Cultivation of Science), “How do 3*d* Transition Metal Clusters Behave When Encapsulated Inside BN Cages and Nanotubes?”

16: H. Chen (Fudan University), “Edge States and Electronic Devices in Graphene Nanoribbons”

17: Michael R. Philpott (University of California Berkeley), “Multi-radical Ground State and Magnetism of Neutral, Charged and Chemically Modified Zigzag Edged Graphene Nanopatches”

18: K. Iyakutti (Madurai Kamaraj University), “Investigation of Wigner Crystallization in Graphene”

19: Vijay Kumar (Dr. Vijay Kumar Foundation), “Band-gap Engineering of Graphene by BN Doping and Effects of Metal Contacts: *Ab-initio* Calculations”

20: Masanori Tachikawa (Yokohama City University), “Path Integral Simulation for Hydrogen Bonded Systems: Protonic Quantum Nature and H/D Isotope Effect”

21: Shin-ichi Orimo (Tohoku University), “Hydrogen Storage and Ionics in Complex Hydrides”

22: Yuan Ping Feng (National University of Singapore), “Stabilizing Metal Atoms and Clusters on Graphene for Catalytic and Hydrogen Storage Applications”

23: V. R. Belosludov (Tohoku University), “Prediction of Structure, Composition and Phase Behavior of Helium Clathrate Hydrates”

24: Qiang Sun (Peking University), “Enhancing Hydrogen Storage with an Applied Electric Field”