

Minutes of ACCMS Working Group Meeting on Clusters and Nanomaterials

Sendai, 7-9 September 2006

This first Working Group Meeting of ACCMS on Clusters and Nanomaterials was held in the Institute of Materials Research in Sendai during 7-9 Sept '06 under the convenership of Prof. Y. Kawazoe. The idea of organizing such a Working Group Meeting originated from the discussion that took place during ACCMS-3 Conference in Beijing in 2005. About 100 participants from 11 countries (China, India, Japan, Korea, Iran, Singapore, Russia, USA, Spain, Sweden, Australia) attended this Meeting. There were 9 scientific sessions covering 14 invited talks, 21 oral presentations. In his inaugural address Prof. G.P. Das gave a panoramic view of nanomaterials research and the role of computational materials science, before summarizing the ACCMS initiative, activity and achievements. The technical sessions spanned a variety of topics such as nanomaterials for hydrogen storage, carbon nanotubes, clusters, low-dimensional systems, spintronics materials, soft matter and nano-biology. Advanced methodologies of electronic structure, quantum transport, correlated molecules and clusters, time-dependent and excited state etc. were discussed. Applications of various density functional, quantum chemical and quantum monte carlo approaches to molecules, clusters and nanomaterials were discussed. There were also several state-of-the-art experimental overviews on free as well as supported clusters, diluted magnetic semiconductors and oxides and other related topics. In the poster session, more than 40 posters were presented by young researchers and these were of consistently high quality. Three prizes for best poster presentations have been awarded to (1) Mohammad Saeed Bahramy from Institute of Materials Research, Sendai (2) Yasunobu Kodama from Department of Physics and Graduate School of Engineering, Yokohama National University and (3) Wei Fa from National Laboratory of Solid State Microstructures and Department of Physics, Nanjing University. On the whole, this Working Group meeting turned out to be successful and intellectually exciting.

An open panel discussion was held on the last day of the working group meeting (9th Sept '06) to discuss the ongoing and future activities of ACCMS. The panelists are Prof. J. Ihm, Prof. R.V. Belosludov, Prof. J. Dong, Prof. T. Kondow, Prof. G.P. Das and Prof. Y. Kawazoe. The Meeting is attended by a large number of participants representing different countries. A summary of the views expressed by different representatives is summarized below.

1. Prof. Y. Kawazoe presented a flow-chart of the ACCMS activities during the past 6 years. He emphasized the importance of the working group formation for more active collaborations in specific areas related to computational materials science. Under the "Clusters and Nanomaterials" subgroup, three sub-areas are suggested and unanimously accepted by the audience viz. (a) Nanotubes, nanowires, and nanobundles (b) Hydrogen storage materials and (c) Clusters, especially transition metal based.
2. Prof. G.P. Das initiated discussion on the new working groups to be formed and the choice will be amongst the following topics suggested : (a) Semiconducting electronics (b) Nano- and Surface magnetism (c) Tackling larger systems (d) Quantum many-body approach to real materials (e) Nano-biology and biologically inspired computation.

3. Prof. J. Ihm and Prof. J. Dong advocated for the first topic viz. Semiconducting electronics, including magneto-, spin- and molecular electronics. The current upsurge in this field all over the world, makes this quite relevant for being taken up as a Working Group topic. Prof. Kondow wanted to include magnetic and magneto-electronic devices in the new working group.
4. Prof. R.V. Belosludov spoke about the current resurgence of interest on Hydrogen storage materials, both bulk (in the form of clathrates etc.) and nano-materials. He also emphasized the need for pursuing our working group activities on novel materials for hydrogen storage.
5. Prof. J. Ihm who is the principal organizer of the 4th ACCMS conference in Seoul, Korea, briefed the audience about the preparation they are taking for hosting this event. The details such as venue, exact dates (it will be in the month of September 2007) and other details will be made available in the website which will be created shortly and will also be linked with the main ACCMS website. Prof. Ihm also declared that Prof. Kwang-Ryeol Lee from KIST will be the co-organizer of this event and that for any query, emails can be sent to either Prof. Ihm (jihm@snu.ac.kr) or Prof. Lee (krlee@kist.re.kr).
6. Prof. G.P. Das mentioned about the forthcoming International Meeting in our areas of interest :
 - (a) International Conference on Advanced Materials (IUMRS-ICAM-2007) to be held in Bangalore, India during 8-13 October, 2007, in which there are 25 Theme Symposia, one of which is on "Computational Materials Science" (Web-site : <http://www.icam2007.com/> Contact person: Prof. G.P. Das).
 - (b) "International Symposium on Science and Technology Issues in a Hydrogen Economy" , to be held in Richmond, Virginia, USA during 12-15 November, 2007 (Web-site : <http://has.vcu.edu/phy/ishe> contact person Prof. P. Jena)
7. Prof. T. Kondow emphasized the need for stronger interaction between the experimental and computational materials scientists. Dr. C. Majumdar suggested the need for a tie-up between the experimental and computational group so that any new findings can be shared even before they are sent for publication.
8. Prof. Kawazoe hinted at the possible formation of some "Virtual Organization" linked with ACCMS, so that the various active groups in Asian countries can be linked together through some kind of grid and the computational infrastructure can be shared. He has already been assured by the government agency of financial support for such VO formation. This, however, needs to be reciprocated by the other countries in Asia, so that some active link can be established. This suggestion is welcomed by the audience.

All the members present in the meeting unanimously agreed that we need to put more efforts on the exchange of scientists and students as well as to mobilize more funding to develop human and computational resources in our Asian region. More publicity should be given to the ACCMS activities through web and other means. A strong role is expected to be played by scientists who are originally from Asian countries, but are currently working in laboratories in the west.

The meeting ended with a vote of thanks to the chairperson Prof. Kawazoe and to the members of the organizing team of this working group meeting.

G.P. Das