

## A brief report on ACCMS-4

Seoul, Korea, 12-16 September, 2007

The 4<sup>th</sup> Conference of the Asian Consortium for Computational Materials Science (ACCMS-4) was held in KIST (Korean Institute of Science and Technology), Seoul (12-16 September, 2007). The three earlier conferences were held at Bangalore (2001), Novosibirsk (2004) and Beijing (2005). The total number of registered participants was more than 200, with 170 papers presented which includes 32 invited papers, 25 oral presentations and 113 posters. The participation from 16 different regions of Asia viz. Bangladesh, China, India, Iran, Japan, Korea, Russia, Singapore, Taiwan, Thailand, Vietnam (include the rest in alphabetical order) gave a unique flavor to this conference, which has been further enhanced by the invitees from Europe, USA and other countries. The conference was successfully organized by Prof. Jisoon Ihm of the University of Korea and Prof. Kwang Ryeol Lee and his team of scientists from KIST. Apart from the sponsorships received from IBM Korea, Accelrys Korea, Open Network, Centre for Nanostructure Materials Technology, there were also strong support from the Director-General of Fusion Technology Hub, KIST (Prof. Hyung Min Rho) and the Director of National Programme for Tera-level Nano-devices (Dr. Jowon Lee).

The conference started with the welcome address by Prof. Y. Kawazoe and the keynote address by the President of KIST Prof. Dongwha Kum, A wide range of topics were covered viz. both methodologies, such as Density Functional Theory, Molecular Dynamics, Monte Carlo, Multiscale modeling and simulation etc. and application areas from Spintronics to Nano-tubes/wires/ribbons to Energy storage materials, surfaces, interfaces, multilayers and devices. The quality of presentations was consistently of very high level, and the richness of computational materials science is further evident from the wide variety of very impressive poster session. There was a general feeling that more time should be given for poster sessions. Three best poster prizes were selected and awarded to (1) Dr. F. Xu at Institute of Physics, China (2) Mr. Sang Uck Lee at Tohoku University, Japan and (3) Mr. Deajin Kim at Insilicotech, Korea.

A unique feature of the ACCMS-4 Conference was the organization of two short courses on 12<sup>th</sup> September, 2007. The first course was "*Introduction to ab-initio calculations VASP (Vienna Ab-initiation Simulation Package)*" covered by Prog. Georg Kresse (Univ. of Wien, Austria) and Prof. Noejung Park (Dankook Univ, Korea). The second course was on "*Introduction to*

*Molecular Dynamics and Accelerated Molecular Dynamics*", by Dr. A. Voter (Los Alamos National Lab, USA) and Prof. Pil-Ryung Cha (Koomin Univ, Korea). Both these two short course attracted a substantial number of participants (approximately 80 participants in each of the two courses). There was also a special evening programme on "*Introduction to TOMBO (Tohoku Mixed Basis Orbitals ab initio programme package)*" organized by Prof. Y. Kawazoe and Dr. M.S. Baharamy, and aptly supported by Tatsuya Funakubo or the Research Institute for High Performance Computing, Japan.

The organizing committee of ACCMS met on 14<sup>th</sup> September '07 to discuss the progress of the ACCMS initiative and how to extend its boundaries by involving more countries and groups into the realm of the Asian Consortium. Two possible venues for the next ACCMS meeting were suggested viz. Vietnam and Singapore and it was unanimously decided that the ACCMS-5 in 2009 will be held at Hanoi. Dr. Vu Ngoc Tuoc from Hanoi University of Technology (HUT) and Dr. Duc Nguyen Manh from UK who will be responsible for organizing the next meeting, make a brief presentation of the infrastructural facility and strength available in Hanoi, and also welcomed all the delegates to participate in ACCMS-5 in Hanoi.

In the concluding session, Prof. G.P. Das aptly summarized the presentations and organization of the conference, while Prof. J. Ihm delivered the Vote of Thanks. The wide international participation and the high level of talks and presentations in this Seoul Conference are indicative of the fact that ACCMS has reached a matured phase during the last 8 years of its existence. It is hoped that more and more groups and laboratories actively involved with computational materials research will continue to nurture this Asian Consortium.

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