



Osaka University
De La Salle University

The 2nd ASIAN Computational Materials Design (CMD[®]) Workshop – Philippines

September 22-23, 2009

De La Salle University, Philippines

The basic foundations of our technology, and its foreseen development in the 21st century, basically lie on the physical sciences and, if one desires to distinguish, also material science. To meet the ever-increasing demand for novel materials, and at the same time satisfy the growing public concern for the energy/power consumption and environmental impacts, novel routines other than relying on the age-old tradition of trial-and-error/hit-and-miss would be necessary. Given these circumstances, we need to develop novel theoretical routines and techniques that could quickly and efficiently find novel materials for synthesis, which would suit our purposes. The theoretical routines and techniques necessary should incorporate quantum mechanics per se, and should not be dependent on experimental results and/or empirical parameters. Ab-Initio/First Principles Calculations satisfy all these requirements. With recent developments in computational techniques, coupled with the rapid progress in computer efficiency, ab-initio/first principles-based COMPUTATIONAL MATERIALS DESIGN (CMD[®]) is now a reality. Its impact/influence on industrial R&D should increase with the passing years. The purpose of these series of workshops is to provide the participants with a first-hand experience of how COMPUTATIONAL MATERIALS DESIGN (CMD[®]) is carried out, provide them with the basic knowledge and techniques, to better prepare them for the new paradigm in materials science research.

Programme

Time	September 22, 2009	September 23, 2009
0900-0920	<u>Opening Remarks</u> Prof. Hisazumi AKAI <i>Graduate School of Science, Osaka University</i>	
0920-1030	<u>Lecture</u> Prof. Tetsuo OGAWA <i>Graduate School of Science, Osaka University</i> "Toward New Optical Science of Dynamically-Correlated Electron Systems: Quantum Cooperative Phenomena in Photoexcited Semiconductors"	<u>Lecture</u> Prof. Hideaki KASAI <i>Graduate School of Engineering, Osaka University</i> "Computational Materials Design and its applications for various industrial fields"
1030-1050	<u>Break</u>	
1050-1200	<u>Lecture</u> Prof. Koun SHIRAI <i>Institute of Scientific and Industrial Research, Osaka University</i> "First-principles pseudo potential electronic structure calculation code, Osaka 2000, and its applications"	<u>Lecture</u> Prof. Tomoya ONO <i>Graduate School of Engineering, Osaka University,</i> "First-principles calculation code by real-space formalism, RSPACE, and its applications"
1200-1300	<u>Lunch Break</u>	
1300-1700	<u>Tutorial/Hands-on</u> Osaka 2000 Operation Basic practice Advance practice	<u>Tutorial/Hands-on</u> RSPACE Operation Basic practice Advance practice
1700 -		<u>Awarding/Closing</u> Prof. Hisazumi AKAI / Prof. Hideaki KASAI

