

# Highlights of Focus Group

## Condensed Matter Physics

### Focus Group on Computational Materials Research

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National Chung Cheng University

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## I ntroduction

The chief purpose of this program is to enhance the domestic research capacity in computational material science especially quantum mechanics-based *ab initio* electronic structure calculations and molecular dynamics simulations, through promoting exchange and collaboration among local members as well as between Taiwan and foreign members, and also through attracting more young researchers into this field. To this end, we will organize *ab initio* methods study group meetings, mini-schools with leading international scientists as main lecturers, and also program-wide annual conference. The gatherings of this kind have provided an essential channel for fruitful discussions among members of the community, and in particular, benefit our postgraduate students and young postdocs tremendously.

In order to be more productive and to have stronger impact, it is vital that we all interact or collaborate with experimentalists especially the experimentalists at home. To strengthen these connections and also to reach to the wider experimental community in

Taiwan, we plan to have at least two joint meetings with the experimentalists. The first meeting is "The 6th Taiwan-Japan-Korea symposium and the 4th oxide workshop" organized by D. J. Huang (SRRC). It will be held in National Dong Hwa University Hualin, Dec. 1-3, 2005. Another meeting is "The first workshop on *Ab Initio* Simulation on Nanomaterials" organized by C. Cheng (NCKU). It will be held in National Cheng Kung University, Tainan, Jan. 6-7, 2006.

The Asian Workshop on First-Principles Electronic Structure Calculations is a big event in the Asian community of *ab initio* research. This series of workshop is initiated seven years ago by Prof. K. Terakura of Japan and K. J. Chang of Korea, about 100 scientists from the Asian countries such as Japan, Korea, India, China, Hong Kong, and Taiwan, and also four to five leading experts from Europe and USA participate in this workshop. Active discussions between the participants continued through the three days workshop as well as critical comments from outstanding and senior *ab initio* guests. It is a



fruitful experience for the local *ab initio* people as well as the graduate students. The 4<sup>th</sup> Asian Workshop was held in National Taiwan University in 2001, and the 7<sup>th</sup> Asian Workshop was held in Tamkang University in 2004. The next meeting will be held in China and the CMR focused group members will continue being active in this Asian community of *ab initio* research. We also encourage members especially young ones to attend relevant international conferences, workshops and schools. The  $\Psi_k$  2005 Conference took place during September 17-21, 2005 in Schwäbisch Gmund, Germany. As the two previous  $\Psi_k$  meetings (1996, 2000),  $\Psi_k$  2005 covered theoretical and computational research of electronic structure and properties of matter, ranging from new materials to systems of biological interest. It is one of the most important conference in the community of *ab initio* research. We supported W.S Su ( Ph. D. student at NCCU) and Amel Laref (postdoc. at NTU) to attend the  $\Psi_k$  2005 Conference. In the past half year, up to August 31 2005, the major activities of CMRFG can be represented by the following workshops.

### **1. The First-Principles Computational Materials Physics Mini-School 2005: Beyond Local Density Approximation and Generalized Gradient Corrections May 20-21, 2005, National Taiwan University**

This workshop, organized by G.Y. Guo (NTU), is cooperated with Spin-Related Physics in Condensed Matter Focused Group. Density functional theory (DFT) in the local density approximation (LDA) or generalized gradient approximations (GGA) has been a highly successful method for first-principles quantum mechanical calculations of many properties such as atomic structure and phonon

bands, of a variety of materials. Nonetheless, it fails to give accurate excitation properties, e.g., band gaps, excitonic binding energies, of solids. In this Mini-School, world leading scientists, Prof. Steven Louie from UC Berkeley and Prof. Jim Chelikowsky from UT Austin, are invited to lecture on first-principles many-body techniques that go beyond the standard DFT-LDA (GGA). The titles of the lecture are *GW and Bethe-Salpeter methods* by Prof. Steven Louie and *Time-Dependent Density Functional Theory* by Jim Chelikowsky.

### **2. The 6th Annual Conference on First-Principles Computational Materials Physics July 27-29, 2005, Chi-Tou Forest Recreational Area**

This workshop is organized by T. C. Leung (NCCU). The aim of this conference is to promote interaction and collaboration among local physicists. The Program Committee would also like to take this opportunity to hear about interests of the community in order to plan future activities at the Center. Like previous years, all participants including PhD students and young postdocs, were encouraged to give a talk in this conference. Chi-Tou Forest Recreational Area is a popular tourist attraction, and should provide a relaxing atmosphere for fruitful interactions. The scientific program consisted of three 40-minute lectures, five 30-minute research reports and nine 20-minute talks by young postdocs or Ph. D. student. The three lectures were given by G.Y. Guo (NTU) on *Ab Initio Calculation of Intrinsic Spin Hall Effect in Semiconductors*, C. Cheng (NCKU) on *Relative stability for surfaces of different compositions*, and C. M. Chang (NDHU) on *Ab initio study of CO oxidation on Gold-based catalysts*.