Highlights of Programs

Condensed Matter Physics

Focus Group on Computational Materials Research

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I. Introduction

The chief purpose of this group 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, like previous years, we have organized ab initio methods study group meeting, mini-schools with leading international scientists as main lecturers, and also program-wide annual conference. Furthermore, to attract younger researchers as well as experienced ones to the field of CMR and also promote awareness of the important role in the modern scientific research played by the computation using present-day computers, we have also organized spring school (introductory level) and summer school (advanced level) on first-principles computational materials research. We have encouraged members especially young ones to attend relevant international conferences, workshops and schools. Specifically, we supported Ru-Fen Liu (postdoc. at NCKU), C. H. Cho (Ph. D. student at CCU), and C. H. Yao (Ph. D. student at NDHU) to attend international school. We also supported C. Y. Ren (NKNU) and B. R. Wu (CGU) to visit NCTS this summer in order to promote the collaboration among local members. 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 postdoctoral fellows tremendously.

The CMR focus group consists of 42 members (29 faculties and 13 Ph. D. students and postdocs). It is run by a committee from various institutions. The missions of the committee are to allocate the budget, to initiate research activities, to invite the long-term and short-term visitors and to recommend candidates (Ph. D. student or junior scientist) to attend international school, conference, or workshop with the financial support of CMRFG.

II. Activities

1. Mini-School on Time-Dependent Density Functional Theory: Foundations and Applications

The ground-state based nature of the conventional Density Functional Theory (DFT) method has difficulties in tackling electronic excitations. An alternative method which is comparatively simpler in formalism is the time-dependent (TD) DFT. TDDFT has great success in describing excitations in finite systems such as nanoclusters. The Mini-School on Time-Dependent Density Functional Theory: Foundations and Applications, organized by G. Y. Guo (NTU), is held in National Taiwan University in March 16-17, 2007. Two of the leading figures in the field, namely, Prof. Eberhard K. U. Gross (Berlin Free Univ.) and Prof. Shih-I Chu (Univ. of Kansas and National Taiwan Univ.), gave five lectures on the foundations, recent new developments, and applications of TDDFT.

2. Mini-School on Tight Binding Simulation on Nanomaterials

The ability to perform reliable simulations of molecules and solids systems with thousands of atoms has enormous payoffs in many fields. The Mini-School on Tight Binding Simulation on Nanomaterials, organized by T. C. Leung (CCU), is held in NCTS in June 22-23, 2007. Prof. C. W. Wang from Ames Lab. (USDOE) gave four lectures to review the tight binding theory, formulism and the development of tight binding potentials for molecular simulation of materials. Application of tight binding molecular dynamics to the studies of nanoclusters, carbon nanotubes, and surface-based nanostructures were discussed.

3. The 7th Workshop on First-Principles Computational Materials Physics

The 7th Workshop on First-Principles Computational Materials Physics, organized by S. F. Tsay (NSYSU), was held on Jan. 29-31, 2007 in National Sun Yat-sen University. 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 workshop. The workshop will cover the subjects related to our program such as description of physics and computational methods or report of results. The scientific program consisted of four 40-50-minutes lectures, eight 30-minutes research reports and ten 20-minutes talks by student.

4. Spring school on First-Principles Computational Materials Research - Introductory Level

The spring school on first-principles computational materials research-introductory level, lectured by T. C. Leung (CCU), is held in National Center for High-Performance Computing. The purpose of this school is to offer an introduction to the fundamentals of *ab initio* density functional theory, of pseudopotentials, and large scale calculations, as well as a practical hands-on training for young students and non-specialists. The response from both young students and non-specialist researchers were very positive, there were more than hundred participants in this spring school.

5. Summer School on First-Principles Computational Materials Research – Advanced Level

The summer school on first-principles computational materials research – advanced level, organized by C. Cheng (NCKU) and T. C. Leung (CCU), is held in NCTS. The purpose of this school is to offer the audiences a deeper understanding on the fundamentals of *ab initio* density functional theory, of pseudopotentials, and large scale calculations. Particular emphasis will be laid on a thorough discussion of the problems that can be solved directly with the basic code. There were more than fifty participants in this summer school.

6. Asian Workshop on First-Principles Electronic Structure Calculations

The 9th Asian Workshop on First-Principles Electronic Structure Calculations was held in Korea, Nov. 1 – 3, 2006. This is a big event in the Asian community of ab initio research. This series of workshop is initiated at 1998 by Prof. K. Terakura of Japan and K. J. Chang of

Korea, more than 100 scientists from the Asian countries such as China, Hong Kong, Japan, Korea, India, Singapore, and Taiwan, and also four to five leading experts from Europe and USA participate in this workshop. The 4th Asian Workshop was held in National Taiwan University in 2001, the 7th Asian Workshop was held in Tamkang University in 2004, and the 11th Asian Workshop will be held in National Sun Yat-sen University. Eighteen members of CMRFG participate the 9th Asian Workshop last year. The next meeting will be held in Japan and we will continue being active in this Asian community of *ab initio* research.

7. OpenMx Study Group Meeting

It is well known that the computing time of currently popular electronic structure methods based on Density Functional Theory scale like N^{2-3}, with N being the number of atoms in the simulation cell. In the last few years, much effort has been devoted to overcome this problem, and a number of methods have been developed with "order – N "[O(N)] scaling, i.e., whose computational cost scales only linearly with the number of atoms. One of the successful order N *ab initio* computing code is OpenMx (Open source package for Material explorer) developed by Dr. Taisuke Ozaki from National Institute of Advanced Industrial Science and Technology in Japan. In order to familiar with the principles used in the program and how they are implemented so that the program can be properly applied to the systems we want to study, several study group meeting on OpenMx was organized by T. C. Leung (CCU) and held in NCTS. The key members involved in this project are C. S. Hsue (NTHU), Y. T. Lu (NCKU), W. C. Kuo (NSYSU), T. L. Li (NCYU), T. C. Leung (CCU), Y. C. Hsu (NCKU), S. F. Tsay (NSYSU), G. Y. Guo (NTU), S. H. Chiou (ITRI), C. Y. Ren (NKNU), and B. R. Wu (CGU).

8. Excited State Study Group Meeting

The conventional DFT method fails to give accurate excitation properties, e.g., band gaps, excitonic binding energies, of solids. The GW method has been successfully used to predict electronic properties of a variety of different systems, ranging from bulk materials to surfaces, nanotubes, and molecules, whereas the linear optical response is routinely studied by solving the Bethe-Salpeter Equation (BSE) with comparable success. ABINIT is a package whose main program allows one to study the excited states using the GW approximation. On the other hand, the EXC is an exciton code which uses the output of ABINIT to calculate the dielectric and optical properties for a large variety of systems by solving the Bethe-Salpeter equation. In order to familiar with the principles used in the program and how they are implemented so that the program can be properly applied to the systems we want to study, Exited State Study Group Meeting was organized by G. Y. Guo (NTU) and held in NTU. The key members involved in this project are G. Y. Guo (NTU), T. C. Leung (CCU), Y. J. Tsai (CCU), H. C. Hsueh (TKU) , M. Hayashi (CCMS), C. K. Yang (CGU), H. T. Jeng (AS), and B. R. Wu (CGU).

III. Collaborative Activities

The examples of these collaborations between CMRFG members are listed as follows:

1. C. M. Chang (NDHU), C. Cheng (NCKU) and C. M. Wei (AS) on the Quantum Monte Carlo simulation on nanomaterials.
2. H. T. Jeng (AS) and C. S. Hsue (NTHU) on the Orbital Ordering in transition-metal oxides.
3. C. Y. Ren (NKNU), S. F. Tsay (NSYSU) and F. C. Chuang (NSYSU) on the electronic structure of Au/Si(111) (5x2).
4. B. R. Wu (CGU) and T. C. Leung (CCU) on the electronic and optical properties of ribbon under external electric field.
5. G. Y. Guo (NTU), T. C. Leung (CCU) and H. C. Hsueh (TKU) on the *ab initio* study on excited state of nanomaterials.

International collaborations are listed as follows:

1. K. Terakura (Japan) and G. Y. Guo (NTU)

on the static dielectric response of BN nanotubes from *ab initio* finite electric field calculations,

2. C. T. Chan (Hong Kong) and T. C. Leung (CCU) on the field emission properties of nanomaterials.
3. M. Y. Chou (USA) and C. M. Wei (AS) on the quantum well states in metal thin films.
4. Steven G. Louie (USA) and H. C. Hsueh (TKU) on the quasiparticle excitations in nanomaterials.

IV. Highlights of Research Results

1. Current and strain-induced spin polarization in InGaN/GaN superlattices

Main team members:

G. Y. Guo (NTU) and Y. F. Chen (NTU, experimentalist)

It has been proposed theoretically that a transverse spin current, the so called spin Hall current, can be generated in strongly spin-orbit coupling systems by external electric field. We have investigated the current-induced spin polarization in InGaN/GaN superlattices. It is found that the degree of polarization changes sign as the direction of the current flow is reversed. The strain-induced spin Hall effect discovered here paves an alternative way for the creation of spin polarized current, which should be useful for the realization of the future applications in spintronics.

H. J. Chang, T. W. Chen, J. W. Chen, W. C. Hong, W. C. Tsai, Y. F. Chen, and G. Y. Guo, Phys. Rev. Lett. 98, 239902 (2007).

2. Orbital Ordering and Jahn-Teller Distortion in Perovskite Ruthenate $SrRuO_3$

Main team members:

H. T. Jeng (AS) and C. S. Hsue (NTHU)

Orbital, charge, spin, and lattice degrees of freedom play important roles in the electronic, magnetic, and transport properties of transition-metal oxides. It was proposed that orbital ordering is closely related to magnetic and crystallographic lattices in perovskite manganites such as $La_{1-x}Ca_xMnO_3$ in the low temperature insulating charge ordered phase. We have investigated the electronic structures of $SrRuO_3$ in the distorted orthorhombic structure using LDA+U. The obtained band energies agree well with those from photoemission and X-ray absorption spectroscopy. Our finding unravels the nature of the orbital ordering, the close connection to the JT distortions, and the importance of the on-site correlation U in the relatively extended Ru 4d orbitals.

H. T. Jeng, S. H. Lin, C. S. Hsue, Phys. Rev. Lett. 97, 67002, (2006)

3. Highly Spin-polarized field emission induced by quantum size effects in ultathin films of Fe on W(001)

Main members:

T. C. Leung (CCU) and C. T. Chan (Hong Kong)

Nanostructured systems have enhanced effects due to the confinement of quantized states, and, for the particular case of ultrathin supported films, many amazing structural and electronic properties have been discovered. Although tungsten is the metal of choice for emitter tips, it does not produce spin-polarized field emission currents. We use density functional calculations to study the spin-polarized field emission from pseudomorphic Fe ultathin films on W(001). We found that nearly completely spin-polarized field emission currents can be realized in two and four Fe layers on W(001) and that these systems have the additional advantages of thermal stability and low work functions. The thickness dependent field emission properties are traced to spin-polarized quantum well and surface resonance states localized in the Fe layers.

Bin Li, T. C. Leung, C. T. Chan, Phys. Rev. Lett. 97, 87201 (2006).

Remark: For detail publications, please see the webpage http://phys.cts.nthu.edu.tw/research/focus_group.php