Highlights of Programs

Condensed Matter Physics

Focus Group on Computational Material Research

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I. Brief Description

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, 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 Y. H. Su (Ph. D. student at NCKU), W. S. Su (Postdoc. student at CCU), C. H. Cho (Ph. D. student at CCU), C. L. Huang (Sinica), T. R. Chang (Ph. D. Student at NTHU), and H. L. Huang (Ph. D. student at NTU) to attend international school. We also supported C. Y. Ren (NKNU), J. M. Lu (NCHC), S. P. Ju (NSYSU), and W. S. Su (CCU) 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 56 members (33 faculties and 23 Ph. D. students and postdocs). It is run by a committee from various institutions. The committee members are T. C. Leung (Coordinator, CCU), G. Y. Guo (NTU), M. H. Lee (TKU), C. C. Kuan (Sinica), C. Cheng (NCKU), S. F. Tsay (NSYSU), M. H. Tsai (NSYSU), and C. M. Chang (NDHU). 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-Workshop on Quantum Transport and Current-Driven Dynamics in Molecular-Scale Electronics

Inelastic electron tunneling via molecular-scale junctions can induce a variety of fascinating dynamical processes in the molecular moiety. Potential applications of current-driven dynamics in heterojunctions range from new forms of molecular machines and new modes of conduction, to new directions in surface nanochemistry and nanolithography. This mini-workshop is organized by C. C. Kuan (Sinica) and held in March 7, 2008. Prof. T. Seideman from Northwestern University was invited to give lectures on this issue.

2. Mini-School on Computational Material Physics : Towards an understanding of surface processes and catalysis using density functional theory calculations

It is well known that catalysis plays a very important role in a wide range of scientific and technological problems. It is virtually impossible to provide an insight into catalysis without an understanding of the electronic structures of catalysts. This mini-school was organized by M. H. Lee (TKU) and held in Institute of Atomic and Molecular Sciences in March 29, 2008. Prof. Prof. Peijun Hu from Queen's University gave four lectures on the following topics.

1. A simple thermodynamic rule for the rapid catalyst search
2. CO oxidation on metal and metal oxide surfaces
3. Towards an understanding of Fischer-Tropsch synthesis

3. Summer Workshop on Nanoscale Materials

To provide opportunities for exchange and discussion between theoreticians and experimentalists and also foster collaborations among them, the Summer Workshop on Nanoscale Materials, organized by Dr. J. M. Lu (NCHC), was held in August 21-22 in NCTS. Fourteen theroreticians and experimentalists were invited to present in this workshop. The workshop was well attended and more than eighty participants from all over the country.

4. The 8th Workshop on First-Principles Computational Materials Physics

The 8th Workshop on First-Principles Computational Materials Physics, organized by T. C. Leung (CCU), was held on July 1-3, 2008 in Huisun Forest Station. 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.

5. School on First-Principles Computational Materials Research

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 summer school on first-principles computational materials research – advanced level, organized by T. C. Leung (CCU), is held in NCTS. The purpose of this schools are 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 the spring school and more than fifty participants in the summer school.

6. 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. 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 were organized by T. C. Leung (CCU) and held in NCTS. The key members involved in this project are C. S. Hsue (NTHU), T. C. Leung (CCU), Y. C. Hsu (NCKU), G. Y. Guo (NTU), C. Y. Ren (NKNU), and B. R. Wu (CGU).

7. 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, 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 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, several exited state study group meeting were 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), H. C. Hsueh (TKU) , M. Hayashi (CCMS), C. K. Yang (CGU), H. T. Jeng (Sinica), and B. R. Wu (CGU).

8. Quantum Monte Carlo Study Group Meeting

The quantum monte carlo (QMC) method based on random walk sampling provides a direct treatment of quantum many-particle effects, thus making it beyond the reach of mean-field methods and giving a highly accurate description in electron-electron correlation. QMC provides promising results in the study of real materials and can serve as benchmarks for other techniques may be compared. How to implement QMC methods efficiently is critical. Nowadays, QMC can deal with systems up to hundreds of valence electrons. The aim of this series of study-group meetings is to provide an opportunity of interactions and experience sharing for those who are employing or about to use QMC methods in their research, several QMC study group meeting were organized by C. Cheng (NCKU) and C. M. Wei (Sinica). The key members involved in this project are C. Cheng (NCKU), C. M. Wei (Sinica), C. M. Chang (NDHU).

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 (Sinica) on the Quantum Monte Carlo simulation on nanomaterials.
2. H. T. Jeng (Sinica) , C. Y. Ren (NKNU) and C. S. Hsue (NTHU) on the Orbital Ordering in transition-metal oxides.
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. N. Nagaosa (Japan) and G. Y. Guo (NTU) on the intrinsic spin Hall effect.
2. C. T. Chan (Hong Kong) and T. C. Leung (CCU) on the optical properties of nanomaterials.
3. N. Drummond (UK) and C. M. Wei (Sinica) on the Quantum Monte Carlo simulation on nanomaterials.
4. Steven G. Louie (USA) and H. C. Hsueh (TKU) on the quasiparticle excitations in nanomaterials.

IV. Highlights of Research Results

(1) Intrinsic Spin Hall Effect in Platinum

G.Y. Guo and his collaborators have studied the Spin Hall effect with first-principles relativistic band calculations for platinum. They show that intrinsic spin Hall conductivity has a peak near the Fermi energy and that the vertex correction due to impurity scattering vanishes. They argue that the large SHE observed experimentally in platinum is of intrinsic nature [14].

(2) Au/Si(111)-(5x2) surface reconstruction

F. C. Chuang and his collaborators have studied the models with a honeycomb chain feature for the Au/Si(111)-(5x2) surface reconstruction using. Their calculation shows that one of these models has a lower surface energy than the previously proposed models. This newly identified model also reproduces certain key features in the angle-resolved photoemission measurement and experimental scanning tunneling microscopy images[11].

(3) Work function of Carbon Nanotubes

T. C. Leung and his collaborators have investigated the work functions of various forms of small radius carbon nanotubes and their derivatives by density functional calculations. They found that the work function can exhibit significant variations depending on the length of the tubes and the way they are arranged. It is interesting to see that for isolated tubes, the tip dipole does not affect the work function, but the density and the sign of the dipole become the crucial factor when the tubes form a bundle [22].

V. References

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