Focus Group on Computational Materials Research

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I. Brief Description

The primary purpose of this program is to enhance the domestic research capacity in the computational material science based on the first-principles quantum mechanical methods through promoting interactions and collaborations among local members as well as between local members and international noted scholars, and also through attracting outstanding young researchers into this field.

The CMR focus group presently consists of more than 50 members, including 40 faculties and 14 postdoctors. According to the interests and the existing expertises of the members, we have identified four frontiers to concentrate on, i.e. calculations of the electronic excited states (ExcS), nanomaterials (NM), quantum Monte Carlo methods (QMC), and quantum transport (QT). Study-group meetings initiated by the members involved in these four topics become one of the main backbone activities in promoting collaborations among members as well as stimulating new ideas and in-depth discussions. So are the corresponding leading international visitors with the held comparable minischools. The Ph.D. students, postdoctors and the junior faculty members are encouraged to attend the relevant international conferences, workshops and schools.

The focus group is run by a committee whose members consists of four coordinators in charge of the activities related to the four frontiers, i.e. HC Hsueh (TKU) for ExcS, FC Chuang (NSYSU) for NM, CM Chang (NDHU) for QMC and CC Kaun(AS) for QT, and another six senior members of the group, i.e. GY Guo (NTU), MH Lee (TKU), TC Leung (CCU), MH Tsai (NSYSU), SF Tsay (NSYSU), and C. Cheng (the coordinator of CMRFG, NCKU). 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 through the financial support of CMRFG.

II. Activities

The activities supported by CMRFG are listed according to the following three categories 1) workshops for all members 2) schools 3) study-group meetings.

1. 7/1-7/3 2009 : 9th Workshop on First-Principles Computational Materials Physics

   7/6-7/10 2009: The 1st Workshop of High-Performance Computing on Nanoscale Materials Research 2009

2. 5/16-5/17 2009 : The school on first-principles computational materials research -- introductory level

   6/06-6/07 2009 : The school on first-principles computational materials research -- introductory level

   7/06-7/10 2009 : The school on first-principles computational materials research -- advanced lever

   12/27 2009: Minischool of LDA+U and GW

methods

3. 4/17 2009 : QMC study group meeting

   5/02 2009 : Excited-state study group meeting

   5/08 2009 : Nanomaterials study group meeting

   6/26 2009 : Excited-state study group meeting

   7/06 2009 : QMC study group meeting

   7/21 2009 : QMC study group meeting

   9/11 2009 : Excited-state study group meeting

   11/06 2009 : Excited-state study group meeting

   11/11 2009 : QMC study group meeting

   11/20 2009 : Nanomaterials study group meeting

- **The 9th Workshop on First-Principles Computational Materials Physics**

This program-wide workshop was held on July 1-3, 2009 in Cheng Ching Lake of Kaohsiung. The aim of this workshop is to promote interactions and collaborations among local members. The CMRFG Committee also takes this opportunity to learn about the general interests of the community in order to organize beneficial activities for the members in the future. All participants, particularly PhD students and postdoctors, are encouraged to give a talk in this workshop.

- **The 1st Workshop of High-Performance Computing on Nanoscale Materials Research**

This workshop is also a program-wide one as most of the CMRFG members involve more or less in the studies of nanoscale systems. The emphasis is especially on the possible combinations of the less CPU time-consuming methods for larger systems with the accurate first-principles methods to identify the crucial mechanisms for the investigated issues.

- **Schools on First-Principles Computational Materials Research**

To help the newcomers in this field overcome the hurdle in the beginning, both the introductory-level spring school and the advanced-level summer school on the first-principles computational materials research are organized. The spring school, lectured by T. C. Leung (CCU), is held in National Center for High-Performance Computing. The summer, organized by T. C. Leung (CCU), is held in NCTS (south). Both schools include the practical hands-on sessions. The responses from both students and non-specialist researchers are much positive as there are more than one hundred participants in the spring school and more than fifty participants in the summer school.

- **Excited State study group Meeting and Minischool of LDA+U and GW methods**

Four study-group meetings are held for the last eight months. The discussions are mainly on the applications of the present available methods, i.e. the GW methods (VASP and Berkeley GW), the Bethe-Salpeter methods (Berkeley GW) and the time-dependent DFT (Turbomol), for the excited-state study of the bulk materials and nanomaterials.

- **Quantum Monte Carlo study group Meeting**

Four study-group meetings are held for the last eight months. The discussed topics cover 1) generation of norm-conserving pseudopotentials with the Opium package 2) atomic or molecular absorption on surfaces using QMC methods 3) magnetic moments of small metallic clusters using QMC methods 4) generation of Wannier functions

III. Visitors and International Collaborations

Examples of collaborations between CMRFG members are listed as follows :

1. CM Chang (NDHU), C Cheng (NCKU) and CM Wei (AS) on the applications of the Quantum Monte Carlo methods.
2. HT Jeng (AS) , CY. Ren (NKNU) and CS. Hsue (NTHU) on the Orbital Ordering in transition-metal oxides and developing a specialized ab initio code for surface problems.
3. BR Wu (CGU) and TC Leung (CCU) on the electronic and optical properties of ribbon under external electric field.
4. GY Guo (NTU), TC Leung (CCU) and HC Hsueh (TKU) on the ab initio study for the excited state of nanomaterials.
5. CC Kaun (AS) and TS Tang (NUU) on the

quantum transport in graphene nanoribbons and in nanomachines.

International collaborations are listed as follows :

1. GY Guo (NTU) and N Nagaosa (Japan) on the intrinsic spin Hall effect.
2. TC Leung (CCU) and CT Chan (HongKong) on the optical properties of nanomaterials.
3. CM Wei (AS) and N. Drummond (UK) on the applications of the Quantum Monte Carlo methods.
4. HC Hsueh (TKU) and SG Louie (USA) on the quasiparticle excitations in nanomaterials.
5. CC Kaun (AS) and G Hong (Canada) on the spin transport in nanostructures
6. CC Kaun (AS) and FM Peeters (Belgium) on the interplay of the transverse discrete modes with a longitudinal supercurrent in a superconducting nanowire

IV. Highlights of Research Results

The community of the first-principles electronic calculations for materials of this country has flourished in the last few years. The number of faculty members in the community started by less than ten is now reaching forty. The members benefits extremely from the interactions through the activities supported by the NCTS. That the members share their individual expertise within the community without reservation also advances the community's strength as a whole. How these could lead directly to the concrete research results, e.g. journal publications or invited talks, is not as straightforward to identify as might have been implied in the performance evaluations required by the funding agency. Not to mention that those concrete research results also benefit mostly from the personal NSC projects of the members as well as, for some, the joint projects.

However, for the last eight months, the majority of the members have benefited enormously by the study-group meetings of the focused topics supported by the CMRFG which could not be acquired from other resources otherwise. Continuous supports of these meetings with extensions through invitations and potential collaborations with the international leading experts are expected to lead to concrete and eminent research results as the pursuit all the time of the NCTS.

(1) Excited State study group meetings

The group explores the applicability of the established codes for the electronic excitation using the GW, the Bethe-Salpeter and the time-dependent DFT methods. Investigations are applied to the covalent and ionic insulators as well as the nanosystems. Extensions of these studies to optical spectrum and absorption spectrum are also developed.

(2) Quantum Monte Carlo study-group meetings

To successfully apply the QMC methods to the systems consisting of the extensive range of the elements in the periodic table, the generation of the physical and cpu-time-affordable norm-conserving pseudopotentials is explored and achieved. The current effort is mainly on the generation of the maximally localized Wannier functions from the DFT calculations in order to construct a much better initial many-body wavefunction for the DMC calculations. In the mean time, the effect of the exchange and correlation on the magnetic moments of magnetic clusters and the stability of the surface absorption of atoms and simple molecules are also undergoing investigations.

(3) Nanomaterials study-group meetings

The major issues of these meetings are to identify the way in making use of the advantages of the capable but coarser methods together with the accurate first-principles methods to resolve problems in considerably large-size systems.

V. Selected Publications

[1] GY Guo, S Maekawa and N Nagaosa, Phys. Rev. Lett., 102, 036401 (2009).

[2] TW Chen and GY Guo, Phys. Rev. B 79, 125301 (2009).

[3] ZR Xiao and GY Guo, J. Chem. Phys., 130, 214704 (2009).

[4] S Ju, TY Cai, and GY Guo, J. Chem. Phys., 130, 214708 (2009).

[5] ZZ Zhu, JC Zheng, GY Guo, Chem. Phys. Lett., 472, p99 (2009).

[6] TH Cho, WH Su, TC Leung, W Ren, CT

Chan, Phys. Rev. B 79, 235123 (2009).

[7] J. P. Chou, H. Y. T. Chen, C. R. Hsing, C. M. Chang, C. Cheng, and C. M. Wei, Phys. Rev. B 80, 165412 (2009).

[8] GY Guo, S Murakami, TW Chen, and N Nagaosa, Phys. Rev. Lett., 100, 096401 (2008).

[9] S. Ju and Guo GY, J. Chem. Phys., 129, 194704 (2008).

[10] S. Ju and G. Y. Guo, Appl. Phys. Lett. 92, 202504 (2008).

[11] I. J. Wu and G. Y. Guo , Phys. Rev. B 78, 035447 (2008).

[12] Y. H. Chiu, Y. H. Lai, J. H, Ho, D. S. Chuu, and M. F. Lin, Phys. Rev. B 77, 045407 (2008).

[13] C. M. Chang, C. Cheng, C. M. Wei, J. Chem. Phys., 128, 124710 (2008).

[14] F.C. Chuang, Chia-Hsiu Hsu, C.-Z. Wang, and K.-M. Ho, Phys. Rev. B 77 153409 (2008).

[15] PA Lin, HT Jeng, and CS Hsue, Phys. Rev. B 77, 085118 (2008).

[16] CK Yang, Appl. Phys. Lett. 92, 033103 (2008).

[17] C Cheng, Phys. Rev. B 78, 132403 (2008).