Focus Group on Computational Materials Research

Period between Nov. 1, 2005 and Oct. 31, 2006
Coordinator : Tsan-Chuen Leung (e-mail: tcleung@phy.ccu.edu.tw)
National Chung Cheng University
Committee members: C.M. Chang (Nat'l Dong Hwa Univ.), C. Cheng (Nat'l Cheng Kung Univ.),
G.Y. Guo (Nat'l Taiwan Univ.), M.H. Lee (Tamkang Univ.), S.F. Tsay (Nat'l Sun Yat Sen Univ.).

Introduction

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 meetings, joint experimental and theoretical workshops, mini-schools with leading international scientists as main lecturers, and also program-wide annual conference. Furthermore, to attract younger researchers as well as the experienced ones to the field of CMR and also to 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. 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. We have encouraged members especially young ones to attend relevant international conferences, workshops and schools. Specifically, we supported Ru-Fen Liu (postdoc. at NCKU) and Chi-Cheng Lee (Ph.D. student at Tamkang Univ.) to attend International Workshop: Density functional theory meets strong correlation. We also supported Chung-Yuan Ren and Bi-Ru Wu visited NCTS (south) last summer in order to promote the collaboration among local members. The 8th Asian Workshop on First-Principles Electronic Structure Calculations was held in Shanghai, Oct. 31 to Nov. 2, 2005. 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, about 100 scientists from the Asian countries such as China, Hong Kong, Japan, Korea, India, 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, and the 7th Asian Workshop will be held in Tamkang University in 2004. We have eighteen members of this focus group participate the 8th Asian Workshop last year. The next meeting will be held in Korea and the member of focus group on Computational Material Research will continue being active in this Asian community of ab initio research. In order to promote the international collaborations, we have invited a couple of distinguished foreign scientists to visit Taiwan for a short period. We have the following visitors from abroad in the past year: Prof. J.P. Lu from Univ. of North Carolina at Chapel Hill (USA) visited J.P. Lu, Prof. Steven Louie from

University of California at Berkeley (USA) visited C. Cheng and G.Y. Guo, Porf. Ku Wei from Brookhaven National Laboratory (USA) visited H.C. Hsueh, Prof. Ferdi Aryasetianwan from AIST (Japan) and Prof. Shiwu Gao from Goeteborgs Univ. (Sweden) visited G.Y. Guo, and Prof. C.T. Chan from Hong Kong Univ. of Sci. and Techno. (HK) vistited T.C. Leung.

The 8th Asian Workshop on First-Principles Electronic Structure Calculations at Shanghai

1. The First Workshop of ab Initio Simulations on Nanomaterials (Jan 6 - 7, 2006)

Nanomaterials, due to their nanoscale, exhibit distinct properties from either bulk or atoms and molecules. Theoretical and computational progresses in ab initio simulations have allowed the method to study static as well as dynamic properties of physical systems. In this workshop we shall bring together the local ab initio researchers, an international speaker as well as a few invited experimentalists to present their studies on nanomaterials. The workshop was organized by C. Cheng and held in National Cheng Kung University. The speakers and titles are as follows :

Engineering electronic properties of CNTs through chemical functionalizations by J.P. Lu (Univ. of North Carolina *at Chape*l Hill), *Introduction of lithium ion batteries and direct methanol fuel cells* by Bing Joe Hwang (Nat'l Taiwan Univ. of Science & Technology), *Design of nanocatalyst systems* by C.Y. Mou (NTU), *Ab initio study of CO oxidation on Au-Ag nanoparticles* by C. M. Chang (NDHU) *Single-walled (5,3) gold and platinum nanotubes – a theoretical study* by C.K. Yang (Chang Gung U.), *Ab initio investigations of some 1-D nano-materials* by G.Y. Guo (NTU), *Giant Stark effect and electro-optical modulation in BN nanotubes* by C.W. Chen (NTU), *One-dimensional nanostructures: from lasing to sensing* by L.C. Chen (NTU), *Adsorption kinetics and interaction mechanism of colloidal nanoparticles onto self-assembled monolayers* by Shangir Gwo (NTHU), *From energy transport to medical imaging: some interesting properties of CNTs and their applications* by J.P. Lu (Univ. of North Carolina at Chapel Hill), *Quantum effect on nanostructure* by C.M. Wei (Academia Sinica), *Work function of carbon nanotubes – a first-principles study* by T.C. Leung (CCU).

2. Spring School on First-Principles Computational Materials Research - Introductory Level (Feb. 25-26 ; March 11-12, 2002)

The spring school on first-principles computational materials research – introductory level, lectured by T.C. Leung (NCCU), 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 hands-

on training will be based on a LINUX platform (Pentium PC's). The response from both the young students and non-specialist researchers were very positive, there were about eighty participants in each session of this spring school. Detailed information on the program of the school can be found on the NCTS's web site.

3. The First Study Group Meeting on TDDFT (April 29, 2006)

Time-dependent density functional theory (TDDFT) is one of the two most frequently employed methods based on the DFT scheme to study electronic excitations in many-electron systems. TDDFT mini-schools lectured by distinguished TDDFT experts from abroad will be scheduled. In order to acquire some background knowledge of TDDFT to make the best out of the coming mini-schools, we held the first study-group meeting on TDDFT for the members of the focus group. The first study group meeting on TDDFT was organized by C. Cheng and held in National Cheng Kung University. The speakers and titles are as follows: *Linear response theory in TDDFT* by Chi-Cheng Lee (Tamkang Univ.), *Computational approach to excited states of finite-size systems* by Michitoshi Hayashi (Center for Condensed Matter Sciences), *Examples of TDDFT applications* by Ru-Fen Liu (NCKU) University), and *The TDDFT method in octopus* by C. Cheng (NCKU).

4. Mini-school on the First-Principles Approaches for Many Fermion Interactions (June 16-17 2006)

Resolving obstacles and developing new methods to understanding the novel phenomena in many-fermion systems from first-principles approaches are one of the frontiers of condensed-matter physics. In this mini-school, Prof. Wei Ku of the Brookhaven National Laboratory, who has had extensive experiences on developing a variety of techniques for applying to realistic systems, will give four lectures about various approaches for first-principles excitations and Wannier functions for strongly correlated systems. The titles of the talk in this mini-school are as follows:

1. *Linear response and time-dependent density functional theory.*
2. *Quasi-particle excitations and finite-temperature many-body perturbation theory.*
3. *Linear response via MBPT and the possible future directions.*
4. *Wannier functions and strongly correlated systems.*

5. Summer School on First-Principles Computational Materials Research - Advanced Level (August 17-22, 2006)

The summer school on first-principles computational materials research- advanced level, organized by C. Cheng (NCKU) and T.C. Leung (NCCU), is held in National Cheng Kung University. The purpose of this summer 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. The hands-on training will be based on a LINUX platform (Pentium PC's). There were about fifty participants in this summer school. The lecturers of the school are G.Y. Guo (NTU), C. Cheng (NCKU), T.C. Leung (NCCU), M.H. Lee (TKU), and C.M. Chang (NDHU). Detailed information on the program of the school can be

found on the NCTS's web site.

6. The First Study Group Meeting on OpenMx (August 16-19, 2006)

The ability to perform reliable simulations of molecules and solid systems with thousands of atoms has enormous payoffs in many fields, especially for the materials and pharmaceutical industries. It is well known that the computing time of currently popular electronic structure methods based on Density Funtional Theory (DFT) 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. OpenMX is a program package for nano-scale material simulations, which is designed for the realization of large-scale ab initio calculations based on a density functional theory (DFT), norm-conserving pseudopotentials, and pseudo atomic localized basis functions. 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, the first study group meeting on Openmx was organized by C. Cheng (NCKU) and T.C. Leung (CCU) and held in National Cheng Kung University. The speakers and titles are as follows: *Introduction of C Language* by Y.T. Lu (NCKU), *Overview of Openmx* by G.Y. Guo (NTU), *Comparison on the magnetic properties of oxides calculated with Openmx and VASP* by H.C. Hsueh (Tamkang Univ.), *Electronic and geometric properties of metal cluster calculated with Openmx* by C.M. Chang (NDHU), *Electronic and geometric properties of metal surface calculated with Openmx* by J.P. Chou (CCU), *Electronic and geometric properties of silicon related system calculated with Openmx* by S.F. Huang (NTU), and *Comparison on the geometric properties of carbon and silicon related material calculated with Openmx and VASP* by S.F. Tsay (NSYU).

7. Mini-school on Time-dependent Density Functional Theory: Principles, Application and Beyond (Sept. 4-5, 2006)

Ab initio density functional theory (DFT) with local density approximation (LDA) or generalized gradient approximation (GGA) has been applied to study many physical properties of a wide variety of solids with tremendous success. Nevertheless, the ground-state based nature of the conventional DFT method has difficulties in tackling electronic excitations in solids. An alternative method which is comparatively simpler in formalism, is the time-dependent (TD) DFT. TD-LDA has great success in describing excitations in finite systems such as nanoclusters. In this mini-school, two of the leading figures in the field will give four lectures: on the fundamentals, applications and also beyond TDDFT. The mini-school cooperated with Focus Group on Spin-related Physics in Condensed Matter, was organized by G.Y. Guo and held in National Taiwan University. The speakers and titles are as follows: *"Introduction to Time-dependent Density Functional Theory"*, and *"GW-Dynamic Mean Field Theory (DMFT): An Overview"* by

Prof. Ferdi Aryasetianwan from AIST (Japan) and *"TDDFT in real time, introduction and perspectives"* and *"Collective Excitations in Nanostructures (Nanoplasmons)"* by Shiwu Gao from Goeteborgs Univ. (Sweden).

8. Mini-school on Photonic Crystal - Manipulating Light Using Man Made Materials and Manipulating Materials Using Light (Sept. 22-23, 2006)

The control of light by artificially structured materials has long been an important topic in both academic and applied research. In recent years, we have witnessed significant advances in the field because of the introduction of new ideas, such as the concept of photonic band gap (PBG) materials and meta-materials, which are man-made composites with artificial structures introduced on length scales that are equal to or much smaller than the wavelength of electromagnetic (EM) waves. Light carries energy, momentum and angular momentum, and thus can be used to move and manipulate small particles. Indeed, optical manipulation has provided scientists with unprecedented access to the microscopic world. This mini-school is organized by T.C. Leung (CCU) and held in National Chung Cheng University. In this mini-school, Prof. C.T. Chan from Hong Kong Univ. of Sci. and Techno. (HK) gave a review on the properties of these man-made materials and showed how light can in fact induce structural stability in matter, forming some sort of soft matter called "optical matter". The titles of the talk in the mini-school are as follows:

1. Photonic crystals: The basics.
2. Guided waves and photonic crystal optics.
3. Meta-materials and double negativity.
4. Manipulating materials using light.

9. Selected Publications of CMR Focused Group Members for 2006

1. *"Measurement of current-induced local heating in a single molecule junction"*, Z.F. Huang, B.Q. Xu, Y.C. Chen, et al., Nano Lett. **6**, 1240 (2006).
2. *"Magic structures of H-passivated <110> Silicon nanowires"*, Tzu-Liang Chan, Cristian V. Ciobanu, Feng-Chuan Chuang, Ning Lu, Cai-Zhuang Wang and Kai-Ming Ho, Nano Lett. **6**, 277 (2006).
3. *"Charge-orbital ordering and verwey transition in magnetite measured by resonant soft X-ray scattering"*, D.J. Huang, H.J. Lin, J. Okamoto, K.S. Chao, H.T. Jeng, G.Y. Guo, C.H. Hsu, C.M. Huang, D.C. Ling, W.B. Wu, C.S. Yang, C.T. Chen, Phys. Rev. Lett. **96**, 096401 (2006).
4. *"Orbital ordering and Jahn-Teller distortion in perovskite ruthenate $SrRuO_3$"*, H.T. Jeng, S.H. Lin, C.S. Hsue, Phys. Rev. Lett. **97**, 067002 (2006).
5. *"Highly spin-polarized field emissions induced by quantum size effects in ultrathin films of Fe on W(001)"*, B. Li, T.C. Leung, C.T. Chan, Phys. Rev. Lett. **97**, 087201 (2006).
6. *"Oxygen-Driven Unzipping of Graphitic Materials"*, Je-Luen Li, Konstantin N. Kudin, Michael J. McAllister, Robert K. Prud'homme, Ilhan A. Aksay and Roberto Car, Phys. Rev. Lett., **96**, 176101 (2006), featured in News & Views, Nature, **414**, 818 (2006) .
7. *"Orientational Order of Molecular Assemblies on Inorganic Crystals"* Dudley A. Saville, Jaehun Chun, Je-Luen Li, Hannes C. Schniepp, Roberto Car, and Ilhan A. Aksay, Phys. Rev. Lett., **96** , 18301 (2006)

8. *"Magic numbers of atoms in surface supported planar clusters"*, Y.P. Chiu, L. W. Huang, C.M. Wei, C.S. Chang and Tien T. Tsong, Phys. Rev. Lett. (accepted 2006).
9. *"Sharp infrared emission from single-crystalline indium nitride nanobelts prepared using guided-stream thermal chemical vapor deposition"*, M.S. Hu, W.M. Wang, T.T. Chen, L.S. Hong, C.W. Chen, C.C. Chen, Y.F. Chen, K.H. Chen, L.C. Chen, Adv. Funct. Mater. 16 , 537 (2006).
10. *"Atomic-scale deformation in N-doped carbon nanotubes"*, C.L. Sun, H.W. Wang, M. Hayashi, et al., J. Am. Chem. Soc. **128**, 8368 (2006).
11. *"Percolation transition and colossal magnetoresistive effects in a complex network"*, S. Ju, T.Y. Cai, G.Y. Guo, et al., Appl. Phys. Lett. **89**, 082506 (2006).
12. *"Comparison of the electronic structures of $Zn_{1-x}Co_xO$ and $Zn_{1-x}Mg_xO$ nanorods using x-ray absorption and scanning photoelectron microscopies"*, J.W. Chiou, H.M. Tsai, C.W. Pao, K.P.K. Kumar, S.C. Ray, F.Z. Chien, W.F. Pong, M.H. Tsai, C.H. Chen, H.J. Lin, J.J. Wu, M.H. Yang, S.C. Liu, H.H. Chiang, C.W. Chen, Appl. Phys. Lett. **89**, 043121 (2006).
13. *"Anomalous blueshift in emission spectra of ZnO nanorods with sizes beyond quantum confinement regime"*, C.W. Chen, K.H. Chen, C.H. Shen, et al., Appl. Phys. Lett. **88**, 241905 (2006).
14. *"Photoconductivity and highly selective ultraviolet sensing features of amorphous silicon carbon nitride thin films"*, C.W. Chen, C.C. Huang, Y.Y. Lin, et al., Appl. Phys. Lett. **88**, 073515 (2006)
15. *"Gate-controlled spin splitting in GaN/AlN quantum wells"*, I. Lo, W.T. Wang, M.H. Gau, J.K. Tsai, S.F. Tsay, J.C. Chiang, Appl. Phys. Lett. **88**, 082108 (2006).
16. *"Electronic and magnetic properties of the Ag-doped Fe_3O_4 films studied by x-ray absorption spectroscopy"*, S.H. Liu, H.M. Tsai, C.W. Pao, J.W. Chiou, D.C. Ling, W.F. Pong, M.H. Tsai, H.J. Lin, L.Y. Jang, J.F. Lee, J.H. Hsu, W.J. Wang, C.J. Hsu, Appl. Phys. Lett. **89**, 092112 (2006).
17. *"Effects of strain on the electronic structures and T-C's of the $La_{0.67}Ca_{0.33}MnO_3$ and $La_{0.8}Ba_{0.2}MnO_3$ thin films deposited on $SrTiO_3$"*, H. Chou, M.H. Tsai, F.P. Yuan, et al., Appl. Phys. Lett. **89**, 082511 (2006).
18. *"Comparison of the electronic structures of $Zn_{1-x}Co_xO$ and $Zn_{1-x}Mg_xO$ nanorods using x-ray absorption and scanning photoelectron microscopies"*, J.W. Chiou, H.M. Tsai, C.W. Pao, K.P.K. Kumar, S.C. Ray, F.Z. Chien, W.F. Pong, M.H. Tsai, C.H. Chen, H.J. Lin, J.J. Wu, M.H. Yang, S.C. Liu, H.H. Chiang, C.W. Chen, Appl. Phys. Lett. **89**, 043121 (2006).
19. *"Electronic structures of group-III-nitride nanorods studied by x-ray absorption, x-ray emission, and Raman spectroscopy"*, C.W. Pao, P.D. Babu, H.M. Tsai, J.W. Chiou, S.C. Ray, S.C. Yang, F.Z. Chien, W.F. Pong, M.H. Tsai, C.W. Hsu, L.C. Chen, C.C. Chen, K.H. Chen, H.J. Lin, J.F. Lee, J.H. Guo , Appl. Phys. Lett. **88**, 223113 (2006).
20. *"True nanocable assemblies with insulating BN nanotube sheaths and conducting Cu nanowire cores"*, Z. Zhou, J.J. Zhao, Z.F. Chen, X.P. Gao, J.P. Lu, P.V. Schleyer, C.K. Yang, J. Phys. Chem. B **110**, 2529 (2006).
21. *"Anisotropic Adsorption of Molecular Assemblies on Crystalline Surfaces"* Jaehun Chun, Je-Luen Li, Roberto Car, Ilhan A. Aksay, and Dudley A. Saville, J. Phys. Chem. B, **110**, 16624 (2006)

22. *"Functionalized Single Graphene Sheets Derived from Splitting Graphite Oxide"*, Hannes C. Schniepp, Je-Luen Li, Michael J. McAllister, Hiroaki Sai, Margarita Herrera-Alonso, Douglas H. Adamson, Robert K. Prud'homme, Roberto Car, Dudley A. Saville and Ilhan A. Aksay, J. Phys. Chem. B, **110**, 8535 (2006)
23. *"Transition between icosahedral and cuboctahedral nanoclusters of lead"*, C.M. Wei, C. Cheng, C.M. Chang, J. Phys. Chem. B, accepted (2006).
24. *"Observation of single oxygen atoms decomposed from water molecules on a Si(111)-7x7 surface"*, R.L. Lo, C.M. Chang, I.S. Hwang, et al., Phys. Rev. B **73**, 075427 (2006).
25. *"Effect of atomic geometry on shot noise in aluminum quantum point contacts"*, J. Yao, Y.C. Chen, M. Di Ventra, et al., Phys. Rev. B **73**, 233407 (2006).
26. *"Conserved spin and orbital angular momentum Hall current in a two-dimensional electron system with Rashba and Dresselhaus spin-orbit coupling"*, T.W. Chen, C.M. Huang, G.Y. Guo, Phys. Rev. B **73,** 235309 (2006).
27. *"Robust half-metallic antiferromagnets LaAVOsO(6) and LaAMoYO(6) (A=Ca, Sr, Ba; Y=Re, Tc) from first-principles calculations"*, Y.K. Wang, G.Y. Guo, Phys. Rev. B **73**, 064424 (2006).
28. *"Heterogeneous energy landscapes of individual luminescent conjugated polymers"*, J.J. Liang, J.D. White, Y.C. Chen, C.F. Wang, J.C. Hsiang, T.S. Lim, W.Y. Sun, J.H. Hsu, C.P. Hsu, M. Hayashi, W.S. Fann, K.Y. Peng, S.A. Chen, Phys. Rev. B **74**, 85209 (2006).
29. *"Comparative NMR study of hybridization effect and structural stability in D022-type $NbAl_3$ and NbGa3"*, C.S. Lue, T.H. Su, B. X. Xie, and C. Cheng, Phys. Rev. B.**74**, 094101 (2006).
30. *"Atomic dynamics of In nanoclusters on Si(100)"*, A.A. Saranin, A.V. Zotov, I.A. Kuyanov, M. Kishida, Y. Murata, S. Honda, M. Katayama, K. Oura, C.M. Wei, and Y.L. Wang ,Phys. Rev. B **74**, 125304 (2006).
31. *"Magnetically induced variations in phonon frequencies"*, J.H. Lee, Y.C. Hsue, A.J. Freeman, Phys. Rev. B **73**, 172405 (2006).