

***The 2nd KIAS Workshop on
Electronic Structure Calculations***

Korea Institute for Advanced Study

June 13 – 15, 2005

Abstracts

The 2nd KIAS Workshop on Electronic Structure Calculations

*International Conference Hall
Korea Institute for Advanced Study
June 13 – 15, 2005*

Invited Speakers

<i>K. J. Chang (KAIST)</i>	<i>Y.-H. Kim (KIAS)</i>
<i>H.-Y. Choi (Sungkyunkwan Univ.)</i>	<i>Y.-H. Kim (NREL)</i>
<i>S. Han (Ewha Womans Univ.)</i>	<i>K.-j. Kong (KRICT)</i>
<i>J. Ihm (Seoul Nat'l Univ.)</i>	<i>C. H. Park (Pusan Nat'l Univ.)</i>
<i>S.-H. Jhi (POSTECH)</i>	<i>Y.-G. Yoon (Chung-Ang Univ.)</i>
<i>J. Kang (KAIST)</i>	<i>B. D. Yu (Univ. of Seoul)</i>
<i>T.-S. Kim (Seoul Nat'l Univ.)</i>	<i>J. Yu (Seoul Nat'l Univ.)</i>

Special Invited Speakers on Experiments

<i>Y. Kuk (Seoul Nat'l Univ.)</i>	<i>H.-D. Kim (Pohang Accelerator Lab.)</i>
<i>G. T. Kim (Korea Univ.)</i>	<i>Y. H. Lee (Sungkyunkwan Univ.)</i>

Organized

by

H. J. Choi (KIAS)

Schedule of Events

Monday, June 13

9:00 - 9:30	Coffee and bread
9:30 - 10:00	Opening session
10:00 - 10:30	Yong-Hyun Kim , National Renewable Energy Laboratory (김용현, NREL) <i>Toward development of first-principles theory for molecule-surface interactions in aqueous solutions</i>
10:30 - 11:00	Coffee
11:00 - 12:00	Young Hee Lee , Sungkyunkwan University (이영희, 성균관대학교) <i>Modulation of electronic structures of Carbon Nanotubes</i>
12:00 - 1:00	Lunch
1:00 - 2:00	Young Kuk , Seoul National University (국양, 서울대학교) <i>Chain molecules: Geometric and electronic structures</i>
2:00 - 2:30	Coffee
2:30 - 3:00	Jisoon Ihm , Seoul National University (임지순, 서울대학교) <i>Electronic structure at defects and contacts, and its influence on quantum transport in carbon nanotubes</i>
3:00 - 3:30	Kee Joo Chang , KAIST (장기주, 한국과학기술원) <i>Properties and applications of ZnO</i>
3:30 - 4:00	Photo session / Coffee
4:00 - 5:30	Jaejun Yu , Seoul National University (유재준, 서울대학교) <i>A short introduction to the LDA+U approach to strongly correlated materials</i>
6:00 - 8:00	Banquet

Tuesday, June 14

- 9:00 - 9:30 Coffee and bread
- 9:30 - 10:00 **Chul Hong Park**, Pusan National University
(박철홍, 부산대학교)
Identification of large Jahn-Teller distortion of antisite in ABO_3 perovskite and persistent photorefractivity
- 10:00 - 10:30 **Seungwu Han**, Ewha Womans University
(한승우, 이화여자대학교)
Point defects in transition metal oxides and their relation to transport properties
- 10:30 - 11:00 Coffee
- 11:00 - 12:00 **Yong-Hoon Kim**, KIAS
(김용훈, 고등과학원)
Time-dependent density-functional theory: First-principles approach toward electronic excitations
- 12:00 - 1:00 Lunch
- 1:00 - 1:30 **Ki-jeong Kong**, KRICT
(공기정, 한국화학연구원)
Ab initio study of sensing mechanism of CNT-based FET sensor
- 1:30 - 2:00 **Seung-Hoon Jhi**, POSTECH
(지승훈, 포항공과대학교)
Re-entrant semiconducting behavior of zigzag carbon nanotubes at substitutional doping by oxygen dimers
- 2:00 - 2:30 Coffee
- 2:30 - 4:00 **Han-Yong Choi**, Sungkyunkwan University
(최한용, 성균관대학교)
DMFT in a nutshell
- 4:00 - 4:30 Coffee
- 4:30 - 5:30 **Gyu Tae Kim**, Korea University
(김규태, 고려대학교)
Electrical properties of one-dimensional shaped nanowires

Wednesday , June 15

- 9:00 - 9:30 Coffee and bread
- 9:30 - 10:00 **Hyoung Joon Choi**, KIAS
(최형준, 고등과학원)
Structures and electronic structures of potassium-doped C₆₀ monolayers
- 10:00 - 10:30 **B. D. Yu**, University of Seoul
(유병덕, 서울시립대학교)
Step selectivity of the oxidation on Si(001) surfaces
- 10:30 - 11:00 Coffee
- 11:00 - 12:00 **Hyeong-Do Kim**, Pohang Accelerator Laboratory
(김형도, 포항가속기연구소)
Photoemission spectroscopy studies of Mott-Hubbard systems
- 12:00 - 1:00 Lunch
- 1:00 - 1:30 **Tae-Suk Kim**, Seoul National University
(김태석, 서울대학교)
Inverse tunneling magnetoresistance in nanoscale magnetic tunnel junctions and electronic transport in single-molecule magnets
- 1:30 - 2:00 **Joongoo Kang**, KAIST
(강준구, 한국과학기술원)
Electronic structure and ferromagnetism of Mn-doped GaN
- 2:00 - 2:30 Coffee
- 2:30 - 4:00 **Young-Gui Yoon**, Chung-Ang University
(윤영귀, 중앙대학교)
Car-Parrinello molecular dynamics: A density functional theory approach for quantum molecular simulation
- 4:00 - 4:30 Closing session

***Abstracts
of
Invited Talks***

Monday Morning, 10:00 – 10:30

Toward development of first-principles theory for molecule-surface interactions in aqueous solutions

Yong-Hyun Kim and S.B. Zhang

National Renewable Energy Laboratory, Golden, Colorado 80401, USA

Organic and biological molecule passivation of semiconductor quantum dots has recently attracted much attention not only because the rapid advances in fabricating novel colloidal quantum dots but also because it offers the opportunity to biologically manipulate the dots into desirable assembly. Typically, the interaction between semiconductor surfaces and molecules takes place in aqueous solutions. However, little has been developed to understand such interfaces by *ab initio* approaches. For example, a cysteine (Cys), one of the amino acids, has multi reactive sites whose chemical activity depends critically on the pH value of the solution. If one conducts the calculation in a vacuum condition as many do today, it is practically impossible to control the reactions such that they take place at the sites known experimentally. As such, most of the calculated results are hardly useful. We have recently formulated a method to include the aqueous solutions into first-principles calculations in a surprisingly simple yet completely general way. The method has been applied to a number of molecules such as protonated and deprotonated water molecules, the Cys, the NH_3 and HCOOH where the $-\text{NH}_2$ and $-\text{COOH}$ radicals are the elementary building blocks of the amine group, $\text{R-CH-NH}_2\text{-COOH}$. Our calculations yield good pKa values when compared with experiments. This opens the field for direct first-principles calculations of molecule-surface interactions in aqueous solutions, with modern molecular dynamic simulation techniques, without having to make any unrealistic assumptions.

Modulation of electronic structures of Carbon Nanotubes

Young Hee Lee

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Carbon nanotubes have played an important role in leading the nanoscience and nanotechnology due to their peculiar one-dimensional characteristics and potential applicabilities in various areas. One important feature is its peculiar electronic structure that can be metallic and semiconducting depending on the chirality and diameter of nanotubes. Up to now, it has not been possible to control the chirality of nanotubes systematically by the conventional synthesis approaches such as arc discharge, laser ablation, and (high-pressure) chemical vapor deposition methods. Both metallic and semiconducting nanotubes coexist in the grown sample, which often hinders device applications with high performance. For instance, application to nanoscale transistors and memories requires nanotubes to be semiconducting for clear gate modulation. Therefore, tailoring the metallicity of nanotubes is highly desired.

One approach is to transform the electronic structures by functionalization using gas adsorbates. We will introduce simple gases such as fluorine and hydrogen gases to transform electronic structures from metallic to semiconducting.[1,2]

Another approach is to select either metallic or semiconducting nanotubes from their mixtures. Several methods of selecting semiconducting nanotubes from metallic ones or vice versa using dielectrophoresis, octadecylamine (ODA), bromination, and DNA have been reported. Our aim is to select semiconducting nanotubes from metallic ones in large

quantity with high yield and more importantly without affecting nanotube properties so that the separated nanotubes could be used directly for various applications.

We have found a method for a selective removal of metallic single-walled carbon nanotubes from semiconducting ones by stirring SWNT powder in tetramethylene sulfone (TMS)/chloroform solution with nitronium hexafluoro-antimonate (NO_2SbF_6 : NHFA) and tetrafluoroborate (NO_2BF_4 : NTFB). Positively charged nitronium ions (NO_2^+) were intercalated into nanotube bundles, where the intercalation was promoted also by the counter ions. Nitronium ions selectively attacked the sidewall of the metallic SWNTs due to the abundant presence of electron density at the Fermi level, thus yielding stronger binding energy compared to the counterpart semiconducting SWNTs. The semiconducting SWNTs were left on the filter after filtration, whereas the metallic SWNTs were disintegrated and drained away as amorphous carbons. The effectiveness of selectivity was confirmed by the resonant Raman spectra and absorption spectra.[3] Some other ideas of removing zigzag nanotubes by carbon dioxide gas will be also discussed.[4]

[1] K. H. An *et al.*, Amer. Chem. Soc. **125**, 3507 (2003); K. H. An *et al.*, Appl. Phys. Lett. **80**, 4235; K. A. Park *et al.*, Phys. Rev. B **68**, 045429 (2003).

[2] K. S. Kim *et al.* Adv. Mat. **14**, 181 (2002); K. A. Park *et al.*, Phys. Chem.B, to be published.

[3] K. H. An *et al.* J. Amer. Chem. Soc. **127**, 5196 (2005).

[4] K. Y. Seo *et al.*, J. Amer. Chem. Soc. Comm. **125**, 13946 (2003).

Monday Afternoon, 1:00 – 2:00

Chain molecules: Geometric and electronic structures

Young Kuk

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Chain molecules have drawn much attention to scientific community for their application to interconnection wires, functional devices, energy harvesting materials. Various long chain molecules have been studied with scanning tunneling microscopes, scanning gate microscopes and conventional transport measurements. Many new physics can be learned from the studies on these one dimensional systems, such as 1) deviation from Fermi liquid, 2) different defect bands from the 3-D counter parts, 3) fluctuation in metallic or superconducting wires, 4) energy transfer mechanisms.

Experimentally, carbon nanotubes, azobenzene and pentacene molecules were placed on top of clean single crystal metals or insulating layers on metal substrates. The geometrical and electronic structures were studied with STM. Several new results will be presented in this talk. In some wires, scanning tunneling spectroscopy showed additional standing waves, suggesting spin and charge separation in 1-D. Defect bands are quite different from those in 1D, and they may work as new scattering centers.

Monday Afternoon, 2:30 – 3:00

Electronic structure at defects and contacts, and its influence on quantum transport in carbon nanotubes

Jisoon Ihm

School of Physics, Seoul National University, Seoul 151-747, Korea

Understanding of the electronic structure and the electrical transport properties on the nanoscale becomes increasingly important for the development of the next-generation nanodevices. We have developed a first-principles pseudopotential method to calculate the quantum conductance as well as the self-consistent charge distributions of nanostructures and studied the electronic structure and quantum conductance of carbon nanotubes with impurities or defects. Even if the carbon nanotube is metallic instead of semiconducting, Boron and Nitrogen create acceptor-like and donor-like states which act as scattering centers for conducting electrons. Various defect geometries such as Stone-Wales defects are considered which give rise to interesting localized states and the corresponding conductance characteristics. These localized states are in resonance with the extended states of the metallic nanotube and form quasi-bound states with broadened energy levels leading to novel conductance behaviors. For semiconducting carbon nanotubes, it is shown that various defects located at the junction of two different tubes can produce both shallow and deep defect levels. Theoretical predictions are closely compared with recent Scanning Tunneling Microscopy and Scanning Tunneling Spectroscopy data.

Monday Afternoon, 3:00 – 3:30

Properties and applications of ZnO

K. J. Chang

*Department of Physics, Korea Advanced Institute of Science and Technology, Daejeon
305-701, Korea*

Zinc oxide (ZnO) has attracted much attention because of possible applications for wide-gap optoelectronic devices. Alloying this material with Mg extends applications to the uv range. Despite advantages such as the availability of large area substrates, high radiation resistance, and low material costs, one major problem remains to be solved; it is difficult to obtain low resistivity p-type ZnO. In this work I talk about the compensation mechanism for acceptors in ZnO, based on first-principles pseudopotential calculations within the local-density-functional approximation. Based on the formation energies for various defects, I discuss the defect stability, formation, and concentration as a function of the Fermi level. I show how to enhance doping solubility and doping efficiency to achieve low-resistivity p-type samples. Finally, I discuss the optical characteristics of ZnO doped with acceptors, recent progress in fabricating light emitting diodes based on zinc oxide, and growth and applications of ZnO nanostructures.

Monday Afternoon, 4:00 – 5:30

A short introduction to the LDA+U approach to strongly correlated materials

Jaejun Yu

*School of Physics and Center for Strongly Correlated Materials Research,
Seoul National University, Seoul 151-747, Korea*

Despite successful applications of the density functional theory (DFT) to materials research, strong electron correlations have often become a bottleneck in the electronic structure calculation approach to understanding of various materials properties of transition metal oxides and other so-called strongly correlated materials. In this short tutorial, I will try to describe why the LDA (local density approximation) DFT approach has been so successful in the description of most real materials and when it fails to describe the essential physics of the correlated systems. Among various methods suggested to overcome the shortcomings of LDA, e.g., GW, SIC (self-interaction correction), LDA+U, and DMFT (dynamical mean field theory), I explain the basic idea behind the LDA+U method as a simple way to remedy for the LDA in treating the electron correlations arising from the strong on-site Coulomb interactions, and further introduce our recent development toward the O(N)-LDA+U method based on the localized pseudo-atomic orbital method.

Identification of large Jahn-Teller distortion of antisite in ABO_3 perovskite and persistent photorefractivity

Ho-Hyun Nahm and Chul Hong Park

Pusan National University

The photorefractivity (PR) was discovered in $LiNbO_3$ in 1966, and then in many other perovskite oxides¹. The PR is suggested to be based on the space modulation of photocurrents through charge-transfer from illuminated to dark area by nonuniform illumination. The generation of photocurrent depends on the presence of suitable impurities or defects. Of particular interest is information on the centers supplying charge carriers, on the trapping centers, and on optical excitation. The persistent photorefractivity in ABO_3 -type perovskites has been extensively investigated because of its application to the optical holographic memory with terra-bit capacity and nonlinear optical devices. In spite of the recent significant technical achievement for the long-time persistent robust PR, the microscopic structure responsible for the PR is not yet identified. We identified a large Jahn-Teller distortion of B-antisite in $LiNbO_3$, accompanied with a significant change of the electronic structure: a deep-to-shallow transition. Based on the calculational results, the microscopic mechanism of the persistent PR and related phenomena are discussed.

Tuesday Morning, 10:00 – 10:30

Point defects in transition metal oxides and their relation to transport properties

Seungwu Han

Department of Physics and Division of Nano Sciences, Ewha Womans University

Point defects such as anion and cation vacancies in transition metal oxides play a vital role in determining electronic and optical properties. In this presentation, we present our recent first-principles results on point defects in SrTiO₃, NiO, and TiO₂, and discuss how they can be related to the electronic properties observed in various experiments. We consider anion and cation vacancies as well as interstitials and discuss when the localized trap states appear. The energetics and electronic structures of defect clustering are also discussed. We will compare results between LDA and LDA+U approaches.

Tuesday Morning, 11:00 – 12:00

Time-dependent density-functional theory: First-principles approach toward electronic excitations

Yong-Hoon Kim

Korea Institute for Advanced Study, Seoul 130-722, Korea

In this lecture, I will first review the basics of time-dependent density-functional theory (TDDFT), emphasizing the comparison with the many-body formulation, Hedin's GW approach plus Bethe-Salpeter equation. After presenting several recent developments in its formalism and computational implementations, I will show several examples of its applications taken from the literature to assess its performance. The methodology is still being actively developed, and the theoretical and computational ingredients required for TDDFT to become a reliable and useful tool for the study of electronic excitations will be described throughout the talk.

Tuesday Afternoon, 1:00 – 1:30

***Ab initio* study of sensing mechanism of CNT-based FET sensor**

Ki-jeong Kong

Korea Research Institute of Chemical Technology, Daejeon 305-600, Korea

Electronics based on carbon nanotubes (CNT) and semiconducting nanowires have received a lot of attention recently because of its tremendous application potential, such as active components in nanochips, nanoelectromechanical systems, field-emission display devices, and chemical and biological sensors. However, as with most nanoelectronic systems, successful commercial materialization needs accurate structural control at the molecular level. To this end, computer-aided material design is clearly necessary to understand operation principles, to avoid blind investigation by trial-and-error, and to find more efficient and economic ways to the materializations.

This talk summarizes our computational efforts to address the sensing mechanisms of nanosensors fabricated and operated at KRICT. Examples include the gas sensor of NH_3 and NO_2 , palladium coated CNT sensor that interacts with H_2 molecules, and the humidity sensor made of CNT field effect transistor (FET.) Our approach is based on first-principles density functional theory (DFT) to compute equilibrium structures, electronic density of states, and charge transfer by Mulliken analysis.

Tuesday Afternoon, 1:30 – 2:00

Re-entrant semiconducting behavior of zigzag carbon nanotubes at substitutional doping by oxygen dimers

Seung-Hoon Jhi

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The electronic structures of carbon nanotubes doped with oxygen dimers are studied using the pseudopotential density functional method. The fundamental energy gap of zigzag semiconducting nanotubes shows a strong dependence on the concentration and configuration of oxygen dimer defects that substitute for carbon atoms in the tubes as well as on tube chiral index. For a certain type of zigzag nanotubes, the energy gap is closed and the tubes become semimetallic when doped with oxygen dimers. At higher oxygen-dimer concentrations the gap reopens, and the tubes exhibit semiconducting behavior again. The change of band gap of the zigzag tubes is understood in the frame of their response to the strains caused by the dimer substitutional doping.

DMFT in a nutshell

Han-Yong Choi

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Dynamical mean field theory (DMFT) is probably the most reliable method to describe an interacting many-particle system. The key idea of the DMFT is that, when physics of a problem was determined by the competition of two energy scales, the problem can be made tractable by simplifying other complicating aspects. For the Mott transition, it is the competition between the kinetic and Coulomb energies that determines physics. A prototype model that describes the situation is the Hubbard model. It can not be solved reliably. It is rendered tractable, however, in the seemingly unphysical limit of the infinite spatial dimension, where the competition is fully retained while the less essential momentum dependence is neglected. In that limit, an interacting problem on a lattice is mapped onto an interacting problem on a site. The methods to solve interacting problems on a site were well developed through the Kondo problem such as numerical renormalization group (NRG).

In this tutorial, we will first introduce the basic idea of the DMFT, and then will review how the long standing problem of the Mott transition was successfully understood by applying the DMFT to the Hubbard model. We will then consider the Hubbard-Holstein model, a simplest model that includes both the electron-electron and electron-phonon interactions. The results obtained in our group by applying NRG+DMFT to the Hubbard-Holstein model will be discussed.

Tuesday Afternoon, 4:30 – 5:30

Electrical properties of one-dimensional shaped nanowires

Gyu Tae Kim

Department of Electrical Engineering, Korea University

The electrical properties of one dimensional conductors raised various interesting issues together with the possible application as components of integrated circuits. The one-dimensional shape of nanowires, however, does not guarantee the real one-dimensionality in conduction mechanism and the practical application such as memory devices because of many physical and technical problems including contact resistances and assembly techniques. In this talk, some recent experimental results on electrical properties of nanowires will be presented. In particular, electrical properties of carbon nanotubes, ZnO nanowires, and V_2O_5 nanowires will be discussed.

Structures and electronic structures of potassium-doped C₆₀ monolayers

Hyoung Joon Choi

Korea Institute for Advanced Study, Seoul 130-722, Korea

We present first-principles calculation of structures and electronic structures of K₃C₆₀ monolayers on Ag (111) and (001) surfaces. In case of K₃C₆₀ monolayers on the Ag (111) surface, we consider C₆₀ molecules put in a hexagonal array with the lattice constant of 10.02 Å, and calculate the total energy and the energy-band dispersion for various molecular orientations. We find a C₆₀ molecular orientation whose total energy is very close to the minimum and its LUMO-derived band dispersion has the important features observed by a high-resolution angle-resolve photoelectron spectroscopy (ARPES). The calculated bandwidth, however, is still substantially larger than the measured one, suggesting a renormalization effect in real samples. In case of K₃C₆₀ monolayers on the Ag (001) surface, we study the c(6*4) structure with the inter-fullerene distances of 10.42 and 11.57 Å, and obtain very different LUMO-derived energy-band dispersions. We also study spatial distribution of potassium atoms in C₆₀ monolayers and its effect on the C₆₀-derived energy-band dispersions.

[1] W. L. Yang, V. Brouet, X. J. Zhou, H. J. Choi, S. G. Louie, M. L. Cohen, S. A. Kellar, P. V. Bogdanov, A. Lanzara, A. Goldoni, F. Parmigiani, Z. Hussain, Z.-X. Shen, *Science* **300**, 303 (2003).

[2] V. Brouet, W. L. Yang, X. J. Zhou, H. J. Choi, S. G. Louie, M. L. Cohen, A. Goldoni, F. Parmigiani, Z. Hussain, Z.-X. Shen, *Phys. Rev. Lett.* **93**, 197601 (2004).

[3] Y.-M. Byun, H. J. Choi, S. G. Louie, M. L. Cohen (to be published).

Step selectivity of the oxidation on Si(001) surfaces

B. D. Yu

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Oxidation of silicon surfaces has attracted much attention as one of the most important processes in current and future Si technology. Particularly, control of initial reactions of oxygen with Si surfaces on atomic scale is one of important issues required for better stability and function of Si devices. In this work, we report possible oxygen adsorption structures and oxidation reaction at single-layer steps of Si(001) using first-principles total-energy calculations based on density-functional theory (DFT). In the calculations, we used a (1,1,19) vicinal surface. On each terrace, the orientation of the reconstruction is different, resulting in the formation of alternate single-layer S_A and S_B steps. By employing the DFT calculations, we found that oxygen molecules are preferentially incorporated into sites at the S_B step edges. The resulting oxidation structures consist of -Si-O- chain structures along the step edge, thereby eliminating the energetically unfavorable step-edge dangling bonds. Our results and analysis of the preferential oxidation at the rebonded S_B step provides a natural explanation for the experimental observation that the rebonded step edge acts as strong sink for the oxidation of Si.

Wednesday Morning, 11:00 – 12:00

Photoemission spectroscopy studies of Mott-Hubbard systems

Hyeong-Do Kim

Pohang Accelerator Laboratory

Photoemission spectroscopy has been a powerful tool to probe the electronic structure of solids. Thanks to recent developments in energy and momentum resolutions of an electron energy analyzer, its one-to-one correspondence to a one-particle Green's function of a many-body system enables us to compare directly an experimental spectral function with theoretical one especially for the strongly correlated electron system. In this talk, I will present photoemission spectra of several Mott-Hubbard systems including core-level ones to compare them with the dynamical mean-field theory of the Hubbard model which successfully describes the Mott metal-insulator transition.

Wednesday Afternoon, 1:00 – 1:30

Inverse tunneling magnetoresistance in nanoscale magnetic tunnel junctions and electronic transport in single-molecule magnets

Tae-Suk Kim

School of Physics, Seoul National University, Seoul 151-747, Korea

In this talk I am going to present my recent study of spin-related transport in nanoscale magnetic tunnel junctions (MTJs) and electronic transport in single-molecule magnets (SMMs). In the first part the inverse tunneling magnetoresistance (TMR) effect in nanoscale MTJs will be discussed. The TMR is positive when the transmission probability is close to zero, but can flip its sign when the transmission probability becomes close to a unity. In the second part the transport properties of SMMs will be discussed. The linear response conductance can be controlled by the external magnetic field in a stepwise or oscillatory manner.

Electronic structure and ferromagnetism of Mn-doped GaN

Joongoo Kang and K. J. Chang

*Department of Physics, Korea Advanced Institute of Science and Technology, Daejeon
305-701, Korea*

Mn-doped GaN has currently attracted much attention because of the room-temperature ferromagnetism observed in this material. However, experimental data so far are quite controversial, reporting the Curie temperatures ranging from 10 to 940 K. Very recent experiments showed that Mn δ -doped GaN films have high hole carrier concentrations of about 10^{18} cm^{-3} , which lead to the high Curie temperature and enhanced magnetization.

In this work, we study the electronic and magnetic properties of Mn-doped GaN and the origin of p-type conductance especially for Mn δ -doped films through first-principles pseudopotential calculations within the spin-density-functional theory. The nature of magnetic interactions between two Mn ions is investigated by varying the Mn-Mn distance and their orientation for both GaN bulk and GaN films. The ferromagnetic coupling in GaN bulk has a short-range nature, effective for Mn-Mn distances up to about 7 Å. The magnetic interactions in Mn-doped GaN films also favor a ferromagnetic ordering, with similar coupling strengths to those of bulk GaN. Analyzing the Mn d levels, we suggest that the d - d hybridization between Mn ions is the main reason for stabilizing the ferromagnetic state. The doping effect on ferromagnetism, and the energetics and ferromagnetism of Mn nanoclusters are also investigated. In Mn δ -doped GaN, we find that Ga vacancies are energetically more stable near the Mn layer than in the bulk region of GaN due to the charge transfer from the Mn to Ga vacancy. Our calculations suggest that Ga vacancies near the Mn δ -doped layer are likely to be the origin of p-type conductance observed in Mn δ -doped films.

Wednesday Afternoon, 2:30 – 4:00

Car-Parrinello molecular dynamics: A density functional theory approach for quantum molecular simulation

Young-Gui Yoon

Department of Physics, Chung-Ang University, Seoul 156-756, Korea

Quantum molecular dynamics simulation of real materials from first-principles has been possible since Car-Parrinello introduced a method to treat electronic wavefunctions as dynamical variables. In this tutorial talk, a self-contained explanation of the Car-Parrinello method is given. Some elements of molecular dynamics and density functional theory are introduced if necessary, but emphasis is given to explain how and when the method works. Some applications and advanced techniques such as controlling temperature and pressure during the simulation are briefly introduced.