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Welcome message from Conference Chairman, 5th ACCMS

Dear colleagues,

On behalf of the ACCMS-5 Conference Organizing Committee, it is my great pleasure to extend a warm invitation to you to participate in the Fifth conference of Asian Consortium on Computational Materials Science, and the first ACCMS conference in the South-East Asia region, scheduled to be in Hanoi, Vietnam, from 7th to 11th September 2009.

Over the past 10 years, ACCMS has grown to be the major international conference on Computational Materials Science. The ACCMS-5 continues the ACCMS tradition of high-quality, broad international participation in all advanced and important areas of computational materials science with a record number of 203 accepted contributions from researchers of nearly 30 countries across the world. For comparison, the previous successful ACCMS-1 Conference in Bangalore (India) has received 91 contributions, ACCMS-2 (Novosibirsk, Russia): 154, ACCMS-3 (Beijing, China): 136 and ACCMS-4 (Seoul, Korea): 185 contributions.

The ACCMS-5 covers two main activities:

- The ACCMS-5 conference comprising of 15 technical topics, ranging from Car-Parrinello Molecular Dynamics to computational modeling of mechanical properties of materials under extreme conditions - 3 distinguished keynote talks, invited talks and oral and poster presentations for contributed papers. As is traditional, the ACCMS-5 will award Kawazoe prizes to the best poster presentations in order to encourage young scientists.

- Two-day short courses given by international experts from Germany, Japan, the UK and the USA, focusing on advanced computational methodologies in modeling of materials at the nanoscale.

All of the ACCMS-5 Committees are looking forward to your contribution and participation. For our part, we will do our best to provide a valuable scientific program and to welcome you to Hanoi, soon to be celebrating its thousand years as a city in 2010.

Nguyen-Manh Duc
Chairman of ACCMS-5 Conference
United Kingdom Atomic Energy Authority (UKAEA)

**Welcome message to ACCMS-5 of Prof. Acad. Nguyen Van Hieu
Chairman, Scientific Council of Materials Science, VAST**

Distinguished Guests,
Dear participants of the Conference,
Ladies and Gentlemen's,

The Vietnamese materials science community warmly welcomes the international participants coming to Vietnam from many friendly countries for presenting latest results of their research on Computational Materials Science, discussing new trends in this perspective area of Science and Technology and promoting Vietnamese computational materials scientists to enhance their promising creative activities.

Recently the Scientific Council of Materials Science of Vietnam Academy of Science and Technology has elaborated the strategy of the materials science development in the period 2011–2020 and the vision to the year 2030. The Council has chosen Computational Materials Science as one among a few number of priority research directions in Materials Science. In particular, in the road-map for implementing the strategy of developing the materials science we are intending to create a Center of Excellence for Computational Materials Science. With the gratitude we believe that the 5th Conference of the Asian Consortium on Computational Materials Science will enhance the international cooperation of Vietnamese computational materials scientists and promote their effort toward the foundation and the development of the Center of Excellence for Computational Materials Science in Vietnam. With this believe I would like to express our best wishes for the success of the Conference.

I wish also the pleasant visit of the international participants in Vietnam and their beautiful impressions on the hospitality of Vietnamese colleagues.

<div align="right">

Acad. Nguyen Van Hieu
Chairman
Scientific Council of Materials Science
Vietnam Academy of Science and Technology

</div>

Welcome message to ACCMS-5 of Tooru Matsumiya
Executive Adviser, Nippon Steel Corporation

First of all I would like to congratulate the opening of ACCMS-5. Benefits of application of computational science and engineering to materials and process development are considered to be summarized as follows: First, short time and efficient screening of plant test conditions by computer simulation reduces the development cost and time of materials processing. Second, computer case study under extreme conditions where experiment is difficult and computer observation of process behavior and materials state which are not available by experiment enlarge the possibility of finding of optimum condition out of the extension of conventional direction and clarifying mechanism of phenomena evolving in processing and realize control and optimization of processing based on the mechanism and seeds findings of innovative technology. Third, computational model constructed based on mechanism clarified and verified by crosscheck and fulfillment of experimental data can store the discrete knowledge as scientific database, that is, the set of parameter values used in computation assessed and verified by the comparison with experiment, and be utilized as material and process design aid system. When the modeling becomes sound the parameters in computation come close to materials properties, which also can be estimated by computation including the first principle calculations. The benefit mentioned first becomes fully true only after the computation framework mentioned third is accomplished. Although some modification will be made because of the recent economic crisis, 10P FLOPS computer will be operated in Japan in 2012. Year after year increase of computer performance and cost effectiveness of computation encourage the extended use of the abovementioned benefits. Ranging from continuum mechanics simulation to electronic level simulation, phenomenological simulation and atomistic level simulation in between, various level simulations have been conducted and multi scale/multi physics simulations are being widely developed in recent decades. For instances, refining and continuous casting processes and related phenomena are simulated by CFD and structure mechanics sometimes with the combination of computational thermodynamics in steelmaking, which realized process optimization. Even the estimation of properties of refining slags has been tried by the use of molecular dynamics and abinitio calculation of phase diagrams by the use of Monte Carlo simulation and estimation of thermodynamic properties by electronic band calculation have also been tried. The fruits of these trials will be harvested within not so far future. I hope that abundance of ideas for improvement and new development of computation methodology and scientific targets in materials especially including the environmental and resource issues for sustainable society, which should be solved by the application of computation, and their tackling strategy be nucleated through the vivid discussions and knowledge exchanges among the participants during this ACCMS5 conference and succeeding series of ACCMS.

Conference Sessions

The ACCMS5 Conference is organized in such way that there is no parallel sessions. All talks are either on plenary sessions or posters. The conference will cover the following sessions.

1. Advanced computational methodology: beyond DFT

2. Modelling of Nanotubes, nanowires and quantum dots

3. Modelling of Nano-biological and Polymeric Systems

4. Multi-scale Modeling of Materials

5. Oxydes and Nitrides materials

6. Modeling Materials for Future Energy (I)

7. Modeling of Mechanical Properties of Materials

8. Materials under Extreme Conditions

9. Spintronics and Magnetic Properties of Materials

10. Modeling of Nano-Devices

11. Cluster Modeling

12. Surface, Interface and Thin Films

13. Modeling of Materials for Future Energy (II)

14. Micro-structure Modelling and Phase Transformation

15. Optical and Spectroscopy Properties of Materials

Committees

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Nguyen Van Hieu, Chairman of the Scientific Council on Materials Science, VAST, Vietnam
Bing Lin Gu, President, Tsinghua University, China
Tooru Matsumiya, Fellow, Nippon Steel Corporation, Japan
Debashis Mukherjee, Director of Indian Association for Cultivation of Science, India

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Gour Prasad Das (IACS)

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Hanoi University of Science (HUS, VNUH, Vietnam)

Vietnam National University (HCM city, Vietnam)

International Center for Theoretical Physics (ICTP, Italy)

Asia Pacific Center for Theoretical Physics (APCTP, Korea)

Accelrys Software Inc.

General information

Transportation

To go from Noi Bai International airport to hotels in Hanoi center and vice versa, the best way is to take a taxi from the taxi companies specializing in transportation service between Noi Bai and Hanoi center [Airport Taxi company (phone: 38733333); Noibai Taxi company (phone: 38868888); and Viet Thanh Taxi company (phone: 35636666)]. A taxi to the city-center takes about 40 minutes, and the price for a taxi with 4 places from Noi Bai to any places in Hanoi center is about 16USD (~ 230,000 VND)

During the conference days the participants staying in Hoa Binh hotel, Horison hotel, Trade Union hotel and Kim Lien hotel will be picked up by bus to the conference place and vice versa.

Accommodation

The official Conference hotel is Hanoi Melia Hotel.

Besides Hanoi Melia Hotel, we recommend you the other hotels with which we have negotiated to gain reduced rates for participants of ACCMS-5: Hanoi Horison Hotel, Hoa Binh Hotel, Vietnam Trade Union Hotel, Kim Lien Hotel.
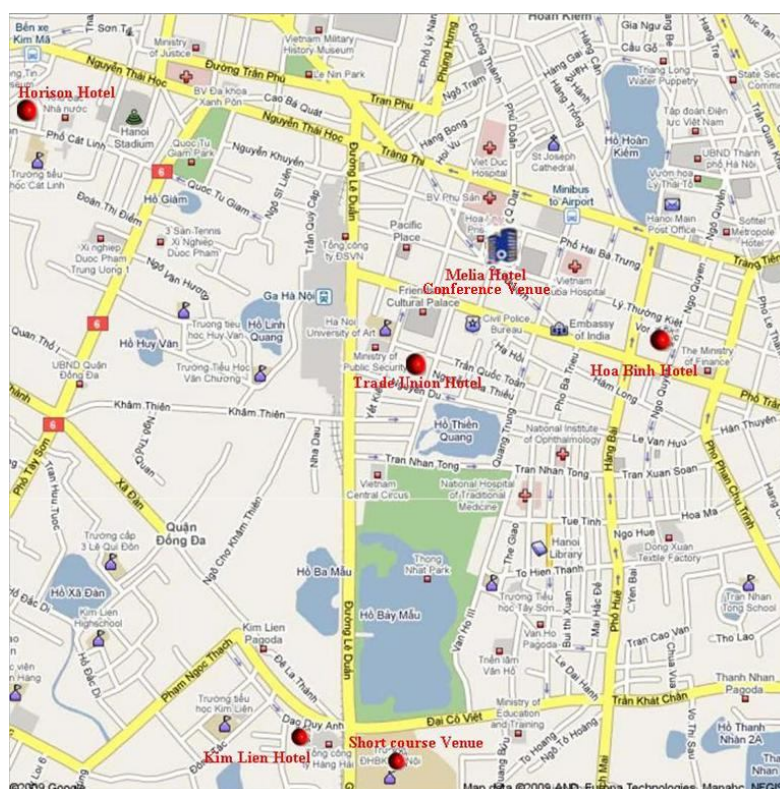
1. Hanoi Melia Hotel (Conference Hotel) (**5 stars hotel**)
   44B Ly Thuong Kiet Street, Hanoi
   Tel: (+84 4) 39343343; Fax: (+84 4) 39343344

2. Hanoi Horison Hotel (**5 stars hotel**)
   40 Cat Linh Street, Hanoi
   Tel: (+84 4) 3733 0808; Fax: (+84 4) 37332625 or 3733 0888

3. Hoa Binh Hotel (**3 stars hotel**)

  27 Ly Thuong Kiet Street, Hanoi

  Tel: (+84 4) 22104621 or 38253315; Fax: (+84 4) 38269818

4. Vietnam Trade Union Hotel (**3 stars hotel**)

  14 Tran Binh Trong Street, Ha Noi

  Tel: (+84 4) 39421776/ 39421764; Fax: (+84 4) 39420762/ 39421786

5. Kim Lien Hotel (**3 stars hotel**)

  7 Dao Duy Anh Street, Dong Da, Hanoi

  Tel: (+84 4) 38522522/35770328; Fax: (+84 4) 38524919/35770463

Tours to Halong Bay (UNESCO World Heritage site)

(participants should pay themselves, it is not included in the conference fee)

Declared as a World Heritage site by the UNESCO, Ha Long Bay is one of Vietnam's most spectacular natural attractions, which was declared a World Natural Heritage site by UNESCO in 1994. Located around 200 km out of Hanoi, the bay covers an area of more than 1500 square kilometers and is dotted with thousands of limestone islands, which are rising from the clear green waters like sculptures carved by the Gods. Come and see that Vietnamese call "the descending dragon"

Option 1: One-day tour to Halong Bay on September 12, 2009:

  Depart from Hanoi at 7h00 AM and arrive back to Hanoi at 19h30 PM on the same day.

  Price in US dollar/ person: 25 $US (The price for group 30 people up only)

Option 2: Two-day tour to Halong Bay with overnight in Hotel on September 12-13, 2009:

  Depart from Hanoi at 7h00 AM on 12 Sep. and arrive back to Hanoi at 13h00 PM on 13 Sep.

  Price in US dollar/ person: 55 $US (The price for group 30 people up only)

Option 3: Two-day tour to Halong Bay with overnight aboard Bhaya Cruises on September 12-13, 2009:

  Depart from Hanoi at 7h00 AM on 12 Sep. and arrive back to Hanoi at 15h00 PM on 13 Sep.

  Price in US dollar/ person: 99 $US (The price for group 30 people up only)

Badge

Your badge contains your name, and affiliation. The badge allows your access to the areas of the convention for which you are enrolled, including access to lunches, dinner and banquet.

Short course
ACCMS-5 SHORT COURSE PROGRAM
Location: Hanoi University of Technology (HUT)
September 7-8, 2009

Time	Monday, Sep. 7	Thursday, Sep. 8
07h30 – 08h00	+ Registration + Hand on documentation + Welcome Address by Vice-President of the HUT + Opening remark by Chairman of the ACCMS-5 Conference	Free time
08h00 – 09h15	Lecture 1 S.D. Kenny	Lecture 1 A.F. Voter
09h15 – 09h30	Coffee Break	
09h30 – 10.45	Lecture 2 S.D. Kenny	Lecture 2 A.F. Voter
10h45 – 12h00	Lecture 1 D.G. Pettifor/R. Drautz	Lecture 1 K. Ohno
	Lunch buffet at HUT Electronic Library (6th or 11th floor's Hall)	
13h00 – 14h15	Lecture 2 D.G. Pettifor/R. Drautz	Lecture 2 K. Ohno
14h15 – 14h30	Coffee Break	
14h30 – 15h45	Lecture 1 Hourahine	Lecture 1 R. Drautz
15h45 – 17h00	Lecture 2 Hourahine	Lecture 2 R. Drautz
	Dinner at HUT Electronic Library Lecturer's Restaurant (2th floor)	Certificate awards to the ACCMS-5 SC's participants by President of the HUT
18h30 – 19h45	Case study of DFTB code (Tutorial on Computer of B. Aradi 1)	Free time
19h45 – 20h00	Coffee Break	
20h00 – 21h00	Case study of DFTB code (Tutorial on Computer of B. Aradi 2)	

SHORT COURSE ABSTRACTS

Abstract 1

Localised orbital based DFT - Methodology and Analysis
Steven D. Kenny

Department of Mathematical Sciences, Loughborough University, Leicestershire, LE11 3TU, UK

This course will start with a brief overview of density functional theory (DFT) specifically focused on how the theory is implemented in localised orbital DFT codes. The main part of the course will then discuss analysis of the results of DFT simulations from a localised orbital perspective, drawing on specific examples of problems to explain why these tools are useful. It will be shown how tools such as the analysis of the density of states and simulated STM approaches can be used to corroborate results with those from experiments, in order to assess the reliability of the results from modelling. The ideas from Bader's Atoms in Molecules will be introduced and it will be shown how these can be used to analyse DFT results to help understand the nature of the bonding in a system. Linkages between these results and new ideas for empirical potentials will be briefly discussed.

Abstract 2

Bond-order potentials: bridging the electronic-atomistic Modelling hierarchies in materials science
Part I: sp-valent materials
David G. Pettifor[1] and Ralf. Drautz [2]

[1] Department of Materials, University of Oxford, Oxford, OX1 3PH, UK

[2] Interdisciplinary Centre for Advanced Materials Simulation Ruhr University, 44780 Bochum, Germany

I. Introduction
- problem: bridging gap from electronic to atomistic modelling hierarchies
- solution: coarse graining from density functional theory (DFT) to tight binding
 (TB) to bond-order potentials (BOPs)

II. Coarse graining I: from DFT to TB
- TB bond model
- TB parametrisation from DFT: sp-valent dimers and screening
- TB prediction of structural trends across periodic table
- interpretation in terms of moments of density of states

III. Coarse graining II: from TB to second-moment approximation (SMA)
- derivation of Finnis-Sinclair and Tersoff-type potentials within SMA
- limitations of SMA: need for higher moments

IV. Coarse graining III: from TB to BOP
- from moments to Lanczos recursion coefficients
- BOP theorem and exact many-atom expansion
- atom-based versus bond-based BOP

V. Applications of bond-based BOP
- hydrocarbons
- silicon
- GaAs

VI. Conclusions

Part II: d-valent transition metals and magnetism

Ralf. Drautz[1] and **D.G. Pettifor** [2]

[1] Interdisciplinary Centre for Advanced Materials Simulation, Ruhr University, 44780 Bochum, Germany

[2] Department of Materials, University of Oxford, Oxford, OX1 3PH, UK

I. Atom-based BOP
- Numerical bond-order potentials
- Analytic bond-order potentials

II. Density matrix and forces
- Density matrix expansion with analytic BOP
- Hellman-Feynman-like forces

III. Structural stability
- Recap: moments and structural stability
- Stability of complex intermetallic phases

IV. Magnetism
- Stoner theory of magnetism
- Magnetic bond-order potentials

V. Current focus and recent developments
- charge transfer
- mixed metallic-covalent bond formation

VI. Conclusions

Abstract 3

Understanding infrequent events and extending the time scale of molecular dynamics simulations of material systems.

Arthur F. Voter

Theoretical Division, Los Alamos National Laboratory, Los Alamos, New Mexico, USA

The molecular dynamics method, although extremely powerful for materials simulations, is limited to time scales of roughly one microsecond or less. On longer time scales, dynamical evolution typically consists of infrequent events, which are usually activated processes. This short course is focused on understanding infrequent-event dynamics, on methods for characterizing infrequent-event mechanisms and rate constants, and on methods for simulating long time scales in infrequent-event systems, including the recently developed accelerated molecular dynamics methods.

Abstract 4

Lattice Monte Carlo method as a powerful tool

Kaoru Ohno

Department of Physics, Yokohama National University, Yokohama 240-8501, Japan

Monte Carlo method is a powerful technique to simulate various stochastic models [1]. I will particularly demonstrate the ability of lattice Monte Carlo method in the analysis of percolation, spin magnetism, pattern growth, order-disorder behavior of alloys, liquid crystals, and polymers. For the systems described by a Hamiltonian, Monte Carlo method allows them to reach thermal equilibrium much faster than molecular dynamics (MD) method. It can describe slow dynamics according to Langevin equations. I will also explain the way of mapping classical or quantum MD systems onto lattice gas models.

[1] K. Ohno, K. Esfarjani and Y. Kawazoe, "Computational Materials Science: From Ab Initio to Monte Carlo Methods", Springer Series on Solid-State Sciences, Vol.129 Springer-Verlag, Berlin, Heidelberg, 1999) pp.1-325.

Abstract 5

Tight-binding modelling with DFTB

Benjamin Hourahine

Department of Physics, University of Strathclyde, John Anderson Building,107 Rottenrow, Glasgow G4 0NG, UK

This lecture and the associated practical laboratory will cover the principles and use of Density Functional based Tight Binding (DFTB). This is an accurate semi-empirical method explicitly derived from Kohn-Sham DFT by making an expansion of the total energy functional around a reference charge density. The zero-th order expansion is similar to standard non-self-consistent tight-binding theory, while the second order leads to transparent parameter-free expressions which include the effects of self-consistent redistribution of Mulliken charges (SCC-DFTB) and spin polarization. DFTB has been successfully applied to many problems where the deficiencies of standard tight-binding become obvious. More information about DFTB is available at http://www.dftb.org

In the last few years the DFTB method has been extended to allow investigation of problems including electronic transport, optical and excited state spectroscopies, hydrogen-bonded, complex magnetic and strongly correlated materials. DFTB also can be used with a range of linear scaling approaches for the simulation of large systems. Applications of DFTB in several areas of materials science will be reviewed in the invited ACCMS-5 conference talk of Dr. Aradi and Prof. Frauenheim.
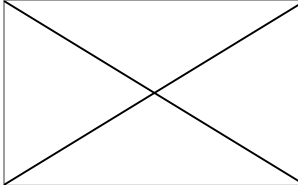
The practical session will give you experience in running the new DFTB+ code, which is available free for academic use as well as a commercial module for the Accelyris materials studio system. DFTB+ can model periodic, embedded and cluster/molecular systems efficiently. Example systems relevant to several of the themes from the main conference will be used to illustrate properties which can .

Conference location:

Melia Hotel (*44B Ly Thuong Kiet Street, Hanoi.*) The Conference hall is at the 7th floor
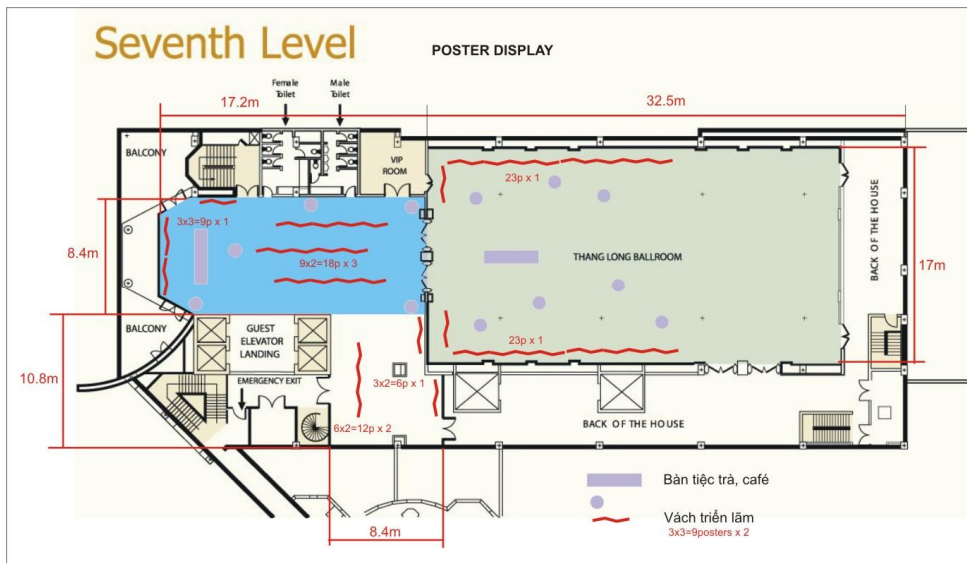
OVERALL CONFERENCE PROGRAM

Time	Wendsday, 09 September 2009	Thursday, 10 September 2009	Friday, 11 September 2009
Morning	Registration: 07:00 - 08:00 Opening: 08h00 - 08:15 Plenary Sessions 1 Plenary Sessions 2	Plenary Sessions 6 Plenary Sessions 7	Plenary Sessions 11 Plenary Sessions 12
Lunch (one hour onsite at the Conference hotel)			
Afternoon	Plenary Sessions 3 Plenary Sessions 4 Plenary Sessions 5	Plenary Sessions 8 Plenary Sessions 9 Plenary Sessions 10	Plenary Sessions 13 Plenary Sessions 14 Plenary Sessions 15
Evening	Accelrys presentation POSTER SESSION Dinner (onsite)	ACCMS5 Banquet (onsite) ACCMS-5 award presentation Kawazoe poster award presentation	

ACCMS-5 SCIENTIFIC PROGRAM
Location: Melia Hotel

44B Ly Thuong Kiet Street, Hanoi. Tel: (+84 4) 39343343; Fax: (+84 4) 39343344

September 8, 2009, Tuesday

17:00-18:00   Conference Registration

September 9, 2009, Wednesday

07:00-08:00   Conference Registration

Conference Opening

08:00   W.1 Welcome address by Chairman of ACCMS-5 Conference

80:05   W.2 Welcome address by Chairman of Scientific Council on Materials Science

08:10   W.3 Welcome address by Chairman of IAB -ACCMS

08:15   W.4 Opening address by Minister of Science and Technology

Session 1 Advanced Computational Methodology: beyond DFT
Chair : Karu Ohno (Yokohama National University, Japan)

08:25-9:00   K1 - 1   Challenges and Progress in Atomistic Simulations

Michele Parrinello

Computational Science, Department of Chemistry and Applied Biosciences, ETH Zurich, USI, Campus, Via Giuseppe Buffi 13, CH-6900 Lugano, Switzerland

09:00-09:25   I1 - 1   Strongly   Correlated   Electrons: Wavefuntion   Based Methods

P. Fulde

Asia Pacific Centre for Theoretical Physics, Korea and Max Planck Institute for the Physics of Complex Systems, Germany

09:25-09:50   I1 - 2   Efficient and Accurate Calculation of Exact Exchange and RPA Correlation Energies in ACFD Theory

Huy-Viet Nguyen, Stefano de Gironcoli, Giulia Galli

Hanoi University of Education and Department of Chemistry, University of California, One Shields Avenue, Davis, CA, 95616 (USA)

09:50-10:05   O1 - 1   Spin-Polarized all-Electron GW+T-Matrix Calculation for Single and Double Quasiparticle Energies of Al Clusters

Y. Noguchi, K. Ohno, I. Solovyev, and T. Sasaki

Institute for Solid State Physics, University of Tokyo, 5-1-5 Kashiwanoha, Kashiwa, Chiba 277-8581, Japan.

BREAK

Session 2 Modelling of Nanotubes, Nanowires and Quantum Dots
Chair: H.T. Diep (Université de Cergy-Pontoise, France)

10:30-10:55   I2 - 1   Modifaction of Electronic Struictures of Carbon Nanotubes with Applied Electric Fields or Adsorbed Molecules

Gunn Kim, Mun-Hyun Cha, J. Bernholc, Jisoon Ihm

FPRD and Department of Physics and Astronomy, Seoul National University, Korea

10:55-11:20   I2 - 2   Electronic Properties of Graphene under One-Dimensional Potentials

V. Lien Nguyen, H. Chau Nguyen, C. Huy Pham, and T. Nguyen Dung

Institute of Physics, Vietnam Academy of Science & Technology

11:20-11:45   I2 - 3   Monatomic Chain Formation and Breaking Process of Zno Nanowires: Molecular Dynamics Simulations

Ya-Pu Zhao, Bin-Bin Wang

State Key Laboratory of Nonlinear Mechanics, Institute of Mechanics, Chinese Academy of Sciences, China, 15 Beisihuanxi Road, Beijing 100190 China

11:45-12:10   I2 - 4   First Principle Study on Wurzite Nano Wire

Vu Ngoc Tuoc

Hanoi University of Technology, Vietnam 01 Dai Co Viet road, Hanoi 10000, Vietnam

12:10-12:35   I2 - 5   A Hierarchical Approach to Study Thermal Behavior of Nano-sized Materials

Jer-Lai Kuo

Institute of Atomic and Molecular Sciences, Academia, Sinica, Taiwan

12:35-12:50   O2 - 1   **Investigation of Chemical Selectivity and Dimer Ordering in One-dimensional Atomic Wires Grown by Co-deposition of In and Sn on Si(100)-2x1 Surface: A Kinetic Monte Carlo Simulation Study**

D.B. Putungan, H.J. Ramos, M.A. Albao

Physics Division, Institute of Mathematical Sciences and Physics, University of the Philippines Los Baños, College, Los Baños, Laguna 4031, Philippines

12:50-13:05   O2 - 2   **Some Theoretical Results on Semiconductor Spherical Quantum Dots**

B. Billaud, M. Picco, T.T. Truong

Université de CERGY-PONTOISE, Laboratoire de Physique Théorique et Modélisation, 2 rue Adolphe Chauvin, F-95302 Cergy-Pontoise, FRANCE

LUNCH

Session 3 Modelling of Nano-biological and Polymeric Systems
Chair: G. Kim (Seoul National University, Korea)

14:15-14:40   I3 - 1   **Resonance Scattering of Phonons-Glass-like Thermal Conductivity in Crystalline Solids**

John S. Tse, Niall J. English

Department of Physics, University of Saskatchewan, 116 Science Place, Saskatoon, Saskatchewan, Canada S7N 0K4

14:40-15:05   I3 - 2   **DFTB - Theory, Parametrization, Recent Applications**

B. Aradi, N. H. Moreira, G. Dolgonos, Th. Frauenheim

Bremen Center for Computational Materials Science, Am Fallturm 1, 28359 Bremen, Germany

15:05-15:20   O3 - 1   **First Principles Studies of the Adsorption of Uracil on SWCNTs**

M. Rajarajeswari, K. Iyakutti and Y. Kawazoe

School of Physics, Madurai Kamaraj University, Madurai,Tamilnadu - 625 02, INDIA

15:20-15:35   O3 - 2   **Monte Carlo Simulation of Coarse-grained Model of Large Polymer Mixtures with Different Chain Topology**

Visit Vao-soongnern

School of Chemistry Institute of Science Suranaree University of Technology Nakhon Ratchasima 30000, Thailand

15:35-15:50 O3 - 3 Adsorption of Polycyclic Aromatic Hydrocarbons on Graphite Surfaces

T. Tran-Duc, N. Thamwattana, Barry J. Cox, J. M. Hill

Nanomechanics Group, School of Mathematics and Applied Statistics, University of Wollongong, Australia

BREAK

Session 4 Multi-scale Modeling of Materials
Chair: S.D. Kenny (Loughborough University, UK)

16:15-16:40 I4 - 1 Accelerated Molecular Dynamics Methods

Arthur F. Voter

Theoretical Division, T-1, MS B268 Los Alamos National Laboratory Los Alamos, New Mexico, 87545, USA

16:40-17:05 I4 - 2 First-Principles Calculation of Microstructural Process in Alloys

T. Mohri

Division of Matrials Scinece and Engineering, Graduate School of Engineering, Hokkaido University, Sapporo 060-8628, JAPAN

17:05-17:30 I4 - 3 Quantum Simulation of Materials at Micron Scales and Beyond

Qing Peng, Xu Zhang, Linda Hung, Emily A. Carter and Gang Lu

Department of Physics, California State University Northridge, 18111 Nordhoff Street, Northridge, CA 91330-8268, USA

17:30-17:55 I4 - 4 Analytic Bond-Order Potentials Including Magnetism

Ralf Drautz and David Pettifor

ICAMS, Ruhr-University Bochum, 44780 Bochum, Germany

17:55-18:10 O4 - 1 A Renormalization Approach to ac Conductivity in Quasicrystals

V. Sanchez, C. Wang

Departamento de Fisica, Facultad de Ciencias, Universidad Nacional Autonoma de Mexico, Apartado Postal 70-542, 04510, D.F., MEXICO

BREAK

Session 5 Oxydes and Nitrides Materials

Chair: S. Limpijumnong (Suranaree University of Technology, Thailand)

18:15-18:40 I5 - 1   **High-k Oxides and Interfaces: Materials Design from First-principles**

M. Yang, Y. F. Dong, G. G. Xu, Y. P. Feng, S. H. Wang, Z. G. Huang, A. C. H. Huan

National University of Singapore Department of Physics, 2 Science Drive 3, Singapore 117542

18:40-18:55 I5 - 2   **Structure Property Correlation forMetal Oxide Structures Designed for Nano-Catalysis with Order N Plane Wave Calculation**

Abhijit Chatterjee

Accelrys 3-3-1 Nishishinbashi Tokyo, Minato-ku 105-0003 Japan

18:55-19:10 O5 - 1   **Investigation on Spin-Flipping near Surface Layers of Perovskite CaMnO3**

Nguyen Thuy Trang, Nguyen Tien Cuong, Nguyen Hoang Linh, and Bach Thanh Cong

Faculty of physics, Hue University of Education

19:10-19:25 O5 - 2   **Carbon and Silicon Impurities in GaAs1-xNx**

Pakpoom Reunchan, Sukit Limpijumnong, Anderson Janotti, and Chris G. Van de Walle

School of Physics Institute of Science, Suranaree University of Technology, Nakhon Ratchasima Thailand 30000

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POSTER SESSION SPONSORED BY ACCELRYS INC.

Chair: Y.P. Feng (National University of Singapore)

ACCELRYS PRESENTATION

19:30-20:00   **Modeling and Simulation to Enterprise Solution: A Passage through Platforms and Tools**

Abhijit Chatterjee

Accelrys 3-3-1 Nishishinbashi Tokyo, Minato-ku 105-0003 Japan

20:00 -

POSTERS PRESENTATION + DINNER

September 10, 2009, Thursday

Session 6 Modeling Materials for Future Energy (I)

Chair: E.G. Wang (Institute of Physics, CAS, China)

08:00-08:35   K6 - 1   Transport Properties and Bonding Characteristics of Nanostructured Materials

Jisoon Ihm

Department of physics and astronomy, Seoul National University, Seoul, 151-747, Korea

08:35-09:00   I6 - 1   Pt Nanoclusters on Carbon Nanotube Support

Dam Hieu Chi

Hanoi University of Science, Vietnam National University Hanoi & JAIST

09:00-09:25   I6 - 2   Phase Behavior Predictions of Various Methane and Hydrogen Clathrate Hydrates

Vladimir R. Belosludov

Nikolaev Institute of Inorganic Chemistry of SB RAS, 3 Lavrentiev av., Novosibirsk, 630090 Russia

09:25-09:50   I6 - 3   Ab Initio Study of Graphene Nanostructures: Metal Binding and Hydrogen Adsorption

G.-B. Kim, S.-M. Choi, N. Park, S.-H. Jhi

Department of Physics Pohang University of Science and Technology Hyojadong San 31, Pohang

09:50-10:25   I6 - 4   Hydrogen-Related Defects and the Role of Metal Additives in the Kinetics of Complex Hydrides

Khang Hoang and Chris G. Van de Walle

Materials Department, University of California, Santa Barbara, California 93106-5050, USA

10:25-10:40   O6 - 1   Single Walled Carbon Nanotubes Coated With Hydrides As Hydrogen Storage Medium

K. Iyakutti, V. J. Surya and Y. Kawazoe

School of Physics, Madurai Kamaraj University, Madurai, Tamil Nadu-625021.

BREAK   CONFERENCE PHOTO

Session 7 Modeling of Mechanical Properties of Materials
Chair: Gang Lu (California State University Northridge, USA)

11:00-11:25 I7 - 1 Stress Dependence of the Peierls Barrier in BCC Metals

V. Vitek and R. Gröger

Department of Materials Science and Engineering, University of Pennsylvania, 3231 Walnut Street, Philadelphia, PA 19104 USA

11:25-11:50 I7 - 2 Bending Analysis of Three-Phase Polymer Composite Plates Reinforced by Glass Fibers and Titanium Oxide Particles

Nguyen Dinh Duc, Dinh Khac Minh

Vietnam National University, Hanoi

11:50-12:15 I7 - 3 A Hybrid Atomistic Simulation for Investigating Spatial Distribution of Alloying Elements and Their Effects on Metallic Materials Properties

Eun Cheol Do, Eun-Ha Kim and Byeong-Joo Lee

Department of Materials Science and Engineering, Pohang University of Science and Technology (POSTECH), Pohang 790-784, Korea

12:15-12:30 O7 - 1 A Molecular Dynamics Study of the Effect of CNT-Al Bond Strength on the Mechanical Properties of CNT-reinforced Al Composite

Byung-Hyun Kim, Kwang-Ryeol Lee, Sang Hak Kim, Do Seok Han, Yong-Chae Chung

KIST, 39-1 Hawolgok-dong, Seongbuk-gu, Seoul, 133-791, Korea

LUNCH   IAB-ACCMS MEETING

Session 8 Materials under Extreme Conditions
Chair: R. Drautz (Bochum University, Germany)

13:30-13:55 I8 - 1 Effect of Impurities on Vacancy Behaviour in Fe-based Alloys from First Principles

Chu Chun Fu

SRMP, CEA-Saclay, 91191 Gif sur Yvette, France

13:55-14:20 I8 - 2 Monte Carlo Models for FeCr Alloys: Prototype Materials for Fusion Applications

M. Yu. Lavrentiev, D. Nguyen-Manh, S. L. Dudarev

Culham Science Centre, Abingdon, OX14 3DB, United Kingdom

14:20-14:45 I8 - 3 On the Electronic Structure of Some Strongly Correlated Electron Systems

Vinh Hung Tran

Polish Academy of Sciences, Institute of Low Temperatures and Structure Research, 50-950 Wroclaw, Poland

14:45-15:00 O8 - 1 First Principles Modeling of Stability Mechanism of Nonstoichiometric Uranium Dioxide

Ying Chen, Hua Y. Geng, Yasunori Kaneta, Motoyasu Kinoshita and Shuichi Iwata

Graduate School of Frontier Sciences, The University of Tokyo, 5-1-5 Kashiwanoha, Kashiwa City, Chiba, 277-8563, Japan

BREAK

Session 9 Spintronics and Magnetic Properties of Materials
Chair: Bach Thanh Cong (Hanoi University of Science, Vietnam)

15:10-15:35 I9 - 1 First Principles Design of DMS and DMO by Transition Metal Codoping

G. P. Das

Indian Association for the Cultivation of Science Department of Materials Science IACS, Jadavpur, Kolkata 700032 INDIA

15:35-16:00 I9 - 2 Monte Carlo Study of the Spin Transport in Magnetic Materials

H. T Diep, K. Akabli, I. Harada, Y. Magnin

Laboratoire de Physique Théorique et Modélisation Université de Cergy-Pontoise, CNRS, UMR8089 2, Avenue A. Chauvin, 95302 Cergy-Pontoise, France

16:00-16:25 I9 - 3 Magnetization Reversal in the Quantum Limit

Frank Marsiglio, Fatih Dogan, Lucian Covaci, and Wonkee Kim

Department of Physics University of Alberta 11322 - 89 Avenue Edmonton, Alberta, CANADA T6G 2G7

16:25-16:50 I9 - 4 Fascinating World of Double Perovskites

Tanusri Saha-Dasgupta

S.N.Bose National Centre for Basic Sciences, Block JD, Sector III, Salt Lake, Kolkata-700098, INDIA

16:50-17:05   O9 - 1   **Spin Orbit Contributions to the Magnetism of Small Iron Clusters**

B. Hourahine, C. Köhler, Th. Frauenheim

Department of Physics, SUPA University of Strathclyde John Anderson Building 107 Rottenrow Glasgow G4 0NG

17:05-17:20   O9 - 2   **New Type of Half-metallic Antiferromagnets and their Applications to GMR and TMR Devices**

Nguyen Hoang Long, Masako Ogura and Hisazumi Akai

Deparment of Physics, Graduate School of Science, Osaka University, Toyonaka 560-0043, Osaka, Japan

17:20-17:35   O9 - 3   **Valence Bond Monte Carlo Study of Random Singlet Phases**

Huan Tran and Nick Bonesteel

Department of Physics and NHMFL, Florida State University, 1800 E. P. Dirac, Tallahassee, FL 32310, USA

BREAK

Section 10 Modeling of Nano-Devices
Chair: S.H. Jhi (Pohang University of Science and Technology, Korea)

17:45-18:10   I10 - 1   **Energy Materials Design: Band Gap Manipulation by First Principles**

S.Y. Chen, W.J Yin, X. G. Gong, S.H. Wei

Department of Physics, Fudan University, Handan Rd 220#, Shanghai 200433, China

18:10-18:35   I10 - 2   **How can a Homogeneous Semiconductor Exhibit Gigantic Dielectric Response?**

Ping Wu, Valeri Ligatchev, Zhi Gen Yu, Jianwei Zheng, Michael B. Sullivan and Yingzhi Zeng

Institute of High Performance Computing, Fusionopolis Way, #16-16 Connexis, Singapore 138632, Singapore

18:35-19:00   I10 - 3   **First-principles Design of Nanomachines**

J. R. Banavar, M. Cieplak, T. X. Hoang, A. Maritan

Institute of Physics, 10 Dao Tan, Ba Dinh, Hanoi

19:00-19:15   O10 - 1   Multi-Paradigm Simulations at the Nanoscale: Methodology and Applications to Functional Carbon Materials

Haibin Su

Divison of Materials Science Nanyang Technological University, Singapore

19.45   ACCMS-5 BANQUET

ACCMS-5 AWARD PRESENTATION

KAWAZOE POSTER AWARD PRESENTATION

September 11, 2009, Friday

Session 11 Cluster Modeling

Chair: Vijay Kumar (Vijay Kumar Foundation, India)

08:00-08:35   K11 - 1   Paradigm Shift of Materials Design by Computer Simulation- from Explanation to Prediction

Y. Kawazoe

Institute for Materials Research, Tohoku University 2-1-1 Katahira, Aobaku, Sendai, 980-8577, Japan

08:35-09:00   I11 - 1   Structure and Properties of Some Doped Metal Clusters: A Quantum Chemical Approach

Minh Tho Nguyen

Department of Chemistry, and Institute for Nanoscale Physics and Chemistry (INPAC), University of Leuven, B-3001 Leuven, Belgium

09:00-09:25   I11 - 2   Charge Separation Dynamics at Molecular Heterojunction of C60 and Zn- Phthalocyanine

Kaoru Ohno and Yasunobu Kodama

Department of Physics,Yokohama National University,79-5 Tokiwadai, Hodogaya,Yokohama 240-8501, Japan

09:25-09:40   O11 - 1   Evaluating Seebeck Coefficient of NaxCoO2 from Molecular Orbital Calculations

T. Seetawan, C. Thanachayanont and V. Amornkitbamrung

680 Nitthayo Road, Sakon Nakhon Rajabhat University, Sakon Nakhon, 47000, Thailand

BREAK

Session 12 Surface, Interface and Thin Films
Chair: Wu Ping (Institute for High Performance Computing, Singapore)

10:00-10:25   I12 - 1   Surface Energy and Surface Proton Order of Ice Ih Basal and Prism Surfaces

Enge Wang

Institute of Physics Chinese Academy of Sciences Box 603, Zhongguancun Beijing 100190 China

10:25-10:50   I12 - 2   Atomistic Modelling of the Growth of Rutile

L.J. Vernon, E. Sanville, S.D. Kenny and R. Smith

Department of Mathematical Sciences, Loughborough University, Loughborough. Leicestershire, LE11 2DH, UK

10:50-11:15   I12 - 3   Ab Initio Modeling of Laser Materials: Segregation of Nd and Gd on YAG Surfaces

Vijay Kumar

Dr. Vijay Kumar Foundation, 1969 Sector 4, Gurgaon 122001, Haryana, India

11:15-11:40   I12 - 4   Influence of Cr and Fe Additions on Grain Boundary Cohesion of Bcc Fe and Cr

A. Kiejna, T. Ossowski, E. Wachowicz

University of Wroclaw, Institute of Experimental Physics, plac M. Borna 9, 50-204 Wroclaw, Poland

11:40-11:55   O12 - 1   First-principles Study of Rectifying Properties of Pt/TiO2 Interface

Tomoyuki Tamura, Shoji Ishibashi, Kiyoyuki Terakura, and Hongming Weng

Research Institute for Computational Sciences (RICS), National Institute of Advanced Industrial Science and Technology (AIST), 1-1-1 Umezono, Tsukuba, Ibaraki 305-8568, Japan

11:55-12:10   O12 - 2   Hydrogen Bonded Bimolecular Monolayers on Au(111): A DFT Study

M. T. Nguyen, D. Passerone, C. Pignedoli

Nanotech@surfaces Empa - Swiss Federal Laboratories for Materials Testing and Research Ueberlandstrasse 129 CH-8600 Duebendorf Switzerland

12:10-12:25 O12 - 3 Molecular Dynamics Simulations Study on the Structure Evolution of Polyethylene Surface by Ar Ion Bombardment

Chansoo Kim1, Sk. Faruque Ahmed, Mina Park1, Minwoong Joe, Myoung-Woon Moon, Kwang-Ryeol Lee

Computational Science Center, Korea Institute of Science and Technology (KIST), P. O. Box 131, Cheongryang, Seoul, 130-650, Korea

12:25-12:40 O12 - 4 A First Principles Calculation on the Polythiophene/Carbon Nanotube Hybrid Nanocomposite

Hsin-An Chen, I-Sheng Chen and Chun-Wei Chen

No. 1, Sec. 4, Roosevelt Road, Taipei, 10617 Taiwan

LUNCH

Session 13   Modeling of Materials for Future Energy (II)
Chair: X.G. Gong (Fudan University, China)

13:45-14:10 I13 - 1 First-principles Determination of Free Energies of Ferroelectric Phase Transitions

Umesh V Waghmare, Anil Kumar

Jawaharlal Nehru Centre for Advanced Sceientific Research Main Campus, Jakkur Post, Jakkur, Bangalore-560 064

14:10-14:35 I13 - 2 Origin of Anisotropy, Metallic Behavior and Thermoelectric Effect in Delafossite $PdCoO_2$, $PtCoO_2$

Khuong P. Ong, Jia Zhang, and Ping Wu

Institute of High Performance Computing, Computational Materials Science and Engineering , 1 Fusionopolis Way, #16-16, Connexis, Singapore 138632

14:35-14:50 O13 - 1 GPU-accelerated Massive Parallel Quantum Molecular Dynamics Simulation

Toshiaki Iitaka

Advanced Science Institute, RIKEN, 2-1 Hirosawa, Wako, 351-198, Japan

14:50-15:05 O13 - 2 Modeling of Pillared Layer Structures as the Hydrogen Storage Material

Daejin Kim, Dong Hyun Jung, Kyung-Hyun Kim, Areum Lee, Seung-Hoon Choi, Jaheon Kim, and Kihang Choi

Insilicotech Co. Ltd., A-1101 Kolontripolis, 210, Geumgok-Dong, Bundang-Gu, Seongnam-Shi, 463-943, Korea

15:05-15:20   O13 - 3   Thermal Diffusivity of Al0.3Ga0.7As by Molecular Dynamics Simulation and Thermograph Method

S.Chitra

Sri Para sakhi college for women, courtallam-627 802, Tamil Nadu, India

BREAK

Session 14   Micro-structure Modelling and Phase Transformation
Chair: Tetsuo Mori (Hokkaido University, Japan)

15:30-15:55   I14 - 1   Liquid Structure as A Guide for Phase Stability in the Solid State: Prediction of a Stable Compound in the Au-Si Alloys System

Marcel H.F. Sluiter, Emre S. Tasci

Department of Materials Science & Engineering, Delft University of Technology, Mekelweg 2, 2628CD Delft, the Netherland

15:55-16:20   I14 - 2   Ab Initio Molecular Dynamics Simulations to Designing Static and Dynamic Properties in Undercooled and Amorphous Materials

A. Pasturel, N. Jakse

SIMAP (G-INP and CNRS) batiment Recherche Phelma 1130 rue de la piscine BP 75, Saint Martin d'Heres 38402 FRANCE

16:20-16:45   I14 - 3   Application of Ab Initio Results in Modelling Phase Diagrams Containing Complex Phases

M. Sob, J. Pavlu, J. Vrestal, A. Kroupa

Faculty of Science Masaryk University Kotlarska 2, CZ-611 37 Brno, Czech Republic

16:45-17:10   I14 - 4   The 'Native Vacancy' and Diffusion Mechanism in Amorphous Alloys

P.K.Hung, L.T.Vinh, P.H.Kien

Hanoi University of Technology, Vietnam

17:10-17:25   O14 - 1   Structural and Dynamic Properties in Undercooled and Amorphous Materials: A Molecular Dynamics Study Cu-Zr Glass Forming Alloys

N. Jakse, A. Nassour and A. Pasturel

Science et Ingénierie des Matériaux et Procédés,INP Grenoble, UJF-CNRS, 1130, rue de la Piscine, BP 75, 38402 Saint-Martin d'Hères Cedex, France

17:25-17:40 O14-2 Kinetic Monte Carlo Simulations of Diffusion-Limited Nucleation

Y. H. Lau, R. Hariharaputran, D. T. Wu

Institute of High Performance Computing, 1 Fusionopolis Way, #16-16 Connexis, Singapore 138632

BREAK

Session 15 Optical and Spectroscopy Properties of Materials
Chair: Umesh V. Waghmare (JNCSR, India)

17:40-18:05 I15 - 1 Using Transformation Optics to Design Materials with Novel Optical Properties

C.T. Chan

PhysicsDepartment, Hong Kong University of Science and Technology Clear Water Bay Hong Kong

18:05-18:30 I15 - 2 Local Structure Analysis by X-ray Absorption Spectroscopy and First Principles Calculations

Sukit Limpijumnong

School of Physics, Suranaree University of Technology and Synchrotron Light Research Institute, Nakhon Ratchasima 30000, Thailand

18:30-18:55 I15 - 3 Beyond LDA in Electronic-Transport Simulations of Single-Molecule Junctions

Hyoung Joon Choi

Department of Physics,Yonsei University 262 Seongsanno, Seodaemun-gu, Seoul 120-749, South Korea

18:55-19:20 I15 - 4 Study of EXAFS Cumulants of Crystals by the Statistical Moment Method and Anharmonic Correlated Einstein Model

Vu Van Hung, Ho Khac Hieu and K.Masuda-Jindo

Hanoi National University of Education, 136 Xuan Thuy street, Cau Giay, Hanoi, Vietnam

19:20-19:35 O15 - 1 Studies of Electronics and Optical Properties of $CaCu_3Ti_4O_{12}$ Using First Principles Calculations

W. Chaiyarat, A. Yangthaisong

Department of Physics Ubonrajathanee University Ubonratchathani THAILAND 34190

POSTER SESSION SPONSORED BY ACCELRYS INC.

Chair: Y.P. Feng (National University of Singapore)

P - 1   **Electronic Structure Property Correlation of Silicon (111) Surface Functionalized with Alkane Molecules**

Abhijit Chatterjee

Accelrys 3-3-1 Nishishinbashi Tokyo, Minato-ku 105-0003 Japan

P - 2   **The investigation of the Effects of Ga-doping on the Electronic Structure and the Optical Properties of ZnO under the Density Functional Theory**

Dinh Son Thach, Tran Nguyen Quynh Nhu

University of Science, VNU-HCM, 227 Nguyen Van Cu str., 5 dist., Hochiminh City, Vietnam

P - 3   **Vibration Control of Piezoelectric Cantilever Plates and Comparision with Experiments**

Tran Ich Thinh, Le Kim Ngoc

Viet Nam Electricity

P - 4   **Simulation of Thermal Dissipation in a Micro-Processor Using Carbon Nanotubes Based Composite**

Bui Hung Thang, Phan Ngoc Hong, Phan Hong Khoi and Phan Ngoc Minh

Institute of Materials Science, 18 Hoang Quoc Viet Str., Caugiay Dist., Hanoi, Vietnam

P - 5   **Interpretation of Hund's First and Second Rules for 3d Atoms**

Takayuki Oyamada, Kenta Hongo, Yoshiyuki Kawazoe, and Hiroshi Yasuhara

Kawazoe Laboratory Institute for Materials Research Tohoku University Katahira 2-1-1, Aoba-ku, Sendai 980-8577 Japan

P - 6   **First Principles Calculations of SrHfO3**

A. Yangthaisong and S. J. Clark

Department of Physics Ubonrajathanee University Ubonratchathani THAILAND 34190

P - 7   **Development of the All-electron Mixed Basis Hartree-Fock Calculation Code**

Yoichi Tadokoro, Kaoru Ohno, Soh Ishii, and Yoshifumi Noguchi

79-5-W708 Tokiwadai Hodogaya-ku Yokohama Japan

P - 8   **Computer Simulation of the Non-Uniform and Anisotropic Diamagnetic Shift of Electronic Energy Levels in Double Quantum Dot Molecules**

L. M. Thu and O. Voskoboynikov

Department of Electronics Engineering, National Chiao Tung University, 1001 Ta Hsueh Rd., Hsinchu, 30010, Taiwan.

P - 9   **Ab-initio Study of the Effect of Size and Shape on the Electronic Properties and Electron Affinity of Hydrogen Terminated Carbon Nanoparticles (Diamondoids)**

N. H. Tuyen, N. M. Tuan, N. T. Loc

Hochiminh City Institute of Physics - 01 Mac Dinh Chi, District 1, Hochiminh City, Vietnam

P - 10   **Highly Photoluminescent Semiconductor Quantum Dots Synthesized in Non-Coordinating Solvent**

Nguyen Hong Quang, Luu Tien Hung

Department of Physics, Vinh University. 182 Le Duan Street, Vinh city, Nghe An Province, VIETNAM

P - 11   **Ab Initio Study of n-type Doping in Anatase TiO2**

Huynh Anh Huynh, Bálint. Aradi, Peter Deák, and Thomas Frauenheim.

Bremen Center for Computational Materials Science Universität Bremen Am Fallturm 1 28359 Bremen, Germany

P - 12   **A Theoretical Approach of Microscopic Solvation of LiCl in Water Cluster: LiCl(H2O)n(n=1-9)**

Manik Kumer Ghosh and Cheol Ho Choi

SINTEF Materials and Chemistry, Department of Hydrocarbon Process Chemistry, P. O. Box 124 Blindern, 0314 Oslo, Norway

P - 13   **Theoretical Prediction of Doubly Charged Hydronium Ions**

Manik Kumer Ghosh and Cheol Ho Choi

SINTEF Materials and Chemistry, Department of Hydrocarbon Process Chemistry, P. O. Box 124 Blindern, 0314 Oslo, Norway

P - 14   **Pair Potential Application for Molecular Dynamics Studies of GaAs Nanoparticles in the Amorphous Phase**

Ngo Huynh Buu Trong, Vo Van Hoang

Department of Applied Physics, Faculty of Apply Sciences, Institute of Technology of HCM City, VNU of HCM, 268 Ly Thuong Kiet District 10 Ho Chi Minh City Viet Nam

P - 15   **Cooling Rate Effects in Liquid and Amorphous Aluminosilicate Nanoparticles: A Molecular Dynamics Computer Simulation**

Nguyen Ngoc Linh, Ngo Huynh Buu Trong, Tran Thi Thu Hanh, Vo Van Hoang

Dept. of Physics, Institute of Technology, National University of HochiMinh City, 268 Ly Thuong Kiet Street, District 10, HochiMinh City-Vietnam.

P - 16   **Effect of Edge Doping on Electronic and Magnetic Properties of Graphene Nanoribbons**

Narjes Gorjizadeh, Amir A. Farajian, Keivan Esfarjani, and Yoshiyuki Kawazoe

Tohoku University IMR, 2-1-1 Katahira, Aoba-ku, Sendai, 980-8577 Japan

P - 17   **Magneton-Phonon Resonance and Line-width in Rectangular Quantum Wire**

Le Dinh, Tran Cong Phong

Hue University-College of Education, 34 Le Loi Hue, Vietnam

P - 18   **Study of Half Metallacity of CrO2 by Using the LSDA and LDA+U Methods**

R. K. Thapa, M. P. Ghimire, Lalmuanpuia and Sandeep

Physics Department, Mizoram University Aizawl 796009, Mizoram INDIA

P - 19   **The Characterization of the Carbon Nanotube-Copper Composites from the First-principle Calculations**

M. Park, K.R. Lee, S.H. Kim, and D.S. Han

Korea institute of science and technology

P - 20 **Controllable Synthesis of Base- and Tip-type of Multiwalled Carbon Nanotubes by a dc Plasma-Enhanced Chemical Vapor Deposition (PECVD) Technique**

Nguyen Hong Quang, Do-Hyung Kim

Department of Physics, Vinh University. 182 Le Duan Street, Vinh city, Nghe An Province, VIETNAM

P - 21 **Calculation of the Field Emission Current from Carbon Nanotubes Using the Bardeen Transfer Hamiltonian Method**

Nguyen Ngoc Hieu, Nguyen Van Hanh, Tran Cong Phong

Le Quy Don Gifted School 106 Hung Vuong Str., Dong Ha, Quang Tri

P - 22 **Totally Symmetric Vibrations of Armchair Carbon Nanotubes**

N.A. Poklonski1, E.F. Kislyakov, Nguyen Ngoc Hieu, S.A. Vyrko1, O.N. Bubel', Nguyen Ai Viet

Institute of Physics and Electronics, Hanoi, Vietnam

P - 23 **An Efficient Tool for Modeling and Prediction of Fluid Flow in Nanochannels**

Samad Ahadian, Yoshiyuki Kawazoe

Laboratory of Materials Design by Computer Simulation, Institute for Materials Research (IMR), Tohoku University, 2-1-1 Katahira, Aoba-ku, Sendai, Japan P. O. Box: 980-8577

P - 24 **Calculation of the Nonlinear Absorption Coefficient of a Strong Electromagnetic Wave by Confined Electrons in Quantum Wires**

Le Thi Thu Phuong, Huynh Vinh Phuc, Tran Cong Phong

Hue University, College of Education 32-34 Le Ioi, Hue, Viet Nam

P - 25 **Waters Mediate Interaction between Proteins: An Observation by data Mining Method**

Ayumu Sugiyama, Taku Mizukami, Dam Hieu Chi, Ho Tu Bao

Japan Advanced Institute of Science and Technology, 1-1 asahidai nomi ishikawa JAPAN

P - 26   **Determine Crystal Structure of Poly(pentamethylene 2,6-naphthalate) by Molecular Modeling Technique**

Thi Cuc Do, Hye-Jin Jeon, Hyun Hoon Song, Kohji Tashiro, Young Ho Kim

Department of Advanced Materials, Hannam University, Daejeon, S. Korea

P - 27   **Computation of Chemical Equilibrium in Multi-component Zzirconium Alloys for Biomaterials Applications**

Pei-Lin Mao and Ping Wu

School of Chemical and Life Sciences, Nanyang Polytechnic, 180 Ang Mo Kio Ave 8, Singapore 569830

P - 28   **Samdwich Microstructure of Tumblebug Cuticle**

B. Chen, Q. Yuan, J Luo, X. Peng

Chen Bin Group, College of Resource and Environment Science, Chongqing University, Chongqing 400044, China

P - 29   **Spiry Microstructure of Aragonite Sheets of Chamidae Shell**

B. Chen, Q. Yuan, J Luo, X. Peng

Chen Bin Group, College of Resource and Environment Science, Chongqing University, Chongqing 400044, China

P - 30   **Anisotropic Diffusion in Disordered Fractals**

Do Hoang Ngoc Anh, Steffen Seeger and Karl Heinz Hoffmann

Dept. of Computational PhysicsTechnische Universit"at Chemnitz 09126 Chemnitz, Germany

P - 31   **Study of Thermodynamic Properties of Cerium Dioxide under High Pressures**

Vu Van Hung, Le Thi Mai Thanh and K.Masuda-Jindo

Hanoi National University of Education, 136 Xuan Thuy Street, Cau Giay, Hanoi, Vietnam

P - 32   **Electrophonon Resonance in Square Quantum Wells of n-GaAs Materials**

Tran Cong Phong, Vo Thanh Lam, Luong Van Tung

Hue University, College of Education 32-34 Le loi, Hue, Viet Nam

P - 33   **The Electronic Properties of MgO under High Pressure from Ab Initio Calculations**

G. Zheng, L. Yu, K.H. He, Z.L. Zeng, Q.L. Chen

School of Mathematics and physics,China University of Geosciences (Wuhan), Wuhan 430074, P. R. China

P - 34   **Complex Characterization of the Nanostructured Materials by Using the Scanning Probe Microscopy Methods**

S.A. Chizhik, Vo Thanh Tung, Nguyen Trong Tinh

A.V.Luikov Heat and Mass Transfer Institute of National Academy of Sciences of Belarus, P Brovki Str. 15, Minsk, Belarus

P - 35   **Another SP3 Bonded Carbon Crystal**

K. Iyakutti, M. Rajarajeswari and Y. Kawazoe

School of Physics, Madurai Kamaraj University, Madurai, Tamil Nadu-625021,. India

P - 36   **Mesoscale Simulation on Phase Behaviour of Triblock Copolymers with Different Chain Architecture in Aqueous Solution**

Mantana Chansuna, Nuttaporn Pimpha, Visit Vao-soongnern

School of Chemistry Inst. of Science Suranaree University of Technology Nakhonratchasima 30000, Thailand

P - 37   **Challenges in Modelling TCP Phase Formation in Ni-based Superalloys**

Bernhard Seiser, Thomas Hammerschmidt, Aleksey Kolmogorov, Ralf Drautz and David Pettifor

Department of Materials, University of Oxford Parks Road Oxford OX1 3PH UK

P - 38   **Fabrication and Calculation of the Friction Coefficient of Cu Matrix Nanocomposites Material is Reinforced by Carbon Nanotubes (CNTs)**

Pham Van Trinh. Tran Bao Trung, Nguyen Ba Thang. Nguyen Van Tu. Duong Ngoc Vinh. Doan Dinh Phuong. Phan Ngoc Minh

Institute of Material Science, Vietnamese Academy of Science and Technology, 18 Hoang Quoc Viet Street, Cau Giay District, Hanoi, Vietnam

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Abstracts

K1 - 1

Challenges and Progress in Atomistic Simulations

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Computer simulation methods based on empirical potentials or on the *ab-initio* approach have made invaluable contributions to our understanding of complex chemical and biochemical processes. However in spite of great progress in hardware, computer simulations often fall short of what is needed for a realistic description of the systems of interest. It suffices here to mention the fields of nanoscience and biomaterials where systems composed of a large number of atoms need to be studied over very long time scales. In order to remedy this situation we are developing novel simulation methods that greatly extend the length and time scale of the simulation. We shall present a new approach to ab-initio molecular dynamics which accelerates simulations by at least one order of magnitude. In addition we shall describe methods for accelerating the study of slow processes and calculating free energies. The application and further development of these methods promises to go a long way towards pushing further the limits of computer simulation.

I1 - 1

Strongly Correlated Electrons: Wavefuntion Based Methods

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Electronic structure calculations for strongly correlated electrons systems based on density-functional theory have faced severe problems. Therefore it is of interest that recently wavefunction based computations became possible for problems of that kind. They apply quantum chemical techniques with well controlled approximations and do not face substantial problems. The computational affords are somewhat larger than those for density functional based calculations. Examples will be presented.

I1 - 2

Efficient and Accurate Calculation of Exact Exchange and RPA Correlation Energies in ACFD Theory

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Recently there have been a renewed interest in the calculation of correlation energy for realistic systems in the Adiabatic Connection Fluctuation-Dissipation (ACFD) formalism, particularly within the Random Phase Approximation (RPA) for the exchange-correlation kernel. RPA correlation energy is an important ingredient in the so-called EXX/RPA(+) scheme, which has been shown to be a promising, though computationally very expensive, scheme to overcome the poor performance of standard LDA/GGA DFT in weakly bound systems [1,2,3,4]. In previous

EXX/RPA(+) calculations, based on plane-wave pseudopotential method [2,3,4], a very time-consuming step is the setup of the Kohn-Sham linear response function by performing summation over valence and conduction bands. In this talk, we will show that this step (and the calculation of the complete conduction state spectrum) is not needed and can be replaced by the iterative diagonalization of the RPA dielectric matrix via Density Functional Perturbation Theory (DFPT)[5]. We will also show that slow convergence of the exact-exchange energy with respect to Brillouin zone sampling can be alleviated by a careful treatment of the integrable divergence. We will demonstrate the efficency and accuracy of our implementation by studying a few bulk, molecular and atomic systems. Since at this stage EXX/RPA(+) scheme is still a perturbative approach, i.e. not being a self-consistent procedure, we will also discuss the role of input Kohn-Sham wave functions used in the calculations.

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Spin-Polarized all-Electron $GW+T$-Matrix Calculation for Single and Double Quasiparticle Energies of Al Clusters

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The Green's function method based on the many-body perturbation theory beyond the density functional theory is one of the most powerful first-principles calculation tools to treat the excited states of the real materials. The one-particle Green's function within GW approximation can estimate the single quasiparticle energy spectra such as the first ionization potential (IP) and electron affinity (EA) [1]. On the other hand, the two-particle Green's function expanded as the ladder diagrams up to the infinite order (T-matrix), which describes the short-range electron correlations between two holes or electrons, can estimate the double quasiparticle energy spectra such as the double ionization energy (DIE) and double electron affinity (DEA) [2].

In this study, we apply the spin-polarized version all-electron $GW+T$-matrix program to Al_n (n = 1-8) with the magnetic moment of 0-2 μ_B and calculate the single and double quasiparticle energy spectra. To check accuracy of the present method, we compare the calculated IP, EA, and DIE with available experimental data. The agreement is fairly good. We also discuss the spin-polarized effect and the cluster size dependence of the resulting spectra in detail.

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I2 - 1

Modifaction of Electronic Struictures of Carbon Nanotubes with Applied Electric Fields or Adsorbed Molecules

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In this talk, we will discuss the modification of electronic structures of carbon nanotubes with applied electric fields or adsorbed molecules. The first study topic is the electronic structure of bundles consisting of two and three CNTs under the applied electric fields. Electrostatic screening between carbon nanotubes (CNTs) in a small CNT bundle leads to novel switching behavior induced by electric field perpendicular to the bundle axis. Using first-principles pseudopotential calculations, we show that the field can lead to band gap closure in semiconducting bundles and opening of a gap in metallic ones, thus enabling considerable modulation of bundle conductivity. The modulation effect originates from the symmetry breaking due to the electrostatic screening in the region between the adjacent tube walls.

The second topic is the single strand DNA-decorated carbon nanotubes. According to our ab initio calculations, a single-walled carbon nanotube (SWNT) shows a transition from a metallic one to a p-type semiconductor after helical wrapping of DNA [1]. Water is found to be critical to activate this metal-semiconductor transition in the ssDNA–SWNT hybrid. Raman spectroscopy confirms the same change in electrical behaviors. a band gap can open up in a metallic SWNT with wrapped ssDNA in the presence of water molecules due to charge transfer.

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I2 - 2

Electronic Properties of Graphene under One-Dimensional Potentials

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Using the Transfer-matrix approach, we have studied the energy band structure and transport properties in different graphene structures formed by one-dimensional electric potentials. While the basic formalism, including expressions for the energy spectrum, the transmission probability, and the ballistic current, is generally developed for any one-dimensional potential, numerical results are shown in detail for the two potential applicable structures: graphene *n-p-n* junctions modeled by a trapezium potential and graphene superlattices with a Kronig-Penney type of periodic potential. For graphene *n-p-n* junctions, we calculated the spectrum of quasi-bound states, the resistance, and the current shot noise, emphasizing the importance of the Klein tunneling and the chiral nature of massless Dirac carriers in graphene. The obtained resistance versus the top gate voltage describes well the experimental data reported by Huard et al. in *Phys. Rev. Lett. 98, 236803 (2007)*. For graphene superlattices, T-matrix gives an expression for the energy dispersion, which shows a clear appearance of new Dirac points as the potential parameters vary and at the same time reveals an easy way for understanding the chirality-induced anisotropic renormalization of the group velocity of low-energy carriers in graphene under a periodic potential. Finally, in the case of relatively narrow structures, when the edge effects could be no longer neglected, we developed an appropriate Tight-binding calculation which is distinguished by explicit expressions for the probability density as well as the group velocity.

I2 - 3

Monatomic Chain Formation and Breaking Process of Zno Nanowires: Molecular Dynamics Simulations

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A monatomic chain (MC) is an ideal prototype of a nanowire for extensibility and mechanical strength study. From view point of electrical properties, MC could transport current with very high density thus has important potential application in electronic devices.

In this report, the probability of the MC formation for ZnO material was studied by molecular dynamics (MD) method under different situations. The process of MC formation was studied extensively, and geometrical information such as bond lengths and bond angles of MC were calculated. It was found that most of the atoms in MC came from the original surface. Temperature and strain rate are two important factors during the formation, and both high temperature and low strain rate in a certain range would be benefit to the formation of MC. Furthermore, the effects of strain rate and temperature could attribute to the energy release mechanism. Potential and kinetic energy per atom were also obtained, which showed that bond energy of MC was larger than that of bulk. These architectures are intriguing objects for possible applications of advanced semiconductor nanodevices.

Keywords: Monatomic chain, Breaking process, ZnO nanowires, MD simulations

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I2 - 4

First Principle Study on Wurzite Nano Wire

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We present a first-principle study on the atomic and electronic structure of II-VI wurtzite ZnO like unsaturated Nanowire and examine the depedence of surface stress on Nanowire lateral size and shape. The hexagonal wire size ranging as 10-16.4-23-30-36(A) and triangular wire ranging from 10-13.2-16.5-19.7-23-26.2(A). We investigate the unsaturated dangling bond state in the region of bandgap with varying the wire's diameter. We also calculated the surface formation energy and find that it decrease with increasing the wire diameter and a greater stability (lower surface formation energy) comes with hexagonal wires. Young's moduli calculation and various tensile test have been applied to show the mechanical properties. The electronics properties of these wires (e.g. bandstructure, Density of State, charge transfer via Mulliken population analysis) also exhibit wire's diameter dependence behaviors

Keyword: Wurtzite Nanowires, Density functional based tight binding simulation.

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I2 - 5

A Hierarchical Approach to Study Thermal Behavior of Nano-sized Materials

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We will present a hierarchical approach starting from empirical models and evolutionary algorithms to explore complex energy landscape of nano-sized clusters. As a case study, the structures of protonated water clusters $H^+(H_2O)_n$ is thoroughly investigated. In particular, the distinct configurational isomers of OSS2 empirical potential for n=5-9 are uncovered and archived systematically using an asynchronous genetic algorithm, which are subsequently refined with first-principle calculations. Using OSS2 model, quantitative agreements in the thermal properties between Monte Carlo and harmonic superposition approximation (HSA) highlighted the reliability of the latter approach for study of small to medium-sized protonated water clusters. From the large sets of collected isomers, finite temperature behavior of the clusters can be efficiently examined at first-principle accuracy with the use of HSA. From the results obtained, evidence of structural changes from single-ring to treelike (n=5-7) and multi-ring to single-ring structures (n=7-9) is observed as expected for the empirical model. Finally, the relevance of these findings to recent experimental data is discussed.

O2 - 1

Investigation of Chemical Selectivity and Dimer Ordering in One-dimensional Atomic Wires Grown by Co-deposition of In and Sn on Si(100)-2x1 Surface: A Kinetic Monte Carlo Simulation Study

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The emergence of one-dimensional atomic wires through co-deposition of In and Sn on Si(100)-2x1 surface was investigated by means of Kinetic Monte Carlo (KMC) simulations. An atomistic lattice gas model incorporating key features (such as C-type defect mediated nucleation, anisotropy of the surface with regards to diffusion and reversible atomic wire growth) pertaining to one-dimensional atomic wires growth through co-deposition was developed, and the corresponding Bortz-Kalos-Liebowitz (BKL) algorithm for the model was implemented. Experimental observations on the codeposition study such as the presence of chemical selectivity in which mixed In-Sn dimers are scarce and the lack of dimer ordering among the atomic wires were considered in the simulations.

Through KMC simulations, it was shown that mix In-Sn dimers pair-interaction energy is negatively valued. This gave rise to mixed In-Sn dimers' instability and thus creating chemical selectivity. On the other hand, ordering was not induced for cases where the pair-interaction energy of the defect-bound odd-sized atomic wires is equal, less or greater than the pair-interaction energy of defect-bound combined oddsized atomic wires. Furthermore, dimer ordering was found out to be dependent on the atomic species being deposited since ordering can be induced by making the pair-interaction energy of the defect-bound odd-sized atomic wires to be considerably small. This could possibly explain why ordering cannot be induced in the co-deposition experiment of In and Sn since they give rise to defect-bound odd-sized atomic wires whose activation barrier is considerably large.

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O2 - 2

Some Theoretical Results on Semiconductor Spherical Quantum Dots

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Many of the quantum effects at the nanometric level have been observed in semiconductor spherical quatum dots. To apprehend correctly their properties, the model of *particle-in-a-sphere* model has been proposed in the effective mass approximation. In this work, we have have improved this model with the introduction of pseudo-potential term, which allows analytical computations to be conducted to a very large extent and which turns out to be very successful in improving agreement of numerical results with experimental data. We have obtained in particular, as a function of the quantum dot radius R in precise domains of validity, the quantum dot excitonic energy, the Stark-shift and the Lamb-shift of its corresponding energy levels. Finally the effect of an electromagnetic cavity on spherical quantum dots is considered and its Purcell factor evaluated. This last result suggests the possibility of having a QD-laser emitting in the range of visible light.

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Resonance Scattering of Phonons-Glass-like Thermal Conductivity in Crystalline Solids

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Crystalline inclusion compounds, such as clathrates, often exhibit an unusual thermal transport with glass-like thermal conductivity close to the Debye temperature but a crystal-like temperature dependence at low temperature. Thermal conductivities of a protypical structure I methane clathrate hydrate and related compounds were computed from classical molecular dynamics calculations using the Green-Kubo formalism. Analysis of the heat flux and local energy correlation functions show that both the crystal structure of the clathrate framework and guest-host interactions contribute to thermal transport processes. The glass-like temperature dependence, however, is governed by the guests and the guest-host interactions. The results are relevant to rationalize apparent conflicting observations in related semi-conductor guest-host compounds.

I3 - 2

DFTB - Theory, Parametrization, Recent Applications

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The Density Functional based Tight Binding (DFTB) method is a fast and efficient way to carry out simulations. It has found widespread application in the atomic study of molecules, solids, surfaces and surface reactions. In the talk an overview of the theory behind the method is given, pointing out the differences to usual ab initio density functional methods. Current and future strategies of the parametrisation are discussed, and the applicability of the method is demonstrated with some recent applications on the functionalization of zinc oxide and titanium oxide surfaces.

O3 - 1

First Principles Studies of the Adsorption of Uracil on SWCNTs

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The interaction of single-walled carbon nanotubes (SWCNTs) with nucleic acid bases[1], proteins and peptides like biological molecules have potential applications in the fields of biosensors, drug delivery and nanoelectronics. We have investigated the interaction of nucleic acid base uracil with carbon nanotubes having different chiralities and curvature. First principles plane wave calculations are performed within Density functional theory with the generalized gradient approximation implemented in VASP. We have considered three types of nanotubes namely zigzag CNT (5, 0) & (10, 0), armchair CNT (5, 5) and chiral CNT (5, 2). Uracil ($C_4H_4N_2O_2$) is a pyrimidine derivative, present in the RNA. Uracil is allowed to adsorb non-covalently on the surface of the carbon nanotubes. After optimization, the structure of the uracil remains planar without any significant bending or wrapping but the upper half of the uracil is closer to the CNT compare to the lower half. The physisorption of uracil on the CNT occurs due to the delocalized electrons of the CNT and the lone pair electrons of the uracil. Bader analysis shows the minimum amount of charge transfer between the two entities. Addition of water molecules inside the CNT reduces the binding of the uracil with CNT and the uracil is desorbed from it[2].

System	Binding Energy (eV)	Diameter (Å)	Electronic Property
C(5, 2) + Uracil	0.28	2.47	Metallic
C(5, 5) + Uracil	0.38	3.43	Metallic
C(5, 0) + Uracil	0.36	1.98	Metallic
C(10, 0) + Uracil	0.69	3.97	Semiconductor

On comparison of the above cases, we conclude that the binding energy of the uracil mainly depends on the chirality and the diameter of the carbon nanotubes and increases in the order of C (5, 2) < C (5, 0) < C (5, 5) < C (10, 0). Generally the binding energy of uracil with the zigzag tube is higher than the armchair and chiral tubes due to the direction of the C-C bonds present in the hexagonal ring of the CNT. Also the tube having large diameter (lesser curvature) enhances the binding of the uracil because the flatter surface reduces the mismatch of the adsorbate with CNT.

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O3 - 2

Monte Carlo Simulation of Coarse-grained Model of Large Polymer Mixtures with Different Chain Topology

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Polyethylene oxide (PEO) with the structure of (CH_3O-[CH_2-CH_2-O]nCH_3) was choosen to illustrate the method of this multiscale modeling. The effect of different chain topology i.e. linear and cylic chain on structure and dynamic properties of polymer mixture. Cyclic polymers, which lack chain ends, are scientifically intriguing, since they defy a simple description in terms of the tube model which has been used rather successfully to describe the properties of linear and branched polymers. A novel lattice Monte Carlo simulation of coarse-grained polymer model was developed and employed to study the statics and dynamics of blends of cyclic and linear poly(ethylene oxide), PEO, blends of varying composition. Local intrachain interactions are from the modified rotational isomeric state model and non-bonded interactions are from a discretized form of the Lennard-Jones (LJ) potential energy function. The simulations were performed at 373 K for the chain length from 50 to 200 repeating units. The relative size of linear/cyclic is $<Rg2>$linear/$<Rg2>$ring ~ 2 which is consistent with the theortetical prediction. The diffusion coefficient of cyclic chain is higherthan linear polymer at high molecular weight. The lower diffusion coefficient of the smaller cyclic polymer was attributed to the high local density within molecular volume. For the binary blends, the sizes of linear and cyclic chains   are relatively unchanged at all composition. As the linear fraction increases, the diffusivities of both cyclic (DC) and linear (DL) decrease. In comparison, DC drops more than DL especially at longer chain length. The decrease in diffusivities is most pronounced at small concentration of linear fraction. Therefore, dynamics of such blends are extraordinarily sensitive to the concentration of linear polymers, as also demonstrated by the linear viscoelastic and self-diffusion studies.

O3 - 3

Adsorption of Polycyclic Aromatic Hydrocarbons on Graphite Surfaces

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Polycyclic aromatic hydrocarbons (PAHs) are the molecules which consist of fused aromatic rings, and do not contain heteroatoms and substituents. They are emitted into the atmosphere as byproducts from the burning of fuel and coal, or from other combustion sources. Once emitted into the atmosphere, PAH's can exist either in the gas phase or they can be adsorbed onto particle surfaces, such as soot and charcoal. They are one of the most widespread pollutants and are known carcinogens and mutagens for human beings. Unfortunately, they are easily inhaled by humans when absorbed on the surfaces of airborne soot particles, produced by the incomplete combustion of carbonaceous fuels. Studying the mechanism of adsorption of PAH's onto soot surfaces is therefore an important problem. However, the number of studies on the interaction mechanism between PAH's and soot surfaces is limited. We comment that using computational methods, such as ab initio or molecular dynamics simulation, is usually not feasible owing to the large molecules involved. In this work, we exploit a continuous atomistic approximation together with the Lennard-Jones potential in order to investigate this problem. Because a soot particle is composed by many graphite layers, the interaction between a PAH and a soot particle can be modeled as the interaction between a PAH and a graphene sheet, which is the model already adopted by some other authors. Due to the large variation in the geometry of PAH's, we choose in particular coronene ($C_{24}H_{12}$) as the typical PAH for modelling the interaction between a PAH and a graphene sheet. That is, we consider the structure and the interaction energy of the system of cororene and gaphene sheet. One of the major results derived here is an analytical expression for the interaction energy.

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Accelerated Molecular Dynamics Methods

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A significant problem in the atomistic simulation of materials, as well as in other areas of chemistry and physics where atomistic simulations are used, is that molecular dynamics simulations are limited to nanoseconds, while important reactions and diffusive events often occur on time scales of microseconds and longer. Although rate constants for these infrequent events can be computed directly using transition state theory (with dynamical corrections, if desired, to give exact rates), this requires first knowing the transition state. Often, however, we cannot even guess what events will occur. For example, in vapor-deposited metallic surface growth, surprisingly complicated exchange events are pervasive. In this talk, I will discuss the accelerated molecular dynamics approach, which we have been developing over the last decade, for treating these complex infrequent-event systems. The idea is to directly accelerate the dynamics to achieve longer times without prior knowledge of the available reaction paths. In some cases, we can achieve time scales with these methods that are many orders of magnitude beyond what is accessible to molecular dynamics. I will give an introduction to the three main methods in this class, hyperdynamics, parallel-replica dynamics and temperature accelerated dynamics, and discuss their relative merits. I will present some illustrative and recent applications to materials problems, such as metallic surface growth, grain boundary slip under applied shear, radiation damage annealing in MgO, and tensile tests on metallic nanowires. I will also discuss some of the ongoing challenges in making these methods as powerful and generally useful as possible.

I4 - 2

First-Principles Calculation of Microstructural Process in Alloys

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Recently, first-principles calculations have been actively performed for clarifying and predicting the phase stability and phase equilibria for a given alloy system. It has been demonstrated that the combination of electronic structure total energy calculation and statistical mechanics method such as Monte Carlo simulation and Cluster Variation Method is a powerful and reliable tool. By further incorporating Phase Field Method, one may perform first-principle calculation of microstructural evolution of an alloy. In order to attempt such microstructural calculation from the first-principles, it is necessary to achieve coarse graining operation. The author has been developing a procedure based on the atomistic description of Cluster Variation Method which is able to incorporate wide range of cluster correlations. In the present talk, first-principles calculations performed on Fe-based alloys are reviewed and the importance of local lattice relaxation is pointed out.

I4 - 3

Quantum Simulation of Materials at Micron Scales and Beyond

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We present a multiscale modeling approach that can simulate multimillion atoms effectively via density functional theory. The method is based on the framework of the quasicontinuum (QC) approach with the density-functional theory (DFT) as its sole energetics formulation. The local QC part is formulated by the Cauchy-Born hypothesis with DFT calculations for strain energy and stress. The nonlocal QC part is treated by a DFT-based embedding approach, which couples DFT nonlocal atoms to local region atoms. The method—QCDFT—is applied to a nanoindentation study of an Al thin film, and the results are compared to a conventional QC approach. The results suggest that QCDFT represents a new direction for the quantum simulation of materials at length scales that are relevant to experiments. If time allows, an application of QCDFT to magnetism-induced dislocation mobility in NiAl alloys will also be presented.

I4 - 4

Analytic Bond-Order Potentials Including Magnetism

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We developed an analytic interatomic bond-order potential (BOP) that depends explicitly on the valence of the transition metal element and describes the structural trend from hcp to bcc to hcp to fcc across the non-magnetic 4d and 5d transition metal series. In this talk we show that the potential may be extended to include magnetic contributions to the binding energy. The resulting magnetic potential displays the experimental trend from anti-ferromagnetic order to ferromagentic order across the 3d transition metal series. For iron, the potential correctly predicts a large magnetic energy for the alpha phase whereas the close-packed gamma and epsilon phases exhibit only a small magnetic contribution to the binding energy.

O4 - 1

A Renormalization Approach to ac Conductivity in Quasicrystals

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Based on the Kubo-Greenwood formula, a renormalization plus convolution method [1] is developed to investigate the frequency-dependent electrical conductivity of quasicrystals. This method combines the convolution theorem with the real-space renormalization technique, being able to address multidimensional quasiperiodic systems in a non-perturbative way. In this work, we report an analytical evaluation of the Kubo-Greenwood formula for the ballistic *ac* conductivity in periodic chains. For Fibonacci chains with two semi-infinite periodic leads, the electrical conductivity is calculated by using the renormalization method and the results show that at several frequencies their conductivities are greater than the ballistic ones. This fact could be due to the resonant scattering process in quasiperiodic systems. Analysis of this behavior in systems with mirror symmetry [2] and in multidimensional quasiperiodic lattices is also presented.

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I5 - 1

High-κ Oxides and Interfaces: Materials Design from First-principles

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The continued downscaling of semiconductor devices into the "nano" era requires the replacement of silicon dioxide (SiO_2) gate dielectric by high dielectric constant (high-κ) materials, as well as polycrystalline Si (poly-Si) gate electrodes by metal gates. However, many issues associated with high-κ oxides remain to be solved. Recent developments in high-κ dielectric oxides in complementary metal-oxide semiconductor (CMOS) devices allow development of MOS devices based on high performance Ge. First-principles method based on density functional theory was used to investigate the properties of high-κ oxides and their interfaces with semiconductors and metal gates. Effects of interfacial structures of semiconductor and high-κ oxide, high-κ oxide and metal gate, on their physical properties were investigated. Variation of work function with composition of metal alloy was also investigated for tuning of Shottky barrier heights. We also propose Ge_3N_4 as a passivation layer to avoid formation of Ge oxide which has poor thermodynamic and electronic properties for Ge-based MOS.

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I5 - 2

Structure Property Correlation forMetal Oxide Structures Designed for Nano-Catalysis with Order N Plane Wave Calculation.

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Transition metal (TM) oxides constitute an important class of inorganic solids exhibiting a very wide variety of structures and electronic and magnetic properties that are due to the nature of the outer d states. They are of great importance for a number of a technological applications such as heterogeneous catalysis, corrosion-protective coating of metals and microelectronic devices. Point defects in TM oxides such as vacancies and interstitials account for the transport properties of ionic solids. In addition, an important issue in TM oxide-based heterogeneous catalysis is the role of surface defects in determining the activity and selectivity of the catalyst. The existence of reduced surface centers — and hence the presence of neutral oxygen vacancies — is sometimes necessary for any activity. [1,2.] We will use the code ONETEP (Order-N Electronic Total Energy Package), which is a parallel density-functional theory code for large-scale first-principles quantum-mechanical calculations developed by Skylaris et al [3]. The distinctive features of ONETEP are linear-scaling in both computational effort and resources, obtained by making well-controlled approximations which enable simulations to be performed with plane-wave accuracy. The computational machinery behind this approach is novel as it makes use of the psinc basis set. In the present study the ONETEP background the oxygen vacancy scenarios will be described for Al_2O_3, GaO_2, and In_2O_3.

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O5 - 1

Investigation on Spin-Flipping near Surface Layers of Perovskite $CaMnO_3$

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The electronic structure of a single-crystal thin film $CaMnO_3$, with Mn-O surfaces were investigated in the framework of density functional theory (DFT) method using generalized gradient approximation (GGA) exchange-correlation function. The results show a splitting among the surface, sub-surface, and bulk e_g bands. There is also a redistribution of charge and spin densities from the film centre to surfaces. We suggest that the missing apical oxygen atoms of $Mn-O_6$ octahedrons at the surface reduced the antiferromagnetic super-exchange interaction in the bulk $CaMnO_3$ and enabled the ferromagnetic double-exchange interaction at the surface and sub-surface layers. Hopping integrals of t_{2g} electrons exhibit a noticeable increase in the direction perpendicular to the film surface.

O5 - 2

Carbon and Silicon Impurities in GaAs$_{1-x}$N$_x$

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Based on first-principles density functional calculations, we investigated the behavior of electrically active impurities incorporated in dilute GaAsN alloys. Contrary to their behavior in the parent compound GaAs, we found that C and Si are not simple substitutional impurities that replace either Ga or As in dilute GaAsN alloys. Instead, they are found to bind to N and form diatomic molecules substituting on the anion sites: $(CN)_{As}$ and $(SiN)_{As}$. The $(CN)_{As}$ acts as a donor under *p*-type conditions but acts as an acceptor under *n*-type conditions [Phys. Rev. B **77**, 195209 (2008)]. The $(SiN)_{As}$ is found to be a deep-acceptor. We used the $(SiN)_{As}$ formation to explain the band gap recovery and donor compensation (mutual passivation effect) that are observed in Si-doped GaAs$_{1-x}$N$_x$ alloys [Phys. Rev. Lett. 100, 045505 (2008)]. Although both C and Si are group IV, the geometries of $(CN)_{As}$ and $(SiN)_{As}$ are quite different. The $(CN)_{As}$ has a geometry of a diatomic molecule CN substituting on an As site, whereas the $(SiN)_{As}$ has a geometry of a traditional split-interstitial defect. As a result, the electronic properties of the two defects are largely different. The vibrational frequencies of the two complexes are also calculated and discussed in detail.

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Modeling and Simulation to Enterprise Solution:
A Passage through Platform and Tools

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This talk will cover our new vision towards expanding modeling to an enterprise solution to a new technology in hand. Pipeline Pilot Enterprise Server (PPES) is a powerful client-server platform that streamlines the integration and analysis of the vast quantities of data flooding research informatics. Designed to meet the critical requirements of the informatics professional, PPES provides an agile development environment, fast and secure deployment, minimal maintenance costs, and application extensibility. With PPES, you can maximize the utility of your information resources through enterprise-scale data flow control, extensive data mining capabilities, and effective reporting. PPES and its graphical orchestration environment, Pipeline Pilot, allow you to graphically compose data processing networks, known as protocols, using hundreds of different configurable components for operations such as data retrieval, manipulation, computational filtering, and display. Material studio being the versatile tool from us for molecular modeling has now have a Materials Component Collection, which is a set of functionality that allows you to access and utilize Materials Studio's premier modeling capabilities within the Pipeline Pilot™ data pipelining environment. Pipeline Pilot captures reoccurring workflows in computational research applications. It integrates a variety of applications, streamlining their execution and facilitating their analysis.

K6 - 1

Transport Properties and Bonding Characteristics of Nanostructured Materials

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In this talk, we report two different computational studies on nanostructured materials. One is the electron transport pattern on defected carbon nanotubes and the other is the analysis of the bonding mechanism of hydrogen on metal atoms for the purpose of hydrogen storage.

When carbon nanotubes have Stone-Wales defects or atomic vacancies, the electron transport exhibits particular flow patterns as a function of incoming electron energy. We analyze the electron flow pattern near the defect and find that loop currents occur which in turn generate magnetic fields around the defect. Different defects show different current patterns, thereby helping identify the type of the defects in the carbon nanotube.

We also report some recent computational results in the study of the hydrogen binding mechanism on metal atoms. Hydrogen molecules are stored by being attached to certain metal atoms which are bound to a backbone matrix consisting of carbon-based nanomaterials or MOFs. Transition metal atoms can bind hydrogen molecules through the simultaneous electron donation and back-donation, which is usually called a ``Kubas interaction''. This interaction is extremely useful for the room-temperature hydrogen storage applications and provides the optimal H_2 binding energy of 0.3 eV (including the zero-point energy correction). We show that there exists competition between the exchange field and the ligand(crystal) field splitting, and the high storage capacity is achievable only when the ligand field dominates. Other metal atoms such as calcium may bind hydrogen molecules through the dipole interaction induced by the ionization of the metal atoms.

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Pt Nanoclusters on Carbon Nanotube Support

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The catalysis plays an innovative role in developing new technologies and catalyst design has become a big issue in industrialization. The combination of nanoclusters and the carbon nanotube supports are strongly proposed as a solution for superior heterogeneous catalysis. Recently we succeeded in establishing a new concept, based on a fundamental bottom-up approach, for synthesizing highly dispersed and size-controlled nanoparticles on carbon nanotube supports.[1] From a theoretical viewpoint, it is suggested that the mixing of the wave functions of the nanotubes and those of the atoms and nanoclusters determine the geometric, electronic, and therefore catalytic properties of the adsorbed clusters.

In this paper, we report our studies on the interplay between single-wall carbon nanotube (SWNT) supports and adsorbed Pt clusters atoms using the first-principles density functional theory (DFT). The cluster formation process, stabilities, electronic structures, and gas adsorption properties of Pt clusters on SWNT will be discussed from the viewpoint of catalyst design.[2,3]

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I6 - 2

Phase Behavior Predictions of Various Methane and Hydrogen Clathrate Hydrates

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The theory developed in our earlier papers [1,2] is extended to predict the thermodynamic functions of binary hydrates of cubic structure I (sI) and II (sII) by accounting for the possibility of multiple filling of small and large cavities by hydrogen molecules. The method is applied to the thermodynamic properties of H_2-CH_4 hydrates, considering both sI and sII, with two types of guest molecules, CH_4 and H_2, and two types of cavities, of which the smaller can hold at most two hydrogen molecules and the larger can accommodate up to four hydrogen molecules while methane molecules can singly fill large and small cages.

The thermodynamic conditions of hydrate formation at equilibrium of guest gas phase with ice are determined. The dependencies of formation pressure and composition of the formed binary H_2-CH_4 hydrates on methane concentration in the gas phase are found. It has been shown that at divariant equilibrium 'gas phase – gas hydrate' with increasing pressure the filling of large cavities by hydrogen proceeds gradually from single to four-fold cluster filling preserving stability of the hydrates.

The pressure of monovariant equilibrium 'ice Ih – gas phase – binary sI hydrate' with increasing methane concentration in the gas phase lowers in comparison with the pressure of pure hydrogen hydrate formation. For the mixed hydrogen-methane hydrates it was demonstrated that thermodynamic stability depends on the filling degree of small cavities by methane molecules and stability area shifts to lower pressure with increasing filling. Regions of stability of hydrate phases sI and sII in T-P plane were determined.

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I6 - 3

Ab Initio Study of Graphene Nanostructures: Metal Binding and Hydrogen Adsorption

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In recent years, we have observed fast growing interest in carbon-based nano-materials such as carbon nanotubes and graphenes. These materials exhibit very intriguing physical properties such as geometry-dependent electronic structures and quantum Hall effects, and have great potentials for application to nanoelectronic devices and energy storage materials. In this presentation, we discuss the binding of alkaline and alkaline earth metals to graphenes and then the adsorption of hydrogen molecules on these metals using the ab initio pseudopotential methods. First we present the binding characteristics of these metals in graphene nanoribbons and show how such metal binding can distinguish the edge geometry of the ribbons[1]. Next we discuss the hydrogen molecular adsorption on the metal atoms, particularly Ca atoms, bound to graphenes and graphene superstructures[2,3]. We particularly focus on the adsorption mechanism of hydrogen molecules on Ca atoms. Implication to the research of hydrogen storage materials is also discussed.

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I6 - 4

Hydrogen-Related Defects and the Role of Metal Additives in the Kinetics of Complex Hydrides

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Complex hydrides such as $LiBH_4$ and $Li_4BN_3H_{10}$ (synthesized from $LiBH_4/LiNH_2$ mixtures) have been identified as promising hydrogen storage materials. These hydrides, however, exhibit limitations in kinetics and reversibility.[1,2] Accurate modeling of hydrogen kinetics in these systems is therefore essential for developing a more complete understanding of the processes that limit the performance of storage materials, and ultimately, for the development of improved materials systems.

In this talk, we present our first-principles studies for $LiBH_4$ and $Li_4BN_3H_{10}$ with a focus on the processes that govern the addition, removal, and diffusion of individual atoms, and the effects of metal additives on such processes. Hydrogen is treated as an "impurity" in the materials, and hydrogen-related defects such as vacancies and interstitials are investigated. One of the key findings is that hydrogen-related defects are positively or negatively charged and their formation energies are therefore Fermi-level dependent. From a materials design perspective, this opens up an opportunity for us to tailor the formation energies (hence the concentrations) of hydrogen-related defects by shifting the Fermi level, as found to be effective in $NaAlH_4$.[3] This can be accomplished by adding appropriate electrically active impurities into the systems.

We have identified a number of transition metal impurities that are effective in shifting the Fermi level of $LiBH_4$ and $Li_4BN_3H_{10}$. A comparison of our calculations with experimental results for the effects of addition of impurities on the kinetics of $LiBH_4$ and $Li_4BN_3H_{10}$ shows qualitative agreement, providing validation for our interpretation of the results and for our proposed model for enhancement of kinetics.

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<div align="right">**O6 - 1**</div>

Single Walled Carbon Nanotubes Coated with Hydrides as Hydrogen Storage Medium

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Among several materials, the carbon based nanostructures are considered as potential candidates for hydrogen storage. We have investigated the hydrogen storage in single walled carbon nanotubes (SWCNTs) using density functional theory as implemented in VASP, a well known plane wave code. Fast and effective kinetics during H_2 adsorption/desorption can be achieved only if H_2 is adsorbed molecularly. The interaction between H_2 and bare SWCNTs is weak and it can't remain attached at ambient conditions. As an alternative measure these SWCNTs are functionalized or doped with metal atoms and then hydrogenated. First these doped metal atoms form their respective hydrides and further H_2 molecules are adsorbed. We, in our study [1, 2], straight away functionalized the SWCNT with hydrides and then hydrogenate them. We considered hydrides like AlH_3, BH_3, NH_3, LiH and NiH_2. All the adsorbates (hydrides) are chemisorbed exohedrally. Among all the systems studied, (CNT+BH_3) is found to satisfy the standards set for an ideal hydrogen storage medium. Though the remaining studied systems have considerable storage capacities, they are not favored because of the weak binding of H_2. The SWCNT functionalized with the light weight, hydrogen rich and electron deficient BH_3 has appreciable hydrogen storage capacity of 11.5 wt% with the binding energy 0.24 eV/H_2. We extended our study to other SWCNTs, (10, 0) and (10, 10) coated with BH_3. The systems (CNT (10, 0)+3BH_3) and (CNT (10, 10)+2BH_3) have the binding energy per H_2 in the range recommended for an ideal hydrogen storage medium. The high storage capacity of (CNT (5, 5)+BH_3) is due to its large curvature when compared to other tubes.

From our present study, we conclude that higher storage capacity at ambient conditions can be achieved by coating light weight hydrides like BH_3 on the SWCNT framework. Also the curvature of the tube plays an important role in enhancing the storage capacity of SWCNTs.

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Stress Dependence of the Peierls Barrier in BCC Metals

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The Peierls barrier of a dislocation is defined as the dependence of the energy of a dislocation on its position along a path between two crystallographically equivalent locations of the dislocation. The Peierls stress is then the stress necessary to surmount this barrier at 0 K and it is related to the maximum derivative of the barrier with respect to the dislocation position. In majority of studies the Peierls barrier has been considered as fixed, determined by the crystal structure and corresponding interatomic interactions in a given material. This implies that the same should apply to the Peierls stress. Nonetheless, recent atomistic studies of ½<111> screw dislocations in transition BCC metals have shown that their Peierls stress is strongly dependent on the applied stress tensor, in particular on shear stresses parallel and perpendicular to the Burgers vector. This implies that the Peierls barrier also depends on the applied stress tensor in asimilar way. However, while the Peierls stress is readily obtained in atomistic calculations, the corresponding Peierls barrier cannot be directly determined. In this paper we show how the stress-dependent Peierls barrier can be ascertained from the atomistic data of the stress dependence of the Peierls stress. This is done by introducing the Peierls potential that is a function of two coordinates that represent the position of the intersection of the dislocation line with the {111} plane perpendicular to the corresponding <111> slip direction. The Peierls barrier is then sought as the lowest energy path over the two-dimensional Peierls potential. This potential that is then self-consistently adjusted such as to reproduce the stress-dependence of the Peierls stress. This procedure is tested using the nudge-elastic-band model to determine the Peierls barrier in a given material without introducing first the Peierls potential. Finally, it is shown that when employing this barrier in the model of the formation of kink-pairs at finite temperatures the observed orientation dependences of the yield stress in molybdenum are well reproduced.

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Bending Analysis of Three-Phase Polymer Composite Plates Reinforced by Glass Fibers and Titanium Oxide Particles

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Mechanical and physical properties of composite materials are usually increased by reinforced particles and fibers. This report presents a method for determining engineering coefficients of three-phase composite materials. Basing these coefficients, bending analysis is carried for three-phase polymer plates composed of reinforced glass fibers and titanium oxide (TiO2) particles, taking into account two important effects are that interaction between titanium oxide particles and matrix materials and shear deformation. Analytical relations of material properties and plate deflection are obtained as functions of properties and volume fractions of constituent materials. These explicit expressions play a important role in design of composite materials as well as optimal behavior of three-phase composite plates.

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A Hybrid Atomistic Simulation for Investigating Spatial Distribution of Alloying Elements and Their Effects on Metallic Materials Properties

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Atomistic simulations such as ab-initio calculations, molecular statics (MS), molecular dynamics (MD) and Monte Carlo (MC) simulations are used to understand the materials behavior in more fundamental level, e.g. the atomic level. Especially, the MD simulation has been widely used to investigate the dynamic behavior of materials during phase transformations or deformations. However, the effect of alloying elements on the transformation or deformation behavior of materials cannot be examined correctly by the MD simulation because of not being able to allow the probable diffusion of alloying elements toward the defects (grain boundaries, crack tip, etc.) during the short simulation time (order of nano-seconds). Allowing modification of atomic positions by inserting an MC routine between MD runs can be easily thought as a solution to overcome the above-mentioned limitation of MD simulations. The MC+MD hybrid simulation can realize the strong interaction between solute atoms and lattice defects, and enable the investigation of the effects of alloying elements on materials properties. However, in the case of interstitial alloys, the MC modification of atomic positions is hardly realized because of the severe local lattice strain around interstitial atoms.

In the present study, we resolve the problem in the MC simulation for interstitial alloys by introducing a molecular statics (MS) relaxation process that allows lattice relaxation just after individual MC attempts. This MS+MC hybrid simulation technique is applied to compute stacking fault energy (SFE) of fcc Fe-N alloys, considering the probable segragation of nitrogen atoms on the stacking fault region. The MS+MC+MD hybrid simulation technique is also applied to investigate the effects of interstitial element atoms, C, N and H on the fracture or deformation behavior of bcc Fe. The non-monotonic effect of nitrogen content on the SFE of fcc Fe and the similarity or difference in the effects of interstitial elements on the mechanical behavior of bcc Fe, which could be investigated only by using the present hybrid simulation, will be presented.

O7 - 1

A Molecular Dynamics Study of the Effect of CNT-Al Bond Strength on the Mechanical Properties of CNT-reinforced Al Composite

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Mechanical properties of CNT-Al nanocomposite are strongly dependent on the bond strength between CNT wall and Al matrix. Recently, aluminum carbide phase between CNTs and matrix were observed by a transmission electron microscope and supposed to bring out the reinforcement by the excellent mechanical properties of CNTs. However, it is required to investigate quantitatively the effect of bond strength between the CNT wall and the Al matrix to understand the mechanism of the reinforcement and to answer how much the bond strength should increase for developing the CNT-Al nanocomposite with effective reinforcement by the CNTs. In this work, classical molecular dynamics method is employed to investigate the mechanical properties of CNT-Al nanocomposite. We prepared an Al single crystal tensile specimen containing a single-wall and open-end carbon nanotube aligned along the tensile axis. The bond strength between the defects on the CNT wall and the Al matrix atoms was artificially modified by changing the parameters of 12/6 Lennard-Jones potential. We found that the CNTs cannot reinforce but rather weaken the CNT-Al nanocomposite unless the interactions between CNT-Al become at least 10 times stronger than the well known Van de Waals interaction of C-Al bond, 0.038 eV. Our results also revealed that the bonds between the open ends of CNTs and Al is much more important than those between the defects of CNT walls and the matrix. Details of the deformation behavior of the CNT-Al nanocomposite will be also presented in the atomic scale.

I8 - 1

Effect of Impurities on Vacancy Behaviour in Fe-Based Alloys from First Principles

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Iron-based alloys play central roles in metallurgical and nuclear technology, in particular, FeCr-based steels are nowadays strong candidates as structural materials for new generation fission and future fusion reactors. Although their mechanical properties have been extensively investigated, relatively little is known about the atomistic origin of their macroscopic behaviour, First principles calculations provide such information, which may not be directly accessible by experiments. The main objective of our work is to reconcile theoretical and experimental results by Density Functional Theory (DFT) calculations. First, to validate our DFT approach, we have performed a systematic study of effects of exchange-correlation functionals, pseudopotentials (norm-conserving, ultrasoft, PAW) and basis sets (plane-wave vs. localized functions) on various collinear and non-collinear structural-magnetic phases of Fe and Cr. We have then focused our study on intrinsic defects, and determined the influence of carbon --one of essential alloying elements in steels-- on the decrease of vacancy diffusivity is quantitatively predicted.

In addition to the self-defects, large amount of He can also been created by transmutation under fast neutron irradiation. Although mechanisms of He diffusion and clustering with vacancies in pure iron are rather well established, how the presence of solutes such as C or Cr may modify these mechanisms remain to be understood. Our results provide a quantitative prediction that C tend to enhance the mobility of He while Cr in a FeCr solid solution may rather decrease the diffusivity of He. These effects of impurities are expected to change significantly the microstructure and mechanical properties of steels induced by He segregation

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Monte Carlo Models for FeCr Alloys: Prototype Materials for Fusion Applications

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Developing materials capable of retaining their engineering properties over extended periods of time under irradiation at high temperature is one of the key challenges for fusion materials science and technology. One of the classes of materials currently under investigation are ferritic-martensitic steels containing close to 10% percent Cr. Developing tools for modelling these steels, and binary FeCr alloys, is one of the objectives for the European fusion programme.

In this presentation we describe two Monte Carlo methods for modelling phase stability of iron and FeCr binary alloys. The first, based on the cluster expansion Hamiltonian, describes effects of configurational disorder in the alloy on thermodynamic properties [1]. The second, recently proposed, "magnetic" cluster expansion (MCE) method, extends the treatment to magnetic degrees of freedom by including magnetic moments of individual atoms as variables [2]. MCE has a unique capability for modeling both structural and magnetic properties of the alloy in a broad range of compositions ranging from pure ferromagnetic Fe to antiferromagnetic Cr. The comparison of the free energies for bcc and fcc Fe, which can be carried out within MCE, offers a way of predicting the α-γ and γ-δ transitions, using only the zero Kelvin *ab-initio* data as input. This work was funded by UK EPSRC and EURATOM.

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I8 - 3

On the Electronic Structure of Some Strongly Correlated Electron Systems

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Electronic band structure (EBS) issues in condensed matter physics have been widely studied for years in order to provide important insights into the properties of matter, since the calculations may predict properties without reference to experiments or may frequently help in understanding how the matter behaves. In strongly correlated electron systems (SCES), where interactions between electrons are very important, new phenomena including heavy-fermion, quantum critical points, non-Fermi liquid behaviour, unconventional superconductivity, and so on, were often observed. For SCES, the most successful electronic structure calculation methods in current use are those of density functional theory. Here, we give a short review on electronic structures of some SCES, namely superconducting Mo_3Sb_7, $ThPt_4Ge_{12}$, ferromagnetic $U_2ScB_6C_3$ and ferrimagnetic Ce_5CuBi_3, obtained with the full-potential linearized-augmented-plane-wave and full-potential local-orbital methods, using the WIEN2k [1] and FPLO [2] packages, respectively. The EBS calculations for Mo_3Sb_7 [3] have indicated that the density of states near the Fermi level is formed by the Mo-4d orbitals and there is negligible overlap between the Mo-4d and Sb-sp orbitals, being consistent with the two-gap feature. Moreover, the Fermi surface calculations have revealed the coexistence of the heavier and lighter bands. In $ThPt_4Ge_{12}$, multiband conduction band and a strong anisotropy can be inferred from the EBS calculations [4]. The EBS calculations for $U_2ScB_6C_3$ [5] have confirmed its metallic and magnetic order properties. In this compound, magnetism is attributed to the polarized $5f^3$-states and a strong hybridization with the spd-states of the B/C atoms involved. In Ce_5CuBi_3, the EBS calculations [6] not only have supported ferrimagnetic ground state but also suggested an inequivalent contribution of Ce atoms at different positions to the density of states.

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First Principles Modeling of Stability Mechanism of Nonstoichiometric Uranium Dioxide

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Uranium dioxide is a widely used fuel materials in nuclear reactor, its performance is quite related to the defects behavior under irradiation which arises the deviation from stoichiometric compounds. To reveal the stability mechanism of nonstoichiometric UO_{2+x}, first-principles calculations has been performed by PAW-LSDA+U method for various complex defects clusters of oxygen atoms [1,2,3]. Calculations revealed that the structural stability of the cuboctahadral embedded into the crystal UO_2 is inherited from U_6O_{12} molecular cluster whereas the energy gain through one additional oxygen's occupying its center makes the cluster win out the competition with point oxygen interstitials and the split quadinterstitial clusters [4] at the ground state. This picture clarified the ambiguousness remaining for long in structure of nonstoichiometric UO_{2+x}. By incorporating the temperature effect, a pseudo phase diagram of temperature and the oxygen concentration has been constructed, and a new physical model of thermodynamic competition between cuboctahadral and point oxygen interstitials is proposed. It shows that at low temperature, the cuboctahadral clusters dominate the stability, whereas at the elevated temperature, point interstitial is more favorite over the cuboctahedral clusters.

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First Principles Design of DMS and DMO by Transition Metal Codoping

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Designing a ferromagnetic semiconductor (DMS) or an oxide (DMO) with a high Curie temperature (T_c above room temperature) is a challenge, and transition metal (TM) doped ZnO and GaN are considered to be the most promising candidates [1]. There are controversies about the nature and origin of the magnetic coupling, the mechanism involved and the possible dependence on various extrinsic factors such as defects, vacancies and cluster formation. First-principles LSDA investigation have been carried out on doped as well as codoped ZnO [2,3] and GaN [4] systems to understand the nature of magnetic interaction. The roles of cation vacancies in stabilizing the long range ferromagnetic order have been emphasized. Codoping either with magnetic materials or with cations and anions with one more or one less valence electron, affects the localized gap states of the TM-dopants that are supposedly responsible for the ferromagnetic half-metallic behaviour. There is a competition between ferromagnetic and antiferromagnetic (or ferrimagnetic in case of two different types of TM dopants) interactions, leading to RKKY type exchange mechanism.

In this talk, we shall present the results of our first principles density functional calculations on codoped ZnO system, in which presence of Zn-vacancy near the TM-dopant pair is found to favor a ferromagnetic ground state within LSDA+U [3]. This is in contrast to the case of (Mn,Cr) codopeed GaN in which ferromagnetism is stabilized via double exchange mechanism between the dopant d-bands. Magnetism in the later system is believed to be carrier mediated and codoping makes it less sensitive to impurity or clustering. [4]

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I9 - 2

Monte Carlo Study of the Spin Transport in Magnetic Materials

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The resistivity in magnetic materials has been theoretically shown to depend on the spin-spin correlation function which in turn depends on the magnetic-field, the density of conduction electron, the magnetic ordering stability, etc. The purpose of this talk is i) to recall some important works which have contributed to the understanding of the resistivity behavior of magnetic systems, and ii) to show by extensive Monte Carlo (MC) simulation the resistivity of the spin current from low-T ordered phase to high-T paramagnetic phase in a ferromagnetic film. We take into account the interaction between the itinerant spins and the localized lattice spins as well as the interaction between itinerant spins themselves. We show that the resisiivity undergoes an anomalous behavior at the magnetic phase transition in agreement with previous theories. The origin of the resistivity peak near the phase transition in ferromagtnets is shown to stem from the existence of magnetic domains in the critical region. We analyze effects of film thickness, surface interactions and different kinds of impurities on the spin resistivity across the critical region. We also solve the Boltzmann's equation in the relaxation-time approximation using numerical data obtained by our simulations. The result is in a good agreement with our MC results. Resistivity in antiferromagnets is briefly shown and comparison with experiments is discussed.

Magnetization Reversal in the Quantum Limit

F. Marsiglio*

Magnetization reversal is a well-studied process with applicability to memory performance in computer hard-drives. More recent work iin this area has focussed on the reversal process instigated by an applied spin current, where, at a minimum,a quantum description of the current is required. We describe some recent work (cond-mat/0905.4708) in which both the spin current and the stationary spins are treated through quantum mechanics. New physics (beyond the semi-classical results) that emerges from this treatment will be discussed.

* work done in collaboration with F. Dogan, L. Covaci, and W. Kim

I9 - 4

Fascinating World of Double Perovskites

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Double perovskite compounds with general formula $ABB'O_6$, have attracted a lot of attention recently due to a variety of properties exhibited by them. In this talk, we will report our recent study on a specific double-perovskite compound, namely the magneto-capacitive compound, La_2NiMnO_6. Our work in the context of La_2NiMnO_6, uncovers the existence of large spin-phonon coupling identifying its super-exchange driven microscopic origin being responsible for the magneto-capacitive behavior observed experimentally [1,2]

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O9 - 1

Spin Orbit Contributions to the Magnetism of Small Iron Clusters

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We present density functional based tight-binding calculations on the magnetic properties of small iron clusters. Extending our earlier studies,[1] energetics and stabilities are presented for collinear and non-collinear spin configurations including the effects of spin-orbit coupling. We discuss a new approach for the L.S contributions to the energy and potential using Mulliken occupation matrices. The geometries presented are obtained via global optimization.

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O9 - 2

New Type of Half-metallic Antiferromagnets and their Applications to GMR and TMR Devices

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A new type of fully spin-compensated ferrimagnetic half-metals (so-called half-metallic antiferromagnets) is designed by use of first-principles KKR-CPA-LDA calculations. These materials consist of two transition metals with total d valence electron number being 10 and chalcogenides or pnictides. Thus designed intermetallic compounds $(AB)X_2$ show significant features of half-metallic antiferromagnets. Moreover, they are chemically stable and the magnetic transition temperature is relatively high, e.g., 817K for $(FeCr)Se_2$.

To demonstrate their applicability to spintronics devices, we calculate the DC conductivity of these new half-metallic systems as well as the superstructure simulating GMR/TMR structures composed of these systems using Kubo-Greenwood formula combined with the first-principles KKR-CPA-LDA method. The results show that those systems function as spintronics materials if used as components of GMR/TMR and magnetic random access memory cells.

Valence Bond Monte Carlo Study of Random Singlet Phases

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In valence-bond Monte Carlo (VBMC) simulations the ground state of a quantum spin system is sampled directly from the valence-bond (VB) basis – a useful basis for visualizing the properties of singlet ground states [1]. For example, the ground state of the uniform AFM spin-1/2 Heisenberg chain is characterized by strongly fluctuating bonds with power-law length distribution, while in the random-singlet phase (RSP) of a *random* Heisenberg chain these bonds lock into a particular VB state on long length scales [2]. In this talk I present our recent results showing that VBMC can be used to directly probe the formation of the RSP by calculating both the average number of bonds n_L leaving a block of L spins (a quantity known as the VB entanglement entropy [3]) and its *fluctuation*, $\sigma_L^2 = \left\langle \left\langle n_L^2 \right\rangle - \left\langle n_L \right\rangle^2 \right\rangle$. For the uniform chain both n_L and σ_L^2 have been calculated exactly [4] and shown to grow logarithmically with L, signaling the presence of long bonds and strong fluctuations. For random chains n_L also grows logarithmically with L [5], but we find that σ_L^2 *saturates* for large L. This saturation signals the "freezing" of the bonds into a particular RSP state, and can be used to determine the length scale on which this freezing occurs

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I10 - 1

Energy Materials Design: Band Gap Manipulation by First Principles

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Energy band gap and band edge alignment are some of the most important physical properties in photovoltaic materials. Searching for and designing the proper energy gap and band alignment are still of great challenge for computational materials sciences. To correctly calculate the band alignment, we have recently developed a new calculation approach by taking into account the hydrostatic absolute deformation potential (ADP) of core states. Using this new approach we have calculated the ADPs of the valence-band maximum (VBM) of group IV, III-V and II-VI semiconductors with zinc-blend structures and obtained the true natural band offsets among these semiconductors.

In this talk, I will give a few examples of our recent work on manipulating the band edge levels and band gaps of semiconductors and oxides by first-principles calculations. We find that: (i) through cation mutation, the band gaps of the analogues chalcogenide compounds decrease from the binary to ternary to quaternary compounds. The VBM levels can be controlled by substituting group IB and IIB cations while the CBM can be controlled by substituting IVA and IIIA cations. We propose, based on our extensive theoretical search, that the quaternary Cu_2ZnSnS_4 and $Cu_2ZnGeSe_4$ have suitable band gaps and optical properties as the cheap absorber materials in thin-film solar cells. (ii) We find that the band gap of anatase TiO_2 could effectively be narrowed under uniaxial strain, which offers an opportunity to reduce the band gap of TiO_2 for the absorption of solar energy. The mechanism of manipulating band gap by applying uniaxial strain along soft direction perpendicular to crystal layer should be applicable to other layer-by-layer energy-related materials. (iii) We have studied the anomalous band gap trends in two technologically important semiconductor alloys, $Ag_xCu_{1-x}GaS_2$ and Sn_xGe_{1-x}, and successfully explained the large band gap bowing in Sn_xGe_{1-x}, and the band gap increase of $Ag_xCu_{1-x}GaS_2$ with the lattice constant. These understanding will be helpful in future band gap engineering of new functional alloys.

I10 - 2

How Can a Homogeneous Semiconductor Exhibit Gigantic Dielectric Response?

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We proposed a new concept to realize gigantic dielectric response in spatially homogeneous semiconductors, which may be used in next generation of microelectronics and energy storage. Non-homogeneities in semiconductors with Gigantic Dielectric Response (GDR) limit their applications in microelectronics and energy storage. We combine first-principle, statistical and phenomenological methods to study heavily Li- and MD- co-doped NiO (MD=Ti, Al, Si), and reproduce the experimental trends in dielectric properties as a function of the dopants and their concentrations. Unlike previous models which depend on heterogenities including grain boundaries, small polaron hopping on the bulk dopant levels is the dominant mechanism resulting in a permittivity of 10^{4-5} for these co-doped nickel oxides. According to our mechanism, GDR can be realized even in a perfectly homogeneous semiconductor.

I10 - 3

First-principles Design of Nanomachines

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Learning from nature's amazing molecular machines, globular proteins, we present a framework for the predictive design of nanomachines. We show that the crucial ingredients for a chain molecule to behave as a machine are its inherent anisotropy and the coupling between the local Frenet coordinate reference frames of nearby monomers. We demonstrate that, even in the absence of heterogeneity, protein-like behavior is obtained for a simple chain molecule made up of just thirty hard spheres. This chain spontaneously switches between two distinct geometries, a single helix and a dual helix, merely due to thermal fluctuations.

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O10 - 1

Multi-Paradigm Simulations at the Nanoscale: Methodology and Applications to Functional Carbon Materials

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Multiparadigm methods to span the scales from quantum mechanics to practical issues of functional nanoassembly and nanofabrication are enabling first principles predictions to guide and complement the experimental developments by designing and optimizing computationally the materials compositions and structures to assemble nanoscale systems with the requisite properties. In this talk, we employ multi-paradigm approaches to investigate functional carbon materials with versatile character, including fullerene, carbon nanotube (CNT), graphene, and related hybrid structures, which have already created an enormous impact on next generation nano devices. The topics will cover the reaction dynamics of C_{60} dimerization and the more challenging complex tubular fullerene formation process in the peapod structures; the computational design of a new generation of peapod nano-oscillators, the predicted magnetic state in NanoBuds; and opto-electronic properties of graphene nanoribbons.

K11 - 1

Paradigm Shift of Materials Design by Computer Simulation
from Explanation to Prediction

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For long time of materials research and development, theory always has had a role to explaining the experimental findings. This fact is really very different compared to the field of elementary particle physics, where theory predicts new particle or phenomena and experiment follows to establish theoretical prediction. Since materials are complex many-body system composed of a number of electrons and nuclei, it has been difficult to compute atomic structure and physical and chemical properties without experimental observations. Recent progress in theory and computer power has changed this situation completely. For any kind of materials we know the governing equation and interation; quantum mechanics and Coulomb force. Therefore, basically we know everything and we can solve to predict new materials without experimental help. This approach is called *ab initio* method and generally used widely, but still not sufficient enough to change the paradigm of materials design. In this talk I will indicate how to overcome this situation, and realize a breakthrough of theoretical materials design to shift "from explanation to prediction", by introducing several examples. This new approach is different from existing methods, and has quality accuarance by itself. When we judge the theory good or not by comparing to existing experimental data, theory can not be independent and has no power of predicting new materials before experiment. Suitable level of theory which should be selected by "accuracy" and "computing cost" will also be given in the talk

I11 - 1

Structure and Properties of Some Doped Metal Clusters:
A Quantum Chemical Approach

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We will present some recent results related to the geometrical and electronic structure as well as the spectroscopic properties of the doped clusters Si_nM_m, Ge_nM_m, Cu_nM and Au_nM, with M = transition metals. Their experimental characterization by far infrared and mass spectrometric methods will be discussed in terms of quantum chemical results. Small metal-doped copper and gold clusters tend to prefer high symmetry, planar but fluxional shape, and their thermodynamic stability can in part be accounted for by a kind of *σ-aromaticity*. The validity of the jellium model in interpreting the structure of metal clusters is also examined.

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I11 - 2

Charge Separation Dynamics at Molecular Heterojunction of C_{60} and Zn- Phthalocyanine

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Molecular heterojunction of C_{60} and zinc phthalocyanine (ZnPc) is one of the prospective candidates of creating efficient organic solar cells [1,2], and the information of its charge separation dynamics is highly desirable. By carrying out semi-classical Ehrenfest dynamics simulations on the basis of the time-dependent density functional theory (TDDFT), the so-called adiabatic LDA, we investigate how the charge separation proceeds between a C_{60} acceptor molecule and a ZnPc donor molecule at different intermolecular distances from 3.0 Å to 5.0 Å when C_{60} is located on top of ZnPc. As a result, we find that the optimal intermolecular distance is around 3.0 Å. In addition, we propose that, if an oligo (*p*-phenylenevynilene) (OPV1) periphery is attached to the ZnPc core, the concurrence of the light-harvesting property of this nearly planer π-congugated complex [3,4] increases the range of the photoabsorption band of the solar cell system.

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O11 - 1

Evaluating Seebeck Coefficient of Na_xCoO_2 from Molecular Orbital Calculations

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We propose the evaluation of the Seebeck coefficeint of Na_xCoO_2 (x = 0.38, 0.67, 0.76, 0.86, and 0.95) compounds by Boltzman theory: Mott expression and Fermi energy from the discrete variational (DV) - $X\alpha$ molecular orbital calculation. This approach was based on molecular orbital calculations using the $Na_8Co_{21}O_{72}$, $Na_{14}Co_{21}O_{72}$, $Na_{16}Co_{21}O_{72}$, $Na_{18}Co_{21}O_{72}$, and $Na_{20}Co_{21}O_{72}$ clusters to obtain special point of the Fermi energy for evaluating the temperature dependent Seebeck coefficient values. The evaluated Seebeck coefficient the Na_xCoO_2 compounds increases with increasing temperature as well as with increasing x values and temperature agrees with experimental data nearly quantitatively.

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I12 - 1

Surface Energy and Surface Proton Order of Ice Ih Basal and Prism Surfaces

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The density functional theory (DFT) calculations are used to study the surface energy and surface proton order of ice Ih. We find that the variation with proton order in the bulk is about 5 meV per H_2O, whereas at the surface it is as much as 100 meV per H_2O molecule. An order parameter which defines the surface energy of ice Ih surfaces is identified to understand the large range of values at ice surface. It is found that this newly established parameter is sensitive on the stability of ice surface and hence likely on ice surface reactivity. A strong linear dependence has been observed between the surface energy and the order parameter. A classical electrostatic model proves useful to explain the physics inside. It is remarkable to see such a simple correlation come out of the sophisticated first principles calculations. We predict that the proton order-disorder transition, which occurs in the bulk at ~72 K, will not occur at the surface at any temperature below surface melting. Our results show that the surface of ice is unexpectedly cold with significantly more proton ordered than the bulk.

I12 - 2

Atomistic Modelling of the Growth of Rutile

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We will present work on modelling the surface growth of the (110) rutile TiO_2 surface. The work has used a combination of ab-initio density functional theory (DFT) and a variable charge empirical potential model to elucidate the available surface and near-surface sites for Ti, O, O_2, TiO and TiO_2 ad-species on the rutile (110) surface. The nudged elastic band and dimer methods have been employed to gain an understanding of the energetics of the possible surface transitions. Furthermore, a combination of molecular dynamics (MD) and long time scale dynamics have been exploited to model the growth of the surface.

We have shown that the SMB-Q variable charge model successfully describes the majority of surface sites found using DFT. The exception to this being any structure involving an O_2 molecule, as the model has a purely repulsive O-O interaction. The structure of the binding sites are generally in good agreement between the two models, the exception to this is the case of the binding site for an O atom above a five-fold coordinated Ti atom. In the variable charge model this is seen to sit immediately above the Ti atom whereas in DFT the O atom is displaced to one side.

Most of the surface diffusion barriers are large in magnitude, greater than 2 eV. Thus implying that the diffusion of these ad-species would not take place on the timescale of the growth of the surface. The exception to this is the diffusion of the O atom along the surface in the [001] direction where a barrier of less than 1 eV was found. A mechanism involving interstitial Ti atoms and this O diffusion will be used to explain surface growth.

I12 - 3

Ab Initio Modeling of Laser Materials:
Segregation of Nd and Gd on YAG Surfaces

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YAG crystal doped with about 1% Nd is widely used as laser material. Currently great efforts are being made to produce high quality laser materials using ceramic powders to develop high power lasers. Segregation of Nd and other dopants on grain boundaries of ceramic YAG samples is an important problem in this effort and segregation can be used to enhance the concentration of the dopants in ceramic samples. We study from *ab initio* calculations the atomic and electronic structures of pure YAG in bulk as well as on (001) and (110) surfaces. The calculated bulk properties obtained within generalized gradient approximation agree remarkably well with experimental data. The atomic structure on surfaces has been fully optimized to allow relaxation/reconstruction and for a given surface, the atomic structure with the lowest energy has been explored. Further we report results of studies on doping of Nd and Gd in small concentrations in bulk as well as on surfaces to understand the segregation behavior.

I12 - 4

Influence of Cr and Fe Additions on Grain Boundary Cohesion of Bcc Fe and Cr

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The macroscopic strength of metals and alloys depends on the cohesion at the boundaries of microscopic grains constituting the metal. Impurities segregated at the grain boundary (GB) can drastically modify its properties. Additionally, the properties of a magnetic host with the magnetic atom additions are affected by a complex interplay between magnetism and different structural settings. In this talk, we present results of systematic computational studies of structural, cohesive, and magnetic properties of two symmetric tilt GBs in pure iron and chromium as well as in the dilute FeCr and CrFe alloys. The calculations were performed within the framework of density functional theory, using the projector-augmented-wave potentials and the plane waves basis set. We will discuss the changes in GBs geometry, energetics, and in their magnetism, caused by Cr (Fe) alloying additions placed in interstitial or substitutional positions at the Fe (Cr) host GBs. The importance of full relaxation of the shape and volume of the supercell, and the relaxation of all position of atoms will be stressed. The segregation of solute atoms at the GBs in Fe and Cr and the embrittling/strengthening effects of the Cr and Fe impurity atoms, and the chemical and mechanical components of the strengthening energy, will be also discussed.

O12 - 1

First-principles Study of Rectifying Properties of Pt/TiO$_2$ Interface

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Reversible resistance-switching phenomena in transition metal oxides have attracted considerable attention for application to ReRAM. Among metal oxides, TiO$_2$ has been also expected as memristive switching material and diode polarity switching material, and the rectifying behavior of Pt/TiO$_2$/Pt structures is required for both switching mechanisms. Although it has been pointed out that the stoichiometry near interfaces affects the conductive property, the microscopic origin is not yet clear. In this study, we have performed first-principles calculations to study the interface electronic structure of Pt/TiO$_2$ and to analyze the rectifying property of the Pt/TiO$_2$/Pt structure, using our in-house computational code QMAS (Quantum MAterials Simulator) based on the projector augmented-wave (PAW) method. For the stoichiometric interface, the metal induced gap states (MIGS) have amplitude appreciably only at the interface TiO$_2$. We will show that the presence of MIGS makes oxygen vacancy formation energy small at the interface. It is therefore expected that the interfacial TiO$_2$ layer can be easily reduced. We will then demonstrate that the Schottky barrier height (SBH) is strongly affected by oxygen deficiency. Accoding to the present calculation, the interface is of Schottky contact type for the fully oxidized interfacial TiO$_2$, while it becomes almost ohmic for strongly reduced one.

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Hydrogen Bonded Bimolecular Monolayers on Au(111): A DFT Study

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Self-assembly of molecular networks on metal surfaces plays an important role in nanotechnology. Its understanding requires the combination of accurate experiments and advanced modelling. We present a complete computational study on hydrogen bonded networks containing the popular perylene-tetracarboxylic-dianhydride (PTCDA) and diamino-p-terphenyl (DATP) on Au(111). Such networks attracted particular interest due to the possible applications in nanoelectronics. Using density functional theory with empirical van der Waals corrections, we start considering isolated adsorbed molecules and show that dispersion forces are important in determining the geometry of the interfaces, which in turn strongly affects the electronic structure. This is true both for physisorbed (PTCDA) and for weakly chemisorbed (DATP) systems. Coming to heteromolecular hydrogen-bonded self-assembled monolayers, a charge density and energy analysis shows that the surface slightly modifies the strength of hydrogen bonding between the molecules and the electronic structure. The change in work function of Au(111) due to the presence of the monolayers is mainly described in terms of Pauli repulsion and charge transfer. Our results are in excellent agreement with the experimental data, particularly concerning the scanning tunneling microscopy (STM) experiments and the relative stability of different adsorbed phases.

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Molecular Dynamics Simulations Study on the Structure Evolution of Polyethylene Surface by Ar Ion Bombardment

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Ion beam bombardment at low energy forms nanosize patterns such as ripples, dots or wrinkles on the surface of polymers in ambient temperature and pressure [1]. It has been known that the ion beam can alter the polymer surface that induces skins stiffer or the density higher by higher compressive stress associated with chain scissions and crosslinks of the polymer. Atomic scale structure evolution in polymers is essential to understand a stress generation mechanism during the ion beam bombardment, which governs the nanoscale surface structure evolution.

In this work, Molecular Dynamics (MD) simulations are employed to characterize the phenomenon occurred in bombardment between the ion beam and polymers that forms nanosize patterns [2, 3]. We investigate the structure evolution of Low Density Polyethylene (LDPE) at 300 K as the polymer is bombarded with Argon ions having various kinetic energies ranging from 70 eV, 200 eV to 1 keV with the fluence of 2.7×10^{19} #/cm^2. These simulations use the Reactive Force Field (ReaxFF), which can mimic chemical covalent bonds and includes van der Waals potentials for describing the intermolecular interactions [4].

The results show the details of the structural evolution of LDPE by the low energy Ar ion bombardment. Analyses through kinetic and potential energy, stresses, number of crosslinks and chain scissions, level of local densification and motions of atoms support that the residual stress on the surface is strongly associated with the number of crosslinks or scissored chains [5].

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O12 - 4

A First Principles Calculation on the Polythiophene/Carbon Nanotube Hybrid Nanocomposite

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In the last decade, polymer solar cells offered the opportunity for fabrication of low-cost, large-area, mechanically flexible photovoltaic devices. One of the popular types is based on polythiophene/inorganic nanocrystal hybrid system. In this work, we have employed the first-principle calculations to investigate the electronic structure of polythiophene/surface-modified CNT hybrid system. Both metallic and semiconducting CNT/polythiophene hybrid systems were calculated.

In a semiconducting CNT/polythiophene system, the band structure shows that a type-II heterojunction can be formed. Different surface modified atoms (ex. H, F and Cl) adsorbed on CNT surface can shift the band alignment between CNT and polymer. In addition, we have found that the surface modifiers assist the interaction between polythiophene and CNT which will change the charge transfer efficiency. Our result provides an insight for the experimentally observed charge transfer and photovoltaic performance in the polythiophene/CNT hybrid system.

First-principles Determination of Free Energies of Ferroelectric Phase Transitions

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We use a combination of (a) constrained polarization molecular dynamics and (b) thermodynamic integration to determine the free energy landscape relevant to structural phase transitions and related phenomena in ferroelectric materials, bridging the gap between first-principles calculations and phenomenological Landau-Devonshire theories. We illustrate it using a first-principles effective Hamiltonian of $BaTiO_3$ to (a) uncover the quantitative features of the free energy function that are responsible for its first-order ferroelectric transitions, and (b) determine the minimum free energy pathway for the polarization switching and (c) evaluate temperature and size dependence of free energy of ferroelectric domain walls. Through a comparison with analysis based on Landau mean field theory of the same hamiltonian, we show that certain terms have to be added to the phenomenological Landau-Devonshire free energy functions to capture the physics of ferroelectric materials. Our method can be readily generalized to any classical microscopic Hamiltonian and ensembles characterized with appropriate constraint.

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Origin of Anisotropy, Metallic Behavior and Thermoelectric Effect in Delafossite $PdCoO_2$, $PtCoO_2$

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$PdCoO_2$ and $PtCoO_2$ have been attracting much concern due to their high electrical conductivity and possible applications in thermoelectrics. But the nature of chemical bonding, origins and cause of high anisotropy in $PdCoO_2$ and $PtCoO_2$ have not been settled yet. In this work, we have studied the electronic structure of $PdCoO_2$, $PtCoO_2$ compounds by using the Full Potential Linearlized Augmented Plane Wave (FP-LAPW) method within the Perdew-Burke-Ernzerhof Generalized-Gradient Approximations (PBE-GGA). The role of the Pd-4d, Pt-5d and Co-3d orbitals to the electrical conduction in $PdCoO_2$, $PtCoO_2$ has been analyzed. Causes and anisotropy in the conductivity behavior of the Pd-/Pt-layer and insulating property of CoO_2-layer have been identified. Conductivity in the c-direction is limited by the anti-bonding Pd-O, Pt-O states and the insulating state of CoO_2 layer. The thermoelectric properties of $PdCoO_2$ and $PtCoO_2$ have been calculated and discussed within the semiclassical Boltzmann theory.

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GPU-accelerated Massive Parallel Quantum Molecular Dynamics Simulation

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Nano-structured carbon materials are playing more and more important roles in materials science due to their potential applications to novel superconductor [1] and electrodes for fuel cell [2,3], solar cell and lithium-sulpfer battery [4] as well as nano-polycrystalline diamond anvil cell for high pressure neutron scattering measurement [5]. Quanutm molecular dynamics simulation of such materials is challenging because the number of atoms necessary for the simulation becomes very large. In this talk I will introduce a massive parallel tight binding molecular dynamics simulation program based on linear scaling methods [6,7] and hardware acceleration with graphic processing unit (GPU) [8].

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O13 - 2

Modeling of Pillared Layer Structures as the Hydrogen Storage Material

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Pillared covalent organic frameworks (PCOFs) have been modeled with the density functional theory (DFT) calculations. Based on the COF-1 structure, one of covalent organic frameworks (COFs), synthesized by the condensation reactions of phenyl diboronic acid $\{C_6H_4[B(OH)_2]_2\}$, we inserted "pillar" molecules between the organic layers for the improvement of physisorption ability for the hydrogen molecules. Pyridine was considered as a candidate for the pillar molecule. The system was extended from the cluster to the periodic systems for the estimation of the effect of insertion, inter-layer distance and energetic stability. We also considered the effect of packing method for COF layers in the presence of "pillar" molecules. Among all the feasible packing structures, two structures in staggered and eclipsed form influence the morphology of the crystal structure. With this calculation, we proposed new PCOF structures to enhance hydrogen storage capacity.

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O13 - 3

Thermal Diffusivity of $Al_{0.3}Ga_{0.7}As$ by Molecular Dynamics Simulation and Thermograph Method

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Aluminium Gallium arsenide is a technologically important material. $Al_{0.3}Ga_{0.7}As$/ GaAs heterostructure system is a promising material system for high speed transistors and optoelectronic device applications. Efficiency and performance of such devices may depend on the defect level present in the material and how likely those defects are to be mobile under device operating conditions. Thermal properties of $Al_{0.3}Ga_{0.7}As$ like thermal diffusivity and thermal conductivity has been studied by photoacoustic technique and molecular dynamics simulation(MDS) /1/ and showed a very good agreement with the literature values/2/. Thermograph, a latest technique is used here presently to determine thermal diffusivity of AlGaAs and compared with the previous methods result.

For MDS, simulation cell of dimension 3 x 3 x 3 having four atoms of Ga and As in every cell is constructed. 216 particles are arranged in the zinc blende type lattice and then 30% of 'Ga' atoms are replaced by 'Al' atoms for the $Al_{0.3}Ga_{0.7}As$ alloy. The three body potential, Tersoff's potential is considered and calculated its parameters for $Al_{0.3}Ga_{0.7}As$ alloy using the parameters of GaAs and AlAs/. After the equilibration of cohesive energy the thermal properties are calculated. Good agreement of thermal diffusivity values with that of phooacoustic study, MDS and the thermograph method using the synthesized $Al_{0.3}Ga_{0.7}As$ sample.

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I14 - 1

Liquid Structure as a Guide for Phase Stability in the Solid State: Prediction of a Stable Compound in the Au-Si Alloys System

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There is an ongoing challenge to truly predict the stable structure of a compound. Among the many approaches to this problem (for a recent comprehensive review see Woodley and Catlow[1]), we can mention the Data Mining Structure Predictor combining data-mining with first-principles calculations by Fischer *et al.*[2] and evolutionary or genetic algorithms coupled with first-principles calculations such as proposed by Oganov and Glass[3] and d'Avezac and Zunger[4]. For certain alloy systems, such as those that form Zintl phases[5] there is a well-documented relationship between local atomic structure in the solid crystalline state and in the liquid state. In the case of eutectic Au-Si alloys there are no extreme changes in the density upon solidification, such as for example in the case of Si[6]. Therefore, one might suspect that atomic coordination in the liquid phase and in the crystal phase are similar. Thus, we use the known coordination number distribution in the liquid phase as a criterion for selecting prototype crystal structures. For the $Au_{80}Si_{20}$ alloy we predict the existence of a stable compound.

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I14 - 2

Ab Initio Molecular Dynamics Simulations to Designing Static and Dynamic Properties in Undercoolled and Morphous Materials.

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An overview of a recent series of ab initio molecular dynamics (MD) simulations for the liquid, supercooled and amorphous states of different materials is presented. Here we use a combination of state-of-the-art computational techniques to resolve the atomic-level structure of such disordered systems. The dynamic properties, such as the self-diffusion coefficients and viscosity, are also studied as a function of temperature in the supercooled regime. By analyzing a range of model systems that involve different chemistry, we elucidate the different types of short-range order that may occur and our findings have strong implications for understanding the nature of the glass forming ability and properties of metallic glasses.

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Application of Ab Initio Results in Modelling Phase Diagrams Containing Complex Phases

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We address the application of ab initio electronic structure calculations to modelling of phase equilibria and to construction of phase diagrams in binary and ternary iron systems containing complex intermetallic phases (Laves phases, sigma phase) in combination with the phenomenological CALPHAD (CALculations of PHAse Diagrams) method. This approach is briefly outlined and utilization of ab initio total energy differences (lattice stabilities) for sigma phase is shown in Fe-Cr, Fe-Cr-Ni and Fe-Cr-Mo systems. Our description of sigma phase is included into a thermodynamic database for calculation of phase equilibria in steels, developed earlier by some of the authors. Theoretical results obtained by new and older models are compared with new experimental data for superaustenitic (high Ni and Cr) steels. In conclusion, some problems and challenges in application of ab initio results in the CALPHAD approach are outlined.

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The 'Native Vacancy' and Diffusion Mechanism in Amorphous Alloys

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The 'native vacancy' and diffusion mechanism have been analyzed for models containing 10^5 atoms and constructing by statistic relaxation method. We found a large number of sets of two spheres with the same radius, where the first sphere contains 5 atoms on its surface, but the second sphere consists of 4 atoms on its surface and one atom lies in a center of the second sphere. The 'native vacancy' is considered to be inside such finding spheres. We approximately estimate the number of native vacancies in five amorphous models $Fe_{80}B_{20}$ with different densities. The self-diffusion enhance in unrelaxed amorphous alloys, the correlation between pre-exponential factor D_0 and activation enthalpy Q are interpreted based on the number of native vacancies for the models considered here.

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Structural and Dynamic Properties in Undercooled and Amorphous Materials: A Molecular Dynamics Study Cu-Zr Glass Forming Alloys

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The understanding of the glass forming ability of metallic alloys from the behavior at the atomic level is one of the unresolved issues in material science. A series of first-principles molecular dynamics simulations the of Cu-Zr alloys in the liquid and undercooled regimes for different compositions in the good glass forming range is presented to give a comprehensive overview of the atomic-level structure and the dynamics through the self-diffusion coefficients viscosity and longitudinal as well as transverse correlation functions. An embedded-atom model is developed within the force-matching technique to address the important question of the evolution of the structural and dynamic properties in approaching the glass transition temperature, namely the fragility, in relation to the glass-forming ability in these materials.

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Kinetic Monte Carlo Simulations of Diffusion-Limited Nucleation

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Nucleation, the stochastic formation of clusters of a stable phase from a metastable phase, is the first step in many phase transformations, including condensation of gases and crystallization of melts.

Due to its simplicity, the classical nucleation theory (CNT) is often used to estimate nucleation rates, but since its derivation depends on the growth rate's being collision (or interface) limited, there has been recent interest to modify CNT for diffusion-limited growth, which involves long-range diffusion and applies, e.g., to oxygen precipitation in silicon and, more generally, to crystallization in alloys. Such a modified theory has been proposed by Kelton[1]. Unfortunately, critical tests of either CNT or Kelton's theory have been prevented by the lack of key input parameters, which are notoriously difficult to obtain experimentally.

We perform kinetic Monte Carlo simulations of diffusion-limited crystallization in 2D to obtain theoretical input parameters, nucleation rates, and size distributions of clusters. The predictions of CNT and Kelton are compared to simulation results.

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I15 - 1

Using Transformation Optics to Design Materials with Novel Optical Properties

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Very recently, a new theoretical technique called "transformation optics" is introduced to establish a correspondence between coordinate transformation and a transformation of material constituent parameters. The most celebrated application of transformation optics is the design and realization of invisibility cloaks that can render an object invisible. Using transformation optics as the starting point, and numerical simulations to refine and demonstrate the optical effects, we designed some conceptual devices that exhibits rather unusual optical properties. Examples of such devices include a frequency-selective "super-absorber" [1], which has unlimited scattering and/or absorption power in the sense that given a fixed device volume, its scattering and/or absorption cross section can be made arbitrarily large. Another interesting example is a device that can "cloak at a distance" [2]so that it can cloak an object with a pre-specified shape and size within a certain distance outside the cloaking shell. [2] We will also show that an extension of that idea can lead to conceptual devices that can optically transform one object into another object.

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I15 - 2

Local Structure Analysis by X-ray Absorption Spectroscopy and First Principles Calculations

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Synchrotron x-ray absorption spectroscopy (XAS) is a very powerful technique to study local structures, especially when used in conjunction with first principles calculations. The main advantage of the technique is that it can selectively excite only the core electrons of a desired element. By using the x-ray energy that matches the core electron energy of the element, only those core electrons are excited into the allowed empty states. Because the shape of the allowed density of states depends on the arrangement of the surrounding atoms, the absorption spectra contain (encrypted) information of the local structure. There is no trivial mean to convert the absorption spectra, especially for the near-edge region of the spectra, to the local structures. However, starting from an assumed local structure model, first principles calculations can be used to generate a theoretical absorption spectrum. By comparing the theoretical spectra generated from various models with the measurement, the actual local structure around the absorbing element can be identified. I will illustrate several successful cases of such combined theoretical/experimental work. I will also show our recent work on aluminum-doped ZnO. For Al-doped ZnO, the combined analysis between the XAS measurements and calculations reveals that majority of Al substitutes for Zn in low Al-content samples. However, for high Al-content samples, the Al starts to form Al_2O_3-like structures. This is consistent with the observed reduction in conductivity for samples with high Al-contents.

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Beyond LDA in Electronic-Transport Simulations of Single-Molecule Junctions

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The density functional theory with the local density approximation (LDA) is an efficient theoretical tool for predicting atomic structures and ground-state energies of electron-ion systems. However, the single-particle energy spectrum from the Kohn-Sham equation underestimates the band gap in semiconductors and insulators, and the HOMO-LUMO gap in molecules. This underestimation may affect the accuracy of the first-principles simulation of electronic conduction in nanometer-scale structures such as single-molecule junctions where the electronic conduction through the molecules is sensitive to the energetic positions of the molecular levels relative to the Fermi energy of metal probes. To achieve a better accuracy beyond the LDA method for the electronic transport through a molecule placed between two metal probes, we consider corrections of the HOMO and LUMO energy levels using the ionization energy and the electron affinity of the molecule and image-charge screening effects of the metal probes. With the corrections, our theoretical method is very successful in describing quantitatively conduction properties of benzene diamine-gold single-molecule junctions, 4,4'-bipyridine–gold junctions, and oligophenyldiamine-gold junctions. The author acknowledges support from the KRF (KRF-2007-314-C00075), the KOSEF (Grant No. R01-2007-000-20922-0, and Grant No. MEST 2009-0081204), and KISTI Supercomputing Center (KSC-2008-S02-0004).

I15 - 4

Study of EXAFS Cumulants of Crystals by the Statistical Moment Method and Anharmonic Correlated Einstein Model

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The moment method in statistical (SMM) dynamics and anharmonic correlated Einstein model (ED) are used to study the cumulants of crystals taking into account the anharmonicity effects of the lattice vibrations. Analytical expressions for the

mean square displacement (MSD) u^2, and the cumulants ($\sigma^{(1)}, \sigma^2, \sigma^{(3)}$) of crystals in the X-ray absorption fine structure (XAFS) have been derived. We have presented the SMM formalism and anharmonic correlated ED by using the Lennard-Jones and Morse interaction potentials. Numerical results for $u^2, \sigma^{(1)}, \sigma^2$ of Pd, Ag, Au, Cu, Pt, Fe, W and Si crystals are found to be in good agreement with experiment.

O15 - 1

Studies of Electronics and Optical Properties of $CaCu_3Ti_4O_{12}$ Using First Principles Calculations

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Recently, an oxide ceramic $CaCu_3Ti_4O_{12}$(denoted as CCTO) has been reported to be very promising due to its high dielectric constant. In this work, first principles pseudopotential calculations based on density functional theory(DFT) have been performed to study the structural, electronic, and optical properties of CCTO. The calculations suggest that the energy gaps of CCTO are 0.50 eV and 0.63 eV eV for local density(LDA) and generalized gradient(GGA) approximations respectively. In addition, the use of the screened exchange method[2], which gives improved band gaps has been investigated. Our result reveals that the energy gap of CCTO is 1.67 eV with sx-LDA calculations, whilst the experimental value is reported to be about 1.5 eV[3].

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P - 1

Electronic Structure Property Correlation of Silicon (111) Surface Functionalized with Alkane Molecules

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The electronic structure at interfaces between molecular and nonmolecular phases, is a subject of considerable recent interest [1,2]. It is very sensitive to basic aspects of the interface, like, molecule-substrate bonding, molecular configuration, and geometric structure. Molecular interfaces with semiconductors are potentially more important in their behavior than those with metals because of the variety of possible band structures and of the potential for controlling their properties via doping, temperature, or optical excitation. We had performed some surface calculation with Silicon surface [3]. Here we elucidate the electronic structure of the Si (111) and alkane interface. We looked into the ground state property the nature of bonding and interaction at the interface. The results were compared with available experimental results.

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P - 2

The Investigation of the Effects of Ga-Doping on the Electronic Structure and the Optical Properties of ZnO under the Density Functional Theory

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The effects of Ga doping on the electronic structure and optical properties of ZnO are studied using the plane-wave pseudopotential method based on the density functional theory (DFT) within the Perdew-Wang 91 generalized gradient approximation (GGA-PW91). The calculated results reveal that due to electron doping, there are lots of carriers in the bottom of conduction band and the Fermi level shifts into conduction bands. Concurrently, the density of states (DOS) shifts towards low energies and the optical band gap is broadened. A sharp resonance attributed to the Ga 4s orbital shows up just below the low-lying Zn 3d valence bands. The width of this peak becomes broader as the amount of the Ga dopant is increased, reflecting an increased interaction with the 2p orbitals of the surrounding O atoms. The calculated result reproduces the pronounced Burstein- Moss shift and the shrinkage of the fundamental band gap. Furthermore, an increase of the Ga content leads the volume of the unit cell to be amplified. The optical properties including the electric function, refractive index, extinction coefficient, absorption coefficient, reflectivity and plasma frequency are also investigated in detailed. The obtained results show that doping concentration strongly affects the optical parameters. The optical parameters shifted to higher energy as increasing doping concentration. The Materials Studio 3.2 software is used for calculating in this work.

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P - 3

Vibration Control of Piezoelectric Cantilever Plates and Comparision with Experiments

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A finite-element model based on the First-order Shear Deformation Theory is developed for the vibration control of a composite plate containing distributed piezoelectric actuator/sensor patches. The piezoelectrics' mass and stiffness are taken into account in the present model. A simple negative velocity feedback control algorithm coupling the direct and converse piezoelectric effects is used to actively control the dynamic response of an integrated structure through a closed control loop. The vibration control and active vibration suppression of a cantilever composite plate are performed as a numerical example to verify the proposed model. The Newmark-β method are used in the numerical simulation to calculate the dynamic response of the piezolaminated composite plate. The numerical results are presented with discussion and in good agreement with experiments.

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P - 4

Simulation of Thermal Dissipation in a Micro-Processor Using Carbon Nanotubes Based Composite

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Currently, the problem of thermal dissipation material for μ-processors, high power lasers and electronic devices becomes a very important issue. In a computer processor, thermal compound between processor and the fan becomes a key factor in thermal dissipation process. Therefore, finding a thermal compound having high thermal conductivity is becoming a major challenge. It is known that carbon nanotubes (CNTs) is one of the most valuable materials with high thermal conductivity (2000 W/m.K compared to thermal conductivity of Ag 419 W/m.K). This suggested an new approach in applying the CNTs as an essential component for thermal paste to improve the performance of computer processor and other high power electronic devices.

In this paper, we present the simulation results of thermal dissipation efficiency using the multi walled carbon nanotubes (MWCNTs) based composites as the thermal dissipation media in a -processor of a personal computer. We used simulation approach to study thermal dissipation process in μ-processor, and the relation between the thermal processor, fan, thermal conductivity of thermal paste and working times. The simulative results showed that the temperature of CPU increases as an exponential function of working time, and this results accord entirely with experimental.

P - 5

Interpretation of Hund's First and Second Rules for 3d Atoms

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Hund's first and second rules have traditionally been interpreted to be ascribed to a reduction in the electron-electron repulsion energy V_{ee}, assuming that the two stationary states being compared have the same set of orbitals. This conventional interpretation, however, is a fallacy since it violates the virial theorem $2T+V=0$ where T is the kinetic energy and V the total Coulomb interaction energy. We have demonstrated the following fact taking due account of correlation in which the virial theorem is fulfilled to high accuracy: The correct interpretation of Hund's rules for 2p and 3p atoms as well as the CH_2 molecule [1~6] are due to the greater electron-nucleus attraction energy V_{en} that is gained at the cost of increasing V_{ee}. In this work, we have extended our study to the titanium atom ($Z=22$) as a first step of investigation of the stability of LS terms for 3d atoms. The $[Ar]3d^2 4s^2$ configuration of the Ti atom is the first configuration to which Hund's empirical rules apply within the ground state of 3d atoms. The experimental order of the total energy E ($=T+V<0$) for LS terms arising from this configuration are as follows: $E(^3F) < E(^1D) < E(^3P) < E(^1G) < E(^1S) < 0$. According to the first rule, the ground term is triplet ($S=1$). Of the two triplet states, ^3F ($L=3$) is more stable than ^3P ($L=1$) in accordance with the second rule. We have interpreted the stabilization mechanism of the above LS terms by Hartree-Fock(HF) and Multiconfiguration HF(MCHF) methods; HF does not include correlation and MCHF takes due account of correlation. Both methods fulfill the virial theorem and reproduce the above order of E even though Hund's empirical rules do not work well between excited terms. The following inequalities obtained from the two methods clarify the stabilization mechanism of the LS terms:

$$V_{en}(^3F) < V_{en}(^1D) < V_{en}(^3P) < V_{en}(^1G) < V_{en}(^1S) < 0,$$
$$V_{ee}(^3F) > V_{ee}(^1D) > V_{ee}(^3P) > V_{ee}(^1G) > V_{ee}(^1S) > 0,$$
$$T(^3F) > T(^1D) > T(^3P) > T(^1G) > T(^1S) > 0.$$

It is concluded that the more stable LS term is due to the greater V_{en} that is gained at the cost of increasing V_{ee}. The greater V_{en} for the more stable LS term is caused by a contraction of 3d orbitals which involves a slight but significant expansion of inner orbitals. We have confirmed the following correlation effect for every LS term that is consistent with our previous study:

$$V_{en}^{corr} = V_{en}^{MCHF} - V_{en}^{HF} < 0, \quad V_{ee}^{corr} = V_{ee}^{MCHF} - V_{ee}^{HF} < 0, \quad T^{corr} = T^{MCHF} - T^{HF} > 0.$$

We have checked the correlational virial ratio $-(V_{en}^{corr}+V_{ee}^{corr})/T^{corr}$ within an accuracy of 2.00.

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P - 6

First Principles Calculations of SrHfO$_3$

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SrHfO3 compound has been reported as a potential gate dielectric for future complementary metal-oxide-semiconductor field-effect transistor(CMOS)[1]. Here we calculate the electronic structure and dielectric properties of cubic SrHfO3 from first-principles pseudopotential calculations[2] based on density functional theory(DFT) within the local density approximation (LDA) and generalized gradient approximaton(GGA). The calculations suggest that the energy gaps of SrHfO3 are 3.5 eV and 3.2 eV for local density(LDA) and generalized gradient(GGA) approximations respectively. In addition, the use of the screened exchange method, which gives improved band gaps[3] has been investigated. Our result reveals that the indirect band gap energy gap of SrHfO3 $(R \rightarrow \Gamma)$ is 6.6 eV with sx-LDA calculations, whilst the optical energy gap as investigated experimentally is reported to be about 6.1 eV[1].

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Development of the All-electron Mixed Basis Hartree-Fock Calculation Code

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In order to describe spatially extended states as well as localized states with reasonable accuracy, it is highly desirable to develop an all-electron Hartree-Fock (HF) calculation code that uses plane waves in addition to atomic orbitals and is applicable to molecules, clusters, surfaces, and crystals. Such a code would provide a physically transparent starting point for more advanced calculations such as the second-order perturbation theory and the *GW* approximation. Here we choose the all-electron mixed basis approach to achieve this requirement. We have successfully applied this code to the perturbation theory [1] and *GW* approximation [2] by beginning with the LDA. For the development of the all-electron mixed basis HF calculation code, we suggest several accurate algorithms to calculate Fock matrix elements. We compare our results of isolated atoms with those of ATSP2K [3] that satisfies the virial thereom. The agreement is quite excellent for H, He, Be, etc..

Details will be presented in the poster.

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P - 8

Computer Simulation of the Non-Uniform and Anisotropic Diamagnetic Shift of Electronic Energy Levels in Double Quantum Dot Molecules.

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In this theoretical study, we present our calculation results for energy states of an electron confined in double asymmetrical InAs quantum dot molecules (QDMs) embedded in GaAs matrix [1] when magnetic field is applied. Based on the effective three-dimensional one band Hamiltonian, the energy and position dependent electronic effective mass approximation, the finite height hard wall three-dimensional confinement potential, and the Ben Daniel-Duke boundary conditions, we perform the calculation for QDMs within complete three-dimensional description. This approach allows us to consider arbitrary directions of the magnetic field. To solve three-dimensional eigen-value problem we apply the nonlinear iterative method [2] for several distances between quantum dots in the molecule by using Comsol Multiphysics package. Increase of the absolute value of the magnetic field leads to the non-uniform diamagnetic shifts for the electronic energy levels [1]. Our simulation results clearly show that application of the magnetic field in various directions generates anisotropic non-uniformity in the diamagnetic shifts (different diamagnetic shift behavior for different directions of the magnetic field). Therefore we dynamically manipulate electronic states not only by varying the magnitude but also changing the direction of the magnetic field.

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P - 9

Ab-initio Study of the Effect of Size and Shape on the Electronic Properties and Electron Affinity of Hydrogen Terminated Carbon Nanoparticles (Diamondoids)

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We show that the electronic properties and electron affinity of hydrogen terminated carbon nanoparticles (diamondoids) are depended on the size and shape of the nanoparticles. By choosing an appropriated basic set at the level of 631G(d) with generalized gradient approximation exchange-correlation functional and the diffusion function added the basics set with hybrid functional in density function theory calculation, the HOMO-LUMO gap is well suit with the result of quantum monte carlo calculation. The nanoparticles have negative electron affinity (NEA) and the quantum confinement effect disappear when the size of nanoparticles increase up to 1nm. Further discussion of rod shaped and chiral higher diamondoids are also included.

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Highly Photoluminescent Semiconductor Quantum Dots Synthesized in Non-Coordinating Solvent

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A conventional and non-coordinated-based approach for synthesis of CdSe and CdSe/ZnS core/shell quantum dots is presented in this work. Simple reagents such as cadmium oxide (CdO), oleic acid (OA), selenium (Se) powder and trioctylphosphine (TOP) with obvious advantages were used to replace for toxic organometallics. This is the first time a CdSe/ZnS core/shell structure was successfully synthesized in noncoordinating solvent without trioctylphosphine oxide (TOPO) [1-3]. The obtained CdSe nanoparticles were characterized by using UV-Vis absorption spectroscopy, photoluminescent (PL) spectroscopy, and transmission electron microscopy (TEM) which confirmed that a series of core CdSe particles with diameter of 1.9 nm~3.5 nm, corresponding to the first peak of absorption spectra at 450 ~ 570 nm range, was successfully achieved. The CdSe/ZnS core/shell structures were then fabricated by coating the previously synthesized CdSe core with various thin ZnS layers. These CdSe/ZnS semiconductor quantum dots exhibited very high photoluminescence. It was about 10-25 times larger than that of the original CdSe core. The narrow bandwidth of the CdSe/ZnS quantum dots indicated that the as-produced quantum dots have uniform size distribution, desirable dispersibility and excellent fluorescent properties, those are the requirements for quantum computational materials [4, 5].

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Ab Initio Study of n-type Doping in Anatase TiO_2

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TiO2 with n-type doping is mainly composed with anisotropic Ti 3d orbitals as a transparent conducting oxide (TCO). We investigate the effect of Nb, V, and Ta substitution of the anion on the electrical properties of anatase single crystals by means of density functional theory, using semilocal (PBE) and hybrid (HSE06) functionals for a supercell.

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A Theoretical Approach of Microscopic Solvation of LiCl
in Water Cluster: $LiCl(H_2O)_n$ (n=1–9)

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The alkali halide-water systems are the best characterized of the ion-solvent systems. Those systems offer optimal opportunity for theoretical study because they are structurally simple, do not react with the solvent, dissociate into singly charged ions, and are ubiquitous in chemistry and biology.[1,2] The smallest alkali halide that fits this description is LiCl. The structure, stability and electronic states of LiCl(H2O)n (n=1-9) clusters have been investigated by Hatree-Fock, MP2 and B3LYP methods with 6-31+G(d) and 6-311++G(2d,2p) basis sets. EFP calculations also performed for comparison with ab-initio and DFT results and it shows the good agreement with HF and MP2 results. We also performed Monte Carlo calculations as an attempt to find the number of low-lying energy structures of the solvated system LiCl(H2O)n (n=1-9). For each value of n the associated structures have been found whereas the dissociated-LiCl structures have been found for n=4–9. In this study the first solvation shell of LiCl has been determined. It is predicated that at least eight water molecules are needed for completion of first solvation shell of LiCl whereas seven water molecules can fully dissociate Li–Cl bond.

Figure: Stable structures of LiCl(H2O)7, LiCl(H2O)8 and LiCl(H2O)9 clusters.
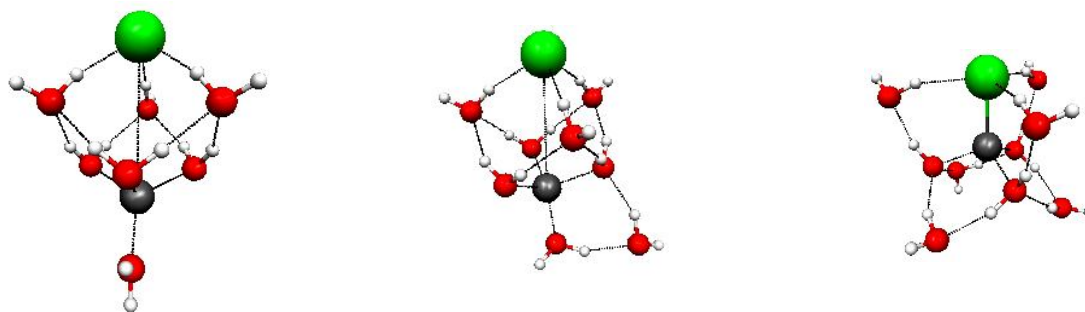
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Theoretical Prediction of Doubly Charged Hydronium Ions

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Two main structural models are well known for the hydrated proton, Eigen[1] and Zundel[2] cations. Eigen proposed each hydrogen of core H_3O^+ strongly hydrogen bonded with every water molecule and possesses $H_9O_4^+$ complex, where as, Zundel proposed one proton shared with two water molecules and possesses $H_5O_2^+$ complex, both are singly charged species. The structure, stability, and electronic state of doubly charged hydronium ions with water, $(H_3O^+)_2(H_2O)_n$ (n=0–10) clusters have been investigated ab initio molecular orbital method, including electron correlation, and DFT methods with 6-31G(d,p) and aug-cc-pVDZ basis sets. Monte Carlo calculations performed as an attempt to find the number of low-lying energy structures of the solvated system for each value of n. Dimerization of hydronium cation without water might be exist but it's extremely unstable whereas after addition two water molecules it become comparatively more stable. The stability of clusters increases with increasing of water molecules. The present study also predicted that hydronium dimmer makes a unique four membered ring core cluster $(H_3O^+)_2(H_2O)_2$ with two water molecules by a strong hydrogen bonds. Solvation shell also discussed.

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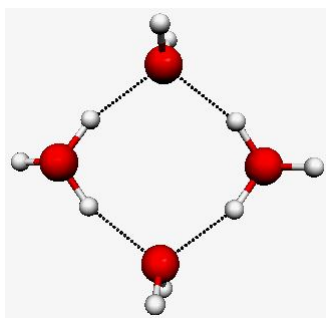
Core Structure, $(H_3O^+)_2(H_2O)_2$
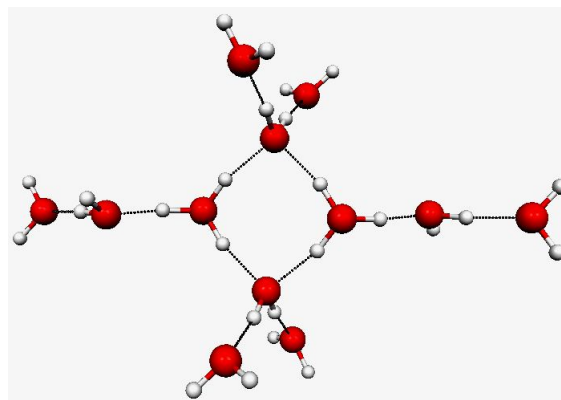
Structure of $(H_3O^+)_2(H_2O)_{10}$

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Pair Potential Application for Molecular Dynamics Studies of GaAs Nanoparticles in the Amorphous Phase

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Structural properties in amorphous gallium arsenide were studied in nano scale with molecular dynamics simulation using the pair potential function proposed by Jin Cai et.al [1]. The defect properties of the models in the size range from 3nm to 5nm were investigated for both core and surface parts by structural quantities such as: interatomic distances, coordination number, bond angle, static structural factor. Moreover, the analyses of shortest-path rings [2] and Voronoi polyhedral were also discussed. In addition, the size dependence of the glass transition temperature and surface energy have been found and discussed.

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Cooling Rate Effects in Liquid and Amorphous Aluminosilicate Nanoparticles: A Molecular Dynamics Computer Simulation

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The cooling rate effects in the liquid and amorphous aluminosilicate nanoparticles have been investigated by Molecular Dynamics (MD) method. Simulations were done in the models of the size of 3 nm under non-periodic boundary conditions with Born-Mayer type pair potentials [1]. The temperature of the system was decreasing linearly in time as $T(t) = T_o - \gamma t$, where γ is the cooling rate, $\gamma = 4.375 \times 10^{12}$, 4.375×10^{13} and 4.375×10^{14} K/s. The cooling rate dependence of thermodynamic properties such as density and potential contributions system was found. Calculations show that with the different cooling rates the dependence of density, with the canonical assemble NPT, is quite pronounced with a clear anomaly minimum around 3000 K for three cooling rates which corresponds to an anomalous of pressure found in the aluminosilicate bulk during cooling with the canonical assemble NVT [2]. Moreover, the microscopic quantities such as coordination number distributions, bond-angle distributions, and partial radial distribution functions (PRDF's) of the amorphous nanoparticles at 350 K have showed such dependences on cooling rates. Namely, beside of the network structure of the amorphous aluminosilicate nanoparticles have a distorted tetrahedral network structure, that is, Al and Si atoms are mainly coordinated to four O atoms, a relatively large mount of structural defects of assumed as $Z_{Al(Si)-O} = 2$ or 3 presents on the surface of nanoparticles, and it is enhanced with the faster cooling rates. Analogously, in the core of nanoparticles the cooling effects on the coordination number distributions have been figured out the trends similar to those observed by the experiments for the bulk counterpart.

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Effect of Edge Doping on Electronic and Magnetic Properties of Graphene Nanoribbons

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Graphene has recently attracted much attention in both theoretical and experimental fields. The development of experimental techniques for fabrication of single sheet graphene has provided practical tools to investigate the properties of a real 2D system. Graphene's unique properties, such as half-integer quantum Hall effect, finite conductivity at zero carrier concentration and half-metallicity make it a promising candidate for application in nanoelectronics and spintronics devices. Graphene nanoribbons, that are slices of graphene, are quasi-1D structures. They can have different edge geometries including zigzag and armchair (Fig. 1). The electronicstructure of the ribbon depends on the edge geometry. Nanoribbons intrinsically have dangling bonds at the edges. Their linear combinations form some of the eigenstates near the Fermi energy, and hence determine the ribbon properties. These dangling bonds also provide active sites for chemical bonding, making the ribbons suitable for doping. As the unique properties of the ribbons are associated with their edge states, engineering the edge will affect the electronic and magnetic properties of the ribbon. In this work we investigate a route for controlling and designing electronic and magnetic devices based on graphene nanoribbons, with wide range of properties, using the same structure mold. We suggest that by doping of the edges of the same ribbon with various atoms, from s-type to d-type transition metals, we can obtain various electronic and magnetic properties. In fact, the same ribbon doped with different dopants can be insulator, semiconductor, metal, ferromagnet (FM) and antiferromagnet (AF). Based on our results we predict that B turns the semiconducting armchair ribbon into a metal, while N, O, and S enlarge the energy gap of the ribbon and make it insulator. Doping with $3d$ transition metals provides systems with FM or AF states at the edges. Armchair ribbons doped with Cr and Co have the most stable structures with large ratios of spin-up to spin-down density of states. Therefore, graphene nanoribbons provide a wide range of possible electronic and magnetic properties based on the same ribbon structure, but different dopant atoms.

Fig.1. (a) graphene nanoribbon with armchair edge (Left) and zigzag edge (Right), as considered in the calculations. (b) magnetic moment per dopant atom. the inset is the ratio of DOS for spin up and down at Fermi E
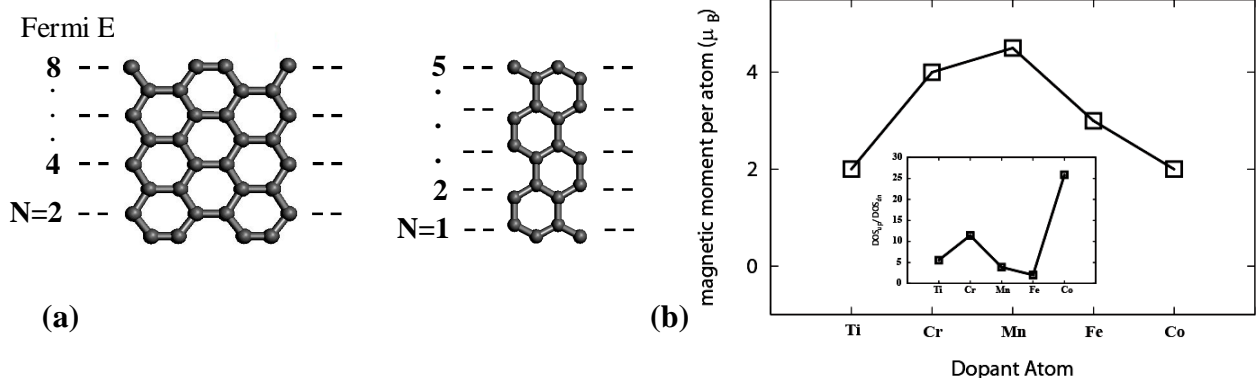
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Magneton-Phonon Resonance and Line-width in Rectangular Quantum Wire

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Using the projection operator technique we obtain the analytical expression of optical conductivity and absorption power in the case of magnetophonon resonance in rectangular quantum wires. Using computational program we draw the graph showing the dependence of absorption power on the temperature and wire's parameters. The line-widths have been obtained as the profile of the curves of graphs. The results show that the splitting of resonant peaks in the presence of laser field can be used for detection of magnetophonon resonance in the wires.

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Study of Half Metallacity of CrO_2 by Using the LSDA and LDA+U Methods

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The unusual half-mettalic electronic structure with an industrial applications, CrO_2 has recently attracted a lot of theoretical and experimental attentions. To understand more about the nature of this material, the local-spin density approximation (LSDA) and LDA+U will be performed. We intend to investigate the electronic and physical properties of CrO_2 in the rutile structure ($P42$ /mnm).The semicore electrons are regarded as valence electrons. From our study, we find that CrO_2 appears to be a half-metallic in character with a direct band gap of 1.8 eV for spin down, and purely mettalic for spin up configurations. We will try to check the difference in the results of DOS, energy bands, magnetic moments etc. by employing the LSDA and LDA+U methods.

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The Characterization of the Carbon Nanotube-Copper Composites from the First-Principle Calculations

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Introduction of carbon nanotubes (CNTs) into a metal matrix is considered to be a promising fabrication technique that can improve the mechanical properties of the metal matrix [1]. In addition to the uniform dispersion of CNTs, interfacial strength between the CNT and the metal matrix is crucial for the improved mechanical properties. However, the binding energy between metals and pristine CNT wall is known to be so small that the interfacial slip between CNT and the matrix occurs at relatively low external stress. Applications of defective CNTs with vacancy or CNTs with various surface functional groups such as –COOH or -OH have attracted great attention. Herein, we report the interaction properties of various hybrid structures composed of the defective or functionalized CNTs and copper (Cu) using the density functional theory calculations based on the generalized gradient approximation. First, differences in the binding energy and electronic structure of the CNT/Cu complexes during the reduction process from copper-oxide (CuO) to Cu are compared. Second, the characteristics of functionalized CNTs interacting with Cu are investigated. Based on these studies, we present the role of vacancy defects or interfacial oxygen atoms from either CuO or oxygen containing functional groups in the improvement of the CNT/Cu interfacial strength, which enables the preparation of high strength CNT/Cu nanocomposites.

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Controllable Synthesis of Base- and Tip-type of Multiwalled Carbon Nanotubes by a dc Plasma-Enhanced Chemical Vapor Deposition (PECVD) Technique

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An approach for synthesis multi-walled carbon nanotubes in controllable regime is presented in this work. Multi-walled carbon nanotubes (MWNT) were grown by a dc plasma-enhanced chemical vapor deposition (PECVD) technique [1-3] in various conditions. The synthesis of the base and tip-type of CNTs was selectively controlled by changing the catalyst size, catalyst film thickness correlated with altering the NH_3 pretreatment plasma current. These types of CNT exhibited distinctive properties in nanotube structure, growth rate and vertical alignment, which were confirmed by scanning electron microscopy (SEM), transmission electron microscopy (TEM), and in situ optical interference measurement. The vertically aligned behavior of CNT was systematically studied by using a fine-patterned catalyst layer with diverse critical dimensions. Freestanding single CNT was successfully realized by optimum tip-type CNT growth, conventional photolithography and wet-etch process. The development of controllable synthesis of carbon nanotube opens a new direction for quantum computer materials and sciences [4, 5].

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Calculation of the Field Emission Current from Carbon Nanotubes Using the Bardeen Transfer Hamiltonian Method

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One of the fields of great interest for carbon nanotube applicability is high brightness electron sources. The problems of the electron field emission from carbon nanotubes are studied by both theoretically and experimentally in recently. In this paper we have theoretically calculated for the field emission current from carbon nanotubes using the Bardeen transfer Hamiltonian method [1], which has used recently to investigate interwall tunneling current in double-walled carbon nanotubes [2]. The tunneling matrix element in proposed modeling of the electron field emission from carbon nanotubes is built and considered based on the tunneling approach of Bardeen. The expressions for the emission as a function of the anode voltage and of the anode plane–nanotube distance are obtained. The influence of the various tube parameters on emission current is also analyzed. The detailed computational results for emission current from carbon nanotubes by Bardeen transfer Hamiltonian method are compared with Fowler–Nordheim theory [3] and some conclusions are drawn from this comparison.

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Totally Symmetric Vibrations of Armchair Carbon Nanotubes

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Low temperature properties of carbon nanotubes (CNT) remain poorly known. Are there Peierls distortions (bond length dimerization) in the ground state of metallic carbon nanotubes or no? In [1, 2] Kekule type distortions of the $(5, 5)$ carbon nanotube in the ground state were quantitatively examined within the framework of semiempirical quantum-chemical PM3 [3] calculations and 0.003 nm bond length difference was predicted.

In this paper we propose to explore the ground state properties of armchair carbon nanotubes in low temperature Raman scattering experiments. In order to qualitatively elucidate totally symmetric vibrations of armchair CNTs in the Brillouin zone center, visible in the Raman scattering experiments, we have developed simple analytical model employing symmetry considerations and nearest neighbor harmonic interactions of CNT's carbon atoms. Parameters of this model (bond stiffnesses) can be adjusted to experiment. We show that quinoid type [1, 2] dimerization (without Peierls gap opening) does not lead to the breathing mode splitting, but to the mixing of radial and tangential displacements in the totally symmetric vibrations of armchair CNTs. Kekule type distortions (with Peierls gap) lead to the breathing mode splitting. Our PM3 calculations using MOPAC 6.0 package [4] give quantitative estimate of this splitting for the case of calculated in [1, 2] geometrical structure of $(5, 5)$ CNT as $10\,\text{cm}^{-1}$. Thus, the problem of the ground state structure of armchair CNTs can be solved experimentally.

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An Efficient Tool for Modeling and Prediction of Fluid Flow in Nanochannels

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Molecular dynamics simulations were performed to evaluate the penetration of two different fluids (i.e., a Lennard-Jones fluid and a polymer) through a designed nanochannel (See Figure 1). For both fluids, the length of permeation as a function of time was recorded for various wall-fluid interactions. An artificial neural network (ANN) approach was then employed for modeling and prediction of the length of imbibition as a function of influencing parameters (i.e., time, the surface tension and the viscosity of fluids and the wall-fluid interaction). It was demonstrated that the designed ANN is capable of modeling and predicting the length of penetration with higher accuracy (i.e., the squared correlation coefficient (R^2) and the mean squared error (MSE) equal 0.9860 and 0.0134, respectively) than that calculated using the Lucas-Washburn equation (i.e., $R^2 = 0.8771$). Moreover, the importance of variables in the designed ANN, i.e., time, the surface tension and the viscosity of fluids and the wall-fluid interaction, was demonstrated with the aid of the so-called *connection weight* approach, by which all parameters are simultaneously considered. It was revealed that the wall-fluid interaction plays a significant role in such transport phenomena, namely, fluid flow in nanochannels.
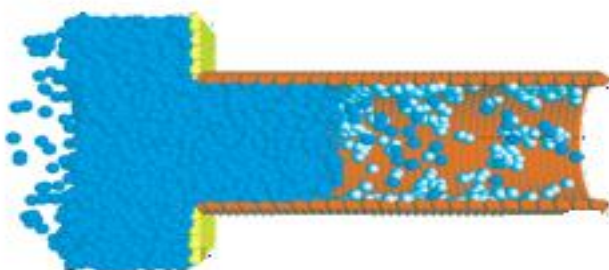
Figure 1. An illustration of the molecular dynamics (MD) simulation of fluid flow through the nanopore

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Calculation of the Nonlinear Absorption Coefficient of a Strong Electromagnetic Wave by Confined Electrons in Quantum Wires

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Analytic expressions for the absorption coefficient of a strong electromagnetic wave (EMW) caused by confined electrons in quantum wires are calculated by using the quantum kinetic equation for electrons for the case of electron – optical phonon scattering. Second-order multiphoton process is included into present account. The dependence of the absorption coefficient on amplitude and photon energy of the EMW, the temperature of the system, and the radius of quantum wire is graphically obtained for a specific quantum wire GaAs/GaAsAl. The results show that the dependence of the absorption coefficient on the amplitude of the EMW is nonlinearity and the dependence of the absorption coefficient on the photon energy or the radius can be use for opticaly detected electrophonon resonance effects in quantum wires.

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Waters Mediate Interaction between Proteins:
An Observation by Data Mining Method

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Dynamics of hydration water surrounding protein is the essential driving force for the specific properties of protein [1]. Many theoretical and experimental studies define the hydration layer from the viewpoint of the distance from the protein surface and discuss the physical properties of each water layer. In this study, we adopt the support vector machine (SVM) techniques for classification problem of solvation water of protein and attempt to distinguish the hydration and bulk waters as the machine learning problem. The dynamics of solvation water are reproduced by molecular dynamics (MD) simulation with AMBER10 program package. CPI-17 (PDBID: 1J2M [2]) protein and designed peptide (PDBID: 1PSV) are adopted for the target protein. From the MD simulation of ideal pure water system and ideal hydration system, water classification SVM are constructed by training RMSD value of each system. Comparing the conventional water counting classification and SVM classification, we propose the new analytical approach for the dynamical structure of solvation water. During the MD simulations with various salvation conditions, we discuss the protein – protein interaction via hydration water molecules.

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Determine Crystal Structure of Poly(pentamethylene 2,6-naphthalate) by Molecular Modeling Technique

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Molecular simulation is a powerful research tool for gaining new insights into polymer chemical structure and processes. This study presents a computational conformation analysis of poly(pentamethylene 2,6-naphthalate). The computational analysis and calculation were performed using the Cerius^2 program (version 4.1), molecular simulation software for material science, designed by Molecular Simulations Incorporated. The total potential energy of a molecular chain consists of the contributions from the intramolecular and intermolecular interactions. The intramolecular interactions consist of the bond stretching, angle bending, torsional, and inversion terms. The intermolecular interactions include van der Waals and Coulomb terms. The COMPASS force field was use to calculate the potential energy of crystal structure, and the Ewald summation method was used in the energy-minimizing calculation.. Standard bond lengths and angles for polyesters were adopted to build repeating unit. It is found that the PPN backbone takes all-*trans* conformation in the pentamethylene unit, and two naphthalene rings are in face-to-face arrangement.

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Computation of Chemical Equilibrium in Multi-component Zirconium Alloys for Biomaterials Applications

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Thermodynamic databases are widely applied in the calculations of chemical equilibrium in multi-component alloy systems, for instance FactSage[1] is a well known software for thermodynamic calculations. It predicts chemical equilibrium involving multi-component and multi-phase systems, based on first principles thermodynamic laws.

In this research, we critically evaluated the solution database of Zr based alloys provided by FactSage[1], and modified the model parameters for sub-binaries whenever necessary. The thermodynamic database can express the Gibbs free energy of the beta-Zr phase and alfa-Zr phase respectively as a function of temperature and composition of the alloy. The re-optimized database will be used to design multi-component beta-zirconium alloys for applications in biomedical load-bearing implant. The new biomaterials are expected to demonstrate good corrosion stability, biocompatibility, low cytotoxicity and a negligible tendency to provoke allergic reactions.

Pure zirconium shows two allotropic modifications with a transition temperature at 863 $_o$C, which are a low temperature alfa-Zr phase of hexagonal closed-packed structure (HCP) and a high temperature beta-Zr phase of body centered cubic structure (BCC). Implant made of beta-Zr is biocompatible due to its low elastic modulus matching that of the surrounding bone tissue. In particular, the patented Oxinium$_R$ (ASTM B550), or a binary Zr-2.5%Nb alloy, is the first new metal alloy adopted in orthopaedic surgery in 30 years. In our study, all beta-phase stabilizer elements besides Nb (like Sn and W) will be tested computationally to further stabilize the single beta-Zr phase range in terms of temperature and composition. New alloys may be designed accordingly.

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Samdwich Microstructure of Tumblebug Cuticle

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Insect cuticle possesses excellent strength, stiffness, fracture toughness and lightweight, which are closely related to its elaborate microstructures optimized through millions of years' evolution. The researches on the microstructures may provide beneficial guidance for developing new high-performance composites, especially, ultra lightweight composites. In this work, a scanning electron microscope (SEM) was used for the observation of the microstructures of a Tumblebug cuticle. The observational result showed that the cuticle is a kind of natural biocomposite consisting of chitin-fiber plies and sclerous protein matrixes. More careful observation showed that there are a kind of chitin-fiber-continuous biosamdwich structure in the cuticle. Based on the SEM observation, a comparatively computational analysis on the ultimate strength between the biosamdwich and the traditional-design samdwich structures was conducted with their representative models. The analytical result shows that the fracture strength of the biosamdwich structure is larger than that of the traditional-design samdwich structures. At last, a biomimetic samdwich structure was designed and fabricated with glass fibers and epoxy resin materials. The ultimate strength of the biomimetic samdwich structure was experimentally investigated and compared with that of the traditional-design samdwich structure. The experimental results validated the computational results of the analytical models.

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Spiry Microstructure of Aragonite Sheets of Chamidae Shell

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Molluscan shell is a kind of natural composite with excellent fracture strength and fracture toughness, which can be attributed to its unique microstructures. The observation of Scanning electron microscope (SEM) shows that Chamidae shell is a kind of bio-ceramic composite consisting of aragonite and organic materials. These aragonite and organic materials distribute in the shell in the form of layers parallel with the surface of the shell. The observation also shows that the aragonite layers consist of numerous thin and long aragonite sheets, which are dozens of nanometers in diameter and can be regarded as aragonite fibers. These aragonite fibers align in different layers with different orientations and compose several particularly distributed microstructures. A kind of particular spiry layup is found. In the layup, the aragonite fibers in arbitrary aragonite layer make a fixed angle with the aragonite fibers in its adjacent aragonite layer. The maximal pull-out force of the spiry layup of the aragonite fibers was analyzed based on its microstructural model, which accounts for the high fracture toughness of the shell. The analytical result was compared with that of the conventional 0° layup. It shows that the maximal pull-out force of the spiry layup is markedly larger than that of the conventional 0° layup, which was validated with a comparative experiment of the maximal pull-out forces of both the spiry and the 0° layups.

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Anisotropic Diffusion in Disordered Fractals

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Porous materials such as metal foam, cements or porous rocks exhibit fractal structure for a range of length scales. Diffusion in porous media under the influence of an external field can be modelled by the anisotropic diffusion in fractal structures. We employ fractals obtained by randomly mixing different Sierpinski carpet generators. The anisotropic diffusion is simulated by the field-biased random walk on such fractal structures. Particularly we study the random-walk exponent d_w, which characterized the anomalous diffusion. For the mixed system, it strongly depends on the mixture composition and the external field. The diffusion can be enhanced or suppressed under the influence of the field.

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Study of Thermodynamic Properties of Cerium Dioxide under High Pressure

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The moment method in statistical (SMM) dynamics is used to study the thermodynamic quantities of cubic flourite cerium dioxide taking into account the anharmonicity effects of the lattice vibrations and hydrostatic pressures. The thermodynamic quantities of CeO_2 are calculated as a function of the pressure. The SMM calculations are performed by using the Buckingham potential for the cerium dioxide. The effects of the 3 different potential parameter sets of the Buckingham potential on some thermodynamic properties for CeO_2 are also investigated.

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Electrophonon Resonance in Square Quantum Wells of n-GaAs Materials

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Electrophonon resonance (EPR) was introduced by Bryskin and Firsov [1]. The EPR effects provide useful information on the transport properties, such as the effective mass of low-dimensional electrons and the energy difference between adjacent electric subband levels of low-dimensional structures, of low-dimensional semiconductors [2, 3]. EPR effects can only be observed for the resonant scattering of electrons confined in electric subband levels by longitudinal optical (LO) phonons whenever the LO phonon energy is equal to the energy separation between two electric subband levels in such low-dimensional structures [4,5]. In most works, EPR conditions are obtained using the linear response limit of the dc conductivity.

In the present work, obtainment for EPR conditions in quantum wells of n-GaAs polar semiconductors with a square potential well is based on a general expression for the nonlinear dc conductivity. The EPR conditions as functions of the well width for are also studied. In particular, anomalous behaviors of the EPR line-width, such as the EPR peaks for the well width and the miniband widths, are discussed. Results show that as the width of well is increased, the width between EPR peaks is decreased. As the well width is increased, the number of the EPR peaks due to the resonance transitions from the subband level n to any n' is increased.

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The Electronic Properties of MgO under High Pressure from Ab Initio Calculations

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MgO is not only one of the most abundant minerals in the Earth, especially in its lower mantle, but a material which is among the least polymorphic solids known, only one solid phase, with the NaCl structure type has been observed in experiments spanning pressures up to several hundreds GPa and temperatures up to several thousand degrees Kelvin. Furthermore, it is known that atsufficiently high compression, all materials should become metallic, but MgO is very difficult to metallize.

In this work, we present a first principles investigation of the electronic properties of MgO, the properties were obtained within density functional theory formalism thathas been proved to be very successful in the previous study for kinds of materials such as manganates [1] and polymers [2]. The electronic properties of the materials and the property evolution with pressure up to hundreds of GPa were studied and comparisons were made. It is found that the results are generally in good agreement with recent theoretical and experimental work. The element iron has a great influence on the magnetic properties when doped in the material.

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Complex Characterization of the Nanostructured Materials by Using the Scanning Probe Microscopy Methods

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The tendencies of miniaturization techniques related with the establishment of the miniature instruments, the micro-electromechanical systems (MEMS), as well as the development of the nanotechnology have required the studying of the new exact characterization methods for the precision surfaces and the nanostructured materials. The extensive opportunities in the development of the experimental methods of the complex analysis for the surface materials on the micro- and nanoscale are opened in the scanning probe microscopy, in particular – the atomic force microscopy. This paper shows the applications of the classical methods atomic force microscopy (the shear-force (lateral force) mapping, the physic-mechanical properties and the static force spectroscopy), as well as the developments of the original methods and the equipments AFM.

The methods of the analysis are shown in the realization process of the nano-drilling based on AFM. The algorithms and the computer software for modelling the contact probe-sample and analyzing the properties of surfaces based on the data AFM for are presented. The models based on the theory of the random fields, the 3D models surface layers, the models based on the method of the finite elements are realized. The geometrical and physico-mechanical heterogeneity in the near-surface layers and the interaction of the surface force of the molecular and the capillary are considered. Furthermore, the examples of the developed application and the analysis of the probe methods in the designing the surfaces of system of magnetic record, the clock component, the microtweezers and the polymeric layers for pressure forming are presented. The investigations have opened the new direction of the development of the techniques in the micro- and nanotribology, as well as the methods scanning probe microscopy.

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Another SP^3 Bonded Carbon Crystal

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The known bulk solid phases of carbon are diamond with sp^3 bonding and graphite with sp^2 bonding. Carbon can assume many structural forms because it can form several distinct types of valence bonds[1]. Recently a new metallic carbon crystal with sp^2 bonding having K$_4$ structure is proposed[2]. Logically if there could be a second sp^2 bonded attractive 3D crystal parallel to graphite, then there could be a second sp^3 bonded interesting 3D crystal parallel to diamond. We predict the possible existence of a new phase of carbon – a simple cubic carbon crystal - exhibiting metallic behavior from the first principles calculations using density functional theory. The interaction between cores (core electrons and nucleus) and valence electrons is modeled by projected augmented wave method. The charge density analysis shows that simple cubic phase of carbon is sp^3 bonded system and confirms the promotion of one electron from 2s to 2p orbital due to the sp^3 hybridization. The six orthogonal bonds made up of p orbitals protrude from the sphere shaped s orbital charge distribution. The bonds between the atoms are semi covalent and weak due to the insufficient valence electrons. This reduction in covalency contrast to diamond induces the metallic nature in the simple cubic carbon. From the total energy calculation, the possibility of pressure induced phase transition from diamond to simple cubic carbon is predicted.
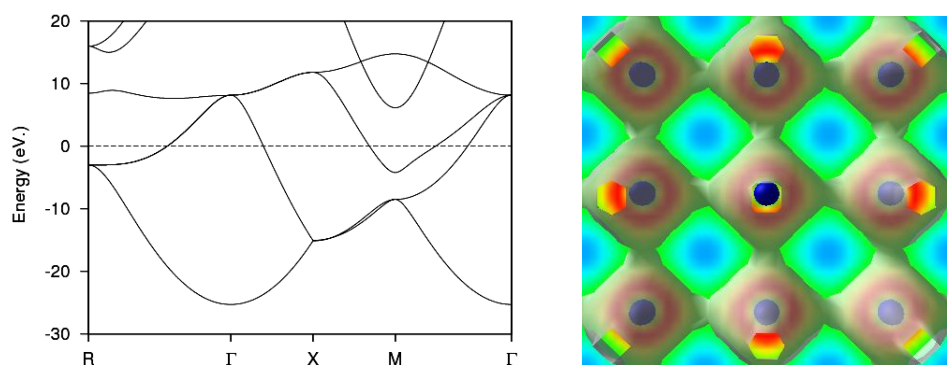
Band structure of simple cubic carbon   Isosurface plot of the simple cubic carbon

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P - 36

Mesoscale Simulation on Phase Behaviour of Triblock Copolymers with Different Chain Architecture in Aqueous Solution

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The mesoscale simulation method called dynamic variant of mean-field density functional theory (MesoDyn) was used to simulate the phase separation behavior of triblock copolymer with various combination of $-[CH_2CH_2O]_n-$ and $-[CH_2CH(CH_3)O]_n-$ (PEO and PPO unit, respectively) in aqueous solutions. The equivalent method was applied to perform the parameterization of the Gaussian chain as established in earlier work by Y.-M. Lam *et al*. With a simple copolymer model, various aggregate structures of block copolymer in water including the micelle, hexagonal, and lamellar phases are produced which can partly reproduce most experimental phase regions. The effect of chain topology such as (1) ABA and BAB arrangement, (2) different A:B ratio, where A = PEO and B = PPO, on the Critical Micelle Concentration (CMC) and (3) copolymer concentration on phase morphology at room temperature was also investigated. The results show that PPO components can aggregate and form an inner core of micelle, surrounded by PEO block. The spherical micelle formed at lower concentration with longer PPO block length in triblock copolymer. The poly(propylene oxide) (PO) block amount is found to influence not only the aggregate morphology but also its formation rate in solution.

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P - 37

Challenges in Modelling TCP Phase Formation in Ni-based Superalloys

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Modelling topologically close-packed (TCP) phase formation in Ni-based superalloys is a challenging task with only the semi-empirical PHACOMP and NewPHACOMP schemes providing some guidance. In this talk we develop a microscopic understanding of the factors that control TCP phase stability by coarse-graining the electronic structure from density functional theory (DFT) to tight-binding (TB) to bond-order potentials (BOPs). These many-body interatomic BOPs are unique in that they depend explicitly on the electron per atom (e/a) ratio, so that they predict the structural sequence from bcc to sigma to khi to hcp that is found, for example, across the W-Re system. The observed stability of the mu and Laves phases requires the additional contribution of size and electronegativity differences. Remaining challenges in modelling TCP phase formation are briefly discussed.

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Fabrication and Calculation of the Friction Coefficient of Cu Matrix Nanocomposites Material is Reinforced by Carbon Nanotubes (CNTs)

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Carbon nanotubes (CNTs) have been considered as an ideal reinforced to improve the mechanical performance of some materials. Because of their exceptionally small diameters ($\approx$ several nm) as well as their high Young's modulus ($\approx$ 1 TPa), tensile strength ($\approx$ 200 GPa) and high chemical stability, CNTs are attractive reinforcement materials for light weight and high strength metal matrix composites. In this paper, our report present some result of fabrication and calculation of the friction coefficient of Cu matrix nanocomposites material is reinforced by carbon nanotubes (CNTs). Cu/CNTs nanocomposites material is fabricated by powder metallurgy method. The microstructure of CNT/Cu nanocomposites consists of two regions including CNT/Cu composite region, where most CNTs are distributed, and CNT free Cu matrix region and showed by SEM. Mechanical properties such as hardness and wear resistance were researched. Base on experimental results, we were calculated of the friction coefficient of Cu/CNTs nanocomposites. The results will be detail discussed in this paper.

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Scanning Probe Microscopy Methods in the Complex Characterization Nanostructured Material and Surface

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The miniaturization tendency in the technique relates to creation of the miniature instruments, micro-electromechanical systems (MEMS), as well as to nanotechnology in common sense. It is necessary to develop the new methods for precise characterization of the surface and nanostructure materials. The big opportunity for creation experimental methods for a complex analysis of the surface and materials at nanoscale is opened in the scanning probe microscopy (SPM), in particular – the atomic force microscopy (AFM).

This paper will discuss about special aspects of the application classical methodology AFM (the shear-force (lateral force) mapping, physic-mechanical properties mapping and the static force spectroscopy), original methods and AFM instruments, which have been developed by us.

The new analyzing method is based on realization procedure "nano-drilling" by AFM. The algorithms and software program for modeling the probe-sample contact based on AFM data of the surface properties will be presented. Realized model is based on the theory of random fields, the Vinklerovski surface layers 3D model and the finite elements method. The geometrical and physic-mechanical heterogeneity of the near-surface layers, interaction of the surface force with molecular and capillary nature are considered for this model. The applications of the developed probe method analysis have been demonstrated in the designing working surface for the magnetic record system, clock component, microtweezer and polymer layer for the nanostamping. The possibility of the applying new methods AFM for characterization biological cells and tissue will be discussed. We also discuss about a tendency and future of the development SPM methods.

P - 40

Effect of Stereochemical Composition on Dynamic Properties of Polypropylene Melts : A Multiscale Molecular Simulation

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The stereochemical effect on the diffusion of polypropylene (PP), was studied with the novel multiscale molecular simulation at 473 K for pure melts of atactic, isotactic and syndiotactic polypropylene chains with a composition of $C_{75}H_{152}$. The simulations of coarse-grained models were performed on a high coordination lattice, with incorporation of short range intramolecular interactions from a rotational isomeric state (RIS) model, and incorporation of long range interactions defined by a Lennard-Jones (LJ) potential function of propane pairs. The efficiency of the simulation on the sparsely occupied high coordination lattice facilitates the equilibration of melts within accessible computer time. Isotactic PP (iPP) was found to diffuse faster than syndiotactic PP (sPP), but a maximum in the diffusion rate at an intermediate stereochemical composition (aPP). Simulation found diffusion coefficient (D) at high P_m several times faster than at low P_m. Sequences of *meso* and *racemo* diads diffuse faster in aPP due to quenched randomness of stereochemical sequences than in iPP and sPP. Mixtures of 50:50 wt% PP with different chain tacticity was also investigated. aPP and iPP are miscible in the melt, but sPP demixes from either aPP or iPP. The demixing is stronger for the iPP/sPP blend than for the aPP/sPP blend. Slowing down of PP chains were observed if sPP was in the mixture. The mechanisms described here for PP may affect the mobility of other polymers in which stereochemical composition is an issue.

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Finite Element Analysis of Magnetic-Mechanical Structures for AFM

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In this paper, design and simulation of two types of cantilever are presented. For the mechanical cantilever, we have designed it using rectangular and triangular structures, which shown the effect of geometry on resonant frequencies and force constant. For the magnetic force driven cantilever, we propose a mechanical model with Ni plate controlled by solenoid coil. We have analyzed some properties such as the effect of Ni plate on the resonant frequencies, the dependence of force on the electric current I and number of solenoid loops N. This is important information for designing more complex MEMS structure in which the mechanical and magneto electric interaction need to be included.
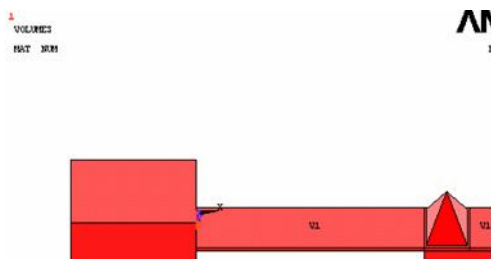
Fig. 1. Model of Si- cantilever coated with a ferromagnetic layer
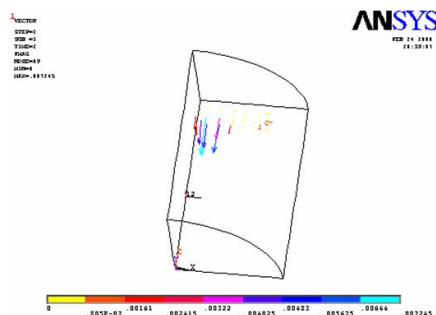
Fig. 2. Effect the F magnetic force applied on Cantilever with N= 500 circle, I = 15 mA

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Multiscale Modelling of Nanoindentation

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Nanoindentation is an experimental technique used to measure the hardness of materials on the nanoscale. Traditionally either molecular dynamics or finite element methods have been used to model this process. The difficulty in applying finite element models to these problems comes from producing a suitable model of the plastic behaviour of the material. Whilst in molecular dynamics models the problem is one of the influence of the boundary conditions on the results.

We will present a 3D multiscale model of nanoindentation that couples a molecular dynamics (MD) model with a finite element (FE) model. The MD model is used to describe the tip and the material around the tip at the atomic scale, allowing for an accurate description of plastic deformation. The FE model is used to describe the long range elastic fields in the material. We will show how this model gives contact pressures, which are in better agreement with experimental results than traditional atomistic only models, illustrating that a correct description of the long range elastic field is essential. We will illustrate the importance of such corrections by applying the methodology to a variety of different systems.

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Spherical Indentation On Ceramic Coatings

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In this paper, the spherical indentation on ceramic coatings was presented. Ceramic coatings have been using of protection and repairing for components of machine and power engines. Mechanical behavior such as deformation, stresses and cranks were carried out in this study by modeling and experimental methods. The coatings with multi-layer have better mechanical behavior in deformation and stress statuses. The thickness of coatings played an important role for mechanical behaviors.

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A New Stiffened Element Using to Analyse the Mechanical Behaviour of Stiffened Laminated Plates under Free Vibration

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A new 9-noded rectangular stiffened plate element for the vibration analysis of laminated stiffened plates based on Mindlin's deformation plate theory has been developed. The stiffened plate element is a combination of basic rectangular element and beam bending component. The element can accommodate any number of arbitrarily oriented stiffeners and obviates the use of mesh lines along the stiffeners. A finite element algorithm and computer program with this element are developed to analyse the mechanical behaviour of stiffened laminated plates under free vibration, and the results are compared with those published.

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Nonlinear Analysis of Stability for Functionally Graded Cylindrical Shells under Mechanical Loads

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This report presents a simple solution of the stability of functionally graded cylindrical shells under mechanical loads. Material properties are assumed to be temperature-independent, and graded in the thickness direction according to a simple power law distribution in terms of the volume fractions of constituents. Equilibrium and compatibility equations for functionally graded cylindrical shells are derived by using the Donnell shell theory taking into account geometrical nonlinearity due to large deflection and initial geometrical imperfection. The resulting equations are analytically solved by Galerkin procedure to obtain explicit expressions of post-buckling load-deflection curves. Stability analysis of a simply supported functionally graded cylindrical shell under mechanical loads shows the effects of the volume fraction index, shell geometry and imperfection on post-buckling behavior of the shell.

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Numerical Simulation of Heat Stresses and Durability of the Combustor Wall

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The development of advanced combustion chambers for the future propulsion systems of airplanes requires the ability to predict the thermal stresses and durability of the combustor wall. This paper presents the study of above mentioned problem in an annular burner, by taking into account the fluid - structure interaction. After having simulated the cooling air introduced around the combustor to reduce the high temperature, the obtained temperature distribution is then used like the thermal load for studing of the wall structure. Results from the study such as the total stress and displacement will assure the good mechanical properties and durability of the material of combustor wall.
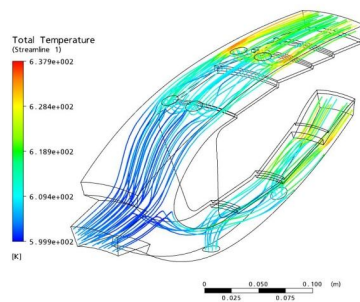
Figure 1: Temperature distribution of cooling air
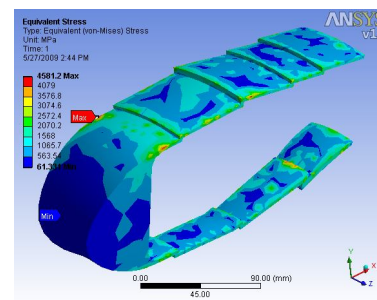
Figure 2: Equivalent stress of the combustor wall

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Study on Mechanical and Thermodynamic Property of Some Cryocrystals

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The mechanical and thermodynamic properties (such as the lattice constant, the molar volume, the isothermal compressibility, the melting temperature, the limiting temperature for absolute stability of lattice state and the fcc-hcp transition temperature, the mean squared displacements, the Debye-Waller factor, the Gruneisen parameter and the Lidemann) of some cryocrystals with fcc and hcp structures (such as N_2, CO and He) at various temperatures and pressures are investigated by the statistical moment method (SMM) in statistical mechanics and compared with the experimental data.

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Effect of Current Crowding on Electromigration Lifetime Investiganted by Simulation and Experiment

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The impact of current crowding on the electromigration lifetime of various interconnect layout designs was investigated through simulations and experiments. Most 2D electromigration simulators use the conventional electromigration model which does not include the effect of current crowding on the electromigration lifetime while electromigration experiments have shown this effect to be important. A new model including this effect is discussed for electromigration simulator improvement in the future. Then the current crowding effect was experimentally investigated in detail in different interconnect layout designs. This has provided a good understanding of the current crowding effect that can be very useful to improve the reliability of multilevel interconnects in the design phase.

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Numerical Simulation of the CUA DAT Dam

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With the size of 1117m long and 117.3m wide, Cua Dat dam which is being built in the upstream of Chu River, Thanh Hoa province becomes one of the biggest dams in Vietnam [1]. Modeling of its structure and behaviors in the pre-construction is critically important to ensure its durability and high performance. The paper presents results of the simulation of Cua Dat dam by Finite Element Method using ANSYS software. Given the large size and complex geometry of the dam, the unstructured mesh with high resolution is used to ensure the highest level of accuracy. The simulation concentrates in the displacement of dam in a wide range of practical conditions, e.g. influence of the dam's body weight, maximum water level in the upstream and downstream, etc. The results obtained from the simulation are important inputs for the design, construction and operation of the dam.
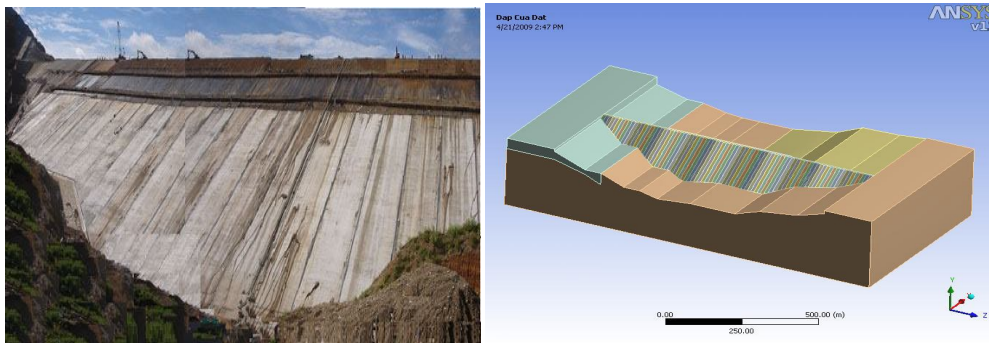
Figure : Cua Dat Dam at Thanh Hoa Province (on the left) and the modelling geometry (on the right)

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An Application of the Meshfree Radial Point Interpolation Method in Solving the Two-Dimensional Node-To-Node Contact Problems

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Meshfree methods have gained more and more attention over the last two decades in analyzing mechanical problems because of their high potentials. In this paper, a meshfree method, Radial Point Interpolation method, is used to solve the two-dimensional node-to-node contact problems. Some examples of normal contact and tangential contact are considered. A Matlab program is also written to implement the method. The results are compared with analytical solutions and with the fine-mesh *FEM* results obtained by software ANSYS where the analytical solutions are not available.

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Finite Element Modeling and Experimental Study on Bending and Vibration of Laminated Stiffened Glass Fiber/Polyester Composite Plates

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In this paper, free vibration and bending behaviour of laminated stiffened glass fiber/polyester composite plates with laminated open section (rectangular or T shaped) and closed section (hat shaped) stiffeners have been studied by finite element method and experiment. A nine-noded isoparametric element with nine degrees of freedom at each node is developed for the plates. The stiffener element is a three-noded isoparametric beam element with five degrees of freedom and the stiffeners can be positioned anywhere within the plate element. The natural frequencies and deflections of the stiffened plates are determined experimentally by Dewebook device and DasyLab 7.0 software. The results of the computational model for above plates under simply support and clamped boundary conditions and subject to uniform load and concentrated load are in good agreement with experiments. The failure problems of these stiffened glass fiber/polyester composite plates are also investigated.

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Finite Element Modeling for Bending and Vibration Analysis of Laminated and Sandwich Composite Plates Based on Higher-Order Theory

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A nine-nodded rectangular element with nine degrees of freedom at each node is developed for the bending and vibration analysis of laminated and sandwich composite plates. The theory accounts for parabolic distribution of the transverse shear strains through thickness of the plate and rotary inertia effects. The parametric effects of plate: aspect ratio, angle of fiber orientation, side-to-thickness ratio and degree of orthotropy on in-plane stresses, transverse shearing stresses, displacements, and fundamental frequencies are shown. Results are compared with existing analytical and numerical solutions.

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Evolution of Void and Constitutive Descriptions of Casting Magnesium Alloy

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Casting magnesium alloy inevitably includes many microscopic voids. The research on the material properties should consider the effect of the evolution of the voids on the material behavior and combine microscopic and macroscopic analysis. The work includes the investigations of void evolution and constitutive equations of the material. The microscopic stresses are obtained through the analyses of the microscopic velocity and the strain fields of a cylindrical void-cell model. The macroscopic stresses obtained based on the approach of micro-to-macro transformation. The void evolution rules consist of void growth and void nucleation ones. The former is obtained from matrix continuity condition, and the latter is derived by assuming that the rate of void nucleation is related to the increment of intrinsic time measure. A nonclassical constitutive equation involving void evolution is obtained by making use of a thermomechanically consistent mechanical model which considers the effects of the void evolution on the material properties. The obtained constitutive equation is applied to the analyses of the deformation and the void evolution of the columned specimens of casting magnesium alloy ZL101. The computational results agree well with experimental data.

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Atomic Structures and the Magnetism of fcc Fe/Cu(111) Films: First-principles Calculations

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The magnetism of fcc Fe/Cu(111) surface system was found to have a strong dependence on the structural charicteristics of the Fe/Cu interface[1], which means the possibility of magnetic property tayloring with the solid relation between the structure and the magnetism of the system. Using the density functional theory[2] calculations, the atomic structures and the magnetism of fcc Fe/Cu(111) films were systematically and quantitatively investigated increasing the amount of adsorbed Fe atoms from one atom to 3 monolayers(ML). Isolated single Fe adatom adsorbed on the surface of a 5ML (111) – (2X2) fcc Cu supercell was found to be antiferromagnetic with the magnetization magnitude higher($3.17\mu_B$) than bulk Fe($2.00\mu_B$). However, as more Fe adatoms were adsorbed, the Fe atoms turned ferromagnetic. With the Fe coverage below 1ML, the ferromagnetic state became unstable as shown by the nearly zero demagnetization energies while the completely filled 1ML Fe was in a stable ferromagnetic state with high demagnetization energy, 0.63eV per Fe atom. For 2 and 3ML Fe coverage, Fe layers were found to favor fcc stacking sequences regardless of the Cu substrate and the demagnetization energies were also higher than the Fe layers in hcp sequences. The demagnetization energy reduction by the intermixing across the Fe/Cu interface could explain the well-known magnetization frustration by the structural imperfection in Fe/Cu systems[1].

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Modelling Gadolinium Doped Gallium Nitride

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Very Dilute GaN:Gd has been suggested as an excellent candidate for a room temperature dilute magnetic semiconductor, with an exceptionally high magnetic moment per Gd atom claimed experimentally.[1] The theoretical literature on this system contains several attempts to explain the observed magnetic ordering, however, all models we are aware of suffer from a range of physically incorrect assumptions. These include excessively high carrier concentrations for semi-insulating materials, coupling is via unstable defects (ignoring the claimed negative-U behavior of this nitrogen vacancies for example) or excessively small cell sizes with associated unphysical Gd concentrations. Additionally, effects such as the strong Gd *4f* spin-orbit coupling are neglected. In an attempt to remedy these deficiencies we present a density-functional based study of GaN:Gd in large cells, correctly considering the thermodynamics of defects present at the experimentally relevant conditions. We also include the effects of spin orbit coupling and strong correlation for the *4f* states via LDA+U and pseudo self interaction corrections.[2]

We discuss magnetic coupling between Gd atoms via states associated with stable defects at physically reasonable concentrations.

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Tailoring Intramolecular Exchange Coupling of Mn_4 Single-Molecule Magnets: A way to Develop Single-Molecule Magnets

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Single-molecule magnet (SMM) is a molecule that can function as magnets below its blocking temperature (T_B). Tailoring intramolecular exchange coupling is an effective way to develop SMMs and SMM-based materials. Tailoring intramolecular exchange coupling requires deeply understanding of magneto-structural correlations of SMMs. Previous theoretical studies [1] of SMMs success in calculating these quantities of synthesized SMMs, however, discussion about magneto-structural correlations of SMMs as well as suggestion for designing new SMMs are still missing. In this paper, we present possibilities of tailoring intramolecular exchange coupling of a fascinating SMM system, i.e. distorted cubane $Mn^{4+}Mn^{3+}_3$ SMMs based on Density-functional theory.

The magneto-structural correlations in $Mn^{4+}Mn^{3+}_3$ SMMs have been explored. We also succeed in establish a method to evaluate the possibility of ligands in forming exchange pathway between Mn ions of $Mn^{4+}Mn^{3+}_3$ SMMs. These results give us an effective method to design new superior $Mn^{4+}Mn^{3+}_3$ SMMs with strong intramolecular exchange coupling.

In conclusion, we have succeeded in exploring possibilities of tailoring intramolecular exchange coupling of $Mn^{4+}Mn^{3+}_3$ SMMs based on DFT. The results strongly support for syntherizing new superior $Mn^{4+}Mn^{3+}_3$ SMMs with strong intramolecular exchange coupling.

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NMR in Nanoscale One-dimensional Spin Chain

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The one-dimensional chain of Cu-O in a quantum system such as the Ca_2CuO_3 exhibits a strong spin ½ antiferromagnetic coupling between the copper atoms [1]. This paper shows how much the Cu-O chains with different lengths and spin states (singlet and doublet) effect the chemical shifts in the NMR signals. The UB3LYP/6-31G(d) was used to calculate the NMR signals and the hyperfine splitting caused by the nuclear spin - electron spin interaction. The obtained values show that there are large differences in splitting of the ^{63}Cu resonances between the copper atoms lying at the beginning, the middle and the ends of the spin chains.

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Density Functional Study of Electronic Properties of Perovskite Systems $La_{1-x}Sr_xFeO_3$

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The electronic properties of perovskite systems $La_{1-x}Sr_xFeO_3$ (x = 0, x = 0.67, x = 0.75, x = 1 for periodic structures and x = 0.5 for clusters) were investigated basing on density functional theory (DFT) and Dmol3 code. Our results show that $LaFeO_3$ is antiferromagnetic insulator and

$SrFeO_3$ expresses itself as conducting material with dominated antiferomagnetic phase. Evidence for an existence of iron ions with different valences is confirmed also by calculation. Especially, for $La_{0.33}Sr_{0.67}FeO_3$ iron ions may have valences $\geq +5$. Investigation on polarization of clustering $La_{0.5}Sr_{0.5}FeO_3$ structure reveals that this system is spontaneously strongly polarized with magnitude of polarization vector $\propto 10^2$ times larger than that of well-known ferroelectric $BaTiO_3$.

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Influence of Doped Rare-Earth Elements on Electronic Properties of $R_xCa_{1-x}MnO_3$ Systems

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Basing on Dmol3 code with density functional theory (DFT), we have investigated the influence of doped rare-earth elements on the electronic properties of oxide systems $R_xCa_{1-x}MnO_3$ (R = La, Nd, Eu, Tb, Ho, Y). We carried out a survey of density of state (DOS), band structure, tolerance factor, and Jahn-Teller distortion, etc. The results show that rare-earth doping elements caused different changes of crystal structure, hopping amplitude, and electrical resistivity of these perovskite systems at the same ratio of Mn^{3+}/Mn^{4+}

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Ground State of Spin Chain System by Density Functional Theory

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The Cu-O based spin chain system A_2CuO_3 (A=Sr, Ca) has attracted considerable attention of scientists during the last decades due to its unique electronic structure. There was not, however, a higher-level theory study of the electronic structure of these compounds and the quantitative analysis with adequate accuracy was not still established. This paper presents the single-point energy calculation using the DFT/B3LYP level theory. In contrast to the Hartree-Fock level that has been involved previously in other studies (e.g. in [1]), the DFT/B3LYP also includes aspects of electron-correlation, which is important for the strongly correlated system. The calculation was carried out on basis of two small model clusters and the respective energy diagrams were obtained.

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Structural Stability, Magnetism and Hyperfine Interactions of Hydrogen Monomer, Dimers, Trimers and Tetramers on Graphen

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Using first-principles electronic structure calculations, we investigate the structural stability, magnetic properties of hydrogen monomer, dimers, trimers and tetramers adsorbed on graphene sheets. We demonstrate that the magnetic behavior of such a systems depends on the geometrical configuration of hydrogen atoms. To predict the stability of the systems two effects become important: the distance between hydrogen atoms and the exchange energy between the local magnetizations. Additionally, for all structures, hyperfine parameters of hydrogen and carbon atoms are calculated. As a result, system with large hydrogen hyperfine coupling represents the large localization of the excess charge. Finally, for two types of defects in graphene, the hydrogen monomer and the vacancy defect, the hyperfine structures are compared.

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The The Monte Carlo Simulation of Magnetic Nanoparticle Systems

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We use Monte Carlo method to study size dependence of peak temperature in magnetic particle systems without interactions. We assume that the size of particles obeys the lognormal distribution. We show the temperature dependence of the magnetization. In the non-interacting model, the peak temperature in zero-field-cooled is simply the average blocking temperature of all the particles. We find that with increasing of the width of the distribution, the peak temperature of system increases. Same time, the mean diameter of the particle system also influences on the peak temperature. Our model is simply, but it can provide the essential information in syntheses and applications of magnetic nanoparticles.

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Atomistic Simulation of the Interlayer Structures and Dynamics of the Hydrated Potassium-Montmorillonite

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Theoretical investigation of the interlayer structure of hydrated montmorillonite (MMT) exchanged with potassium ion (K^+) was studied by a classical forcefield-based molecular dynamic (MD) simulation. The structure of K^+-MMT/PEO nanocomposites model was generated using the optimized forcefield developed by Hienz *et al.*[1] The advantage of these atomistic models is the quantitative reproduction of surface and interface energies relative to experiment, which is a milestone improvement over earlier models with up to 500% deviation, in addition to accurate geometries and vibration spectra. K^+ was observed to slightly diffuse within the tetrahedral pockets of the MMT sheet as well as the centre of the layer spacing. Water molecules in the one-layer hydrate resided at the interlayer midplane, whereas in the two-layer hydrate, they lay in two planes between outer- and inner-sphere K^+ surface complexes, as well as at the midplane. Information from this atomistic simulation will be compared with the Extended X-Ray Absorption Spectra (EXAFS) for the local environment of K+ inside clay gallery.

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Investigation of the Solidification Process of Monatomic Lennard-Jones Systems

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Solidification, structure, various aspects of thermodynamics and stability of eu amorphous state of monatomic Lennard-Jones (LJ) systems at the bulk have been studied by using classical molecular dynamics (MD) method. Models have been obtained by cooling from the liquid at three different cooling rates. Structure of the systems was analyzed via radial distribution function (RDF), static structure factor, mean atomic distances, coordination number and bond-angle distributions. Structure of LJ systems have been analyzed in details. Cooling-rate effects on formation of different solid phases have been found and discussed. The glass transition temperature have been found and the transformation of total energy, potential energy of the models have been investigated.

Keywords: Glasses of monatomic Lennard-Jones systems, MD simulation, Cooling-rate effects.

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Structure and Dynamical Properties in Noblemetal Halide Mixture Include Two Kinds Cations, Ag^+ and Cu^+

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There has been a lot of study of a group of substances with high ionic conductivity comparable to those of liquids though they are still in solid phase. Such substances are called superionic conductors or solid electrolytes. Superionic conductors are applied to various practical devices, e.g. solid state batteries, fuel cells, sensors, etc [1]. The silver and copper halides, e.g. AgI and CuI, are typical examples of superionic conductors in their α phase. However, AgBr and AgCl do not show superionic conduction until their melting point. Therefore it is of particular interest to investigate the mixture of these two different type noble metal halides. However, the study of distributions of cations in the superionic phase of noble metal halides have been executed mainly in the systems with one kind of cation, e.g. Cu^+ or Ag^+. In our previous study, we have carried out the molecular dynamics (MD) simulation to examine the structural properties of $(Ag_xCu_{x-1})Br$ of $x<0.5$ in its superionic phase as an example of the superionic conductor with two kinds of cations, Cu^+ and Ag^+ [2]. The difference in distribution between Ag^+ and Cu^+ ions in superionic phase have been detected by MD results. Concentration dependence in distribution of cations has also been observed. As a serial work, in this study, we investigate the structural and dynamical properties of noblemetal halide mixture $(Ag_xCu_{x-1})I$ by MD using re-examined potentials.

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Modeling of the Phase Transformation sII – sH in Ar Hydrates at High Pressure

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The argon is known to form clathrate hydrates of cubic structure II (sII) at low pressures and hexagonal structure (sH) at high pressure. By now the degrees of filling of large cavities in these structures are under question. The ealier developed method [1] was applied to predict thermodynamic properties of these hydrates. The calculation of thermodynamic properties structure sH and sII with possibility of multiple occupation of large cavities by argon atoms (up to five-fold for hydrate sH and two-fold for sII) was performed to establish the influence of the intermolecular interaction and entropic contributions on structure formation.

It was established that the structure of argon hydrate depends on possibility of multiple occupation of large cavities. It was shown that at high pressures, when the degree of cage filling increases the of entropic contribution is the main structure-determining factor for relatively small molecules such as argon.

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Thermodynamic Prediction of Structural Transitions in Binary Methane-Ethane Hydrates at Low Temperatures

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More then twenty years gas hydrates are in focus of investigations as the alternative energy source which could play an important role in energy production and as perspective materials for environmental projects. Experimental investigations of clathrate gas hydrates are conducted in many countries and now are beginning to be realized in some industrial applications. Low temperature region (less then 0° C) for hydrates formation is especially interesting because hydrates can be a cause of pipeline damages.

Theoretical methods in this field are not sufficiently developed. Moreover, by now there is no clear understanding of nature of structure transitions in gas hydrates with two or more types of guests (binary or mixed gas hydrates) such as ethane-methane hydrates.

We are proposing new theoretical approach that extends modified van der Waals and Platteeuw theory on mixed gas hydrates. Within this approach one can predict dynamic and thermodynamic properties of mixed hydrates and find thermodynamic equilibrium lines of transitions between different gas hydrate structures in a wide region of pressures and temperatures at different compositions of clathrate hydrates. In this approach the host-guest, guest-guest and entropy contributions in Gibbs free energy are taken into account.

The modeling of dynamic and thermodynamic properties of mixed methane-ethane gas hydrates of the cubic structures CS-I and CS-II was performed. Analysis of vibration density of states corresponded to intermolecular vibrations has shown that guest molecules have vibration modes in long-wavelength region and can noticeably influence on dynamic and thermodynamic properties of hydrates. It was found that for this system phase transitions at high temperatures are caused by competition of intermolecular interaction and entropic contribution depending on hydrate composition. Structural transformations at temperatures exceeding 273 K have been observed experimentally. Here the lines of structural transitions in methane-ethane gas hydrate at low temperatures were calculated.

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Influence of Methane Content on Clathrate Hydrate Structure Transformation sI – sII

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The model of mixed hydrates has been developed and applied to predict dynamical and thermodynamic properties of mixed hydrogen - methane clathrate hydrates of cubic I (sI) and II (sII) with multiple filling of cavities by two types of guest molecules. In our study, the small cages can be occupied by single methane molecule or up to two hydrogen molecules. The occupations of the large cages were considered as single for methane and up to four for hydrogen molecule.

It has been confirmed that the structure of clathrate hydrate is very sensitive to methane molar concentration in gas phase. The intermolecular interaction between methane molecules and host water lattice leads to higher thermodynamic stability of sI hydrate even at presence of 2% methane in gas phase. It is shown that for guests which weakly interact with water molecules, such as hydrogen, the entropic contribution is the main structure-determining factor for clathrate hydrates and it is a cause of the hydrate sII formation in this case. The explicit account of the contribution of entropy in the Gibbs free energy allows us to determine the stability of hydrate phases and to estimate the line of structural transition sII to sI in P-T phase diagram. The structural transition between sII and sI in mixed methane - hydrogen hydrates at high pressure has been shown to be the consequence of increasing intermolecular interaction and the degree of occupancy of the large cavities.

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Analysis of Protein Hydration Water by Means of Data Mining Method

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Intensive studies on the relationship between protein and water molecule were done in the last several decades. One of the central interests in this field is the water contribution on the stability and/or dynamics of protein structure that relates strongly to folding, reaction, and functional expression of protein [1]. Most noteworthy point is that protein strongly needs the translational motion of the hydration water for the protein conformational changes [2]. Understanding these strongly coupled dynamics among protein and water is important not only for science but for applications.

In this study, to elucidate the dynamic characteristics of the hydration water molecules, we carried out the classical MD simulation of small globular protein (PDBID: 1psv) and ideal pure water system with AMBER10 program package. The behavior of the hydration water and of the water in bulk condition were quantified by means of data mining techniques for analysis of MD trajectory data. By the comparison of these two dynamic characteristics, we discuss the protein-water interaction and correlation.

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Molecular Dynamics Simulation of Structural and Thermodynamics Properties of Amorphous GeO$_2$ Nanoparticles

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Recent years, there are more and more studies about germania and its applications. In this paper, molecular dynamics (MD) simulation method is used with Born-Mayer potential for studying the structural and thermodynamic properties of amorphous GeO$_2$ nanoparticles with different sizes ranged from 2 to 5nm. Models are generated in liquid state at 5000K and cooling down to 300K, at which the state is amorphous. The partial radial distribution functions, coordination numbers, bond-angle distribution are calculated. We found that Ge-O bond length of GeO$_2$ nanoparticles is about 1.7Å, and they have distorted tetrahedral structure in agreement with the experimental results. The core and surface structure is studied and discussed in details. Moreover, the dependence of glass transition temperature on the finite size is also studied like that done for the surface energy.

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Structure and Diffusion in Simulated Liquid GaAs

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Structure and diffusion of Ga and As ions in simulated liquid GaAs have been studied in a model containing 3000 ions under periodic boundary conditions via Molecular Dynamics simulation (MD). The microstructure of systems has been analyzed through partial radial distribution functions (PRDFs), coordination number distributions, bond-angle distributions and interatomic distances. We found that calculated data agree well with the experimental ones. Temperature dependence of these distributions was obtained. Caculations show that liquid GaAs model with a real density at $5.3176 g.cm^{-3}$ has a distorted tetrahedral network structure with the mean coordination number $Z_{As-Ga} \approx 4$. Diffusion constant D in system has been calculated over temperatures ranged from 5000K down to 1500K. Calculations show that the temperature dependence of the diffusion constant D shows an Arrhenius law at relatively low temperatures above the melting point and it shows a power law, $D \sim (T - T_c)^{\gamma}$, at higher temperatures.

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Molecular Dynamic Simulation Study of
Gold Structure in Amorphous and Liquid States

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Gold has many applications in science and technology. Nowadays, gold is known as a biomedical material. In this article, using Molecular Dynamics simulation we create a 3000-atom model at 2500K with the periodic boundary condition to mimic the characteristics of bulk material form; then we investigate the structure of gold material in amorphous and liquid states. We use Erkoc's pair potential. The amorphous state can be obtained by cooling down the liquid model from 2500K to 50K. Structure of liquid and amorphous Au has been studied via their characteristic quantities such as radial distribution function, interatomic distance, coordination number, angle bond distribution, and Honeycutt-Andersen analysis. The result shows that gold structure in these states matches many experiments as well as a lot of previous simulations. So that, we can use Erkoc's potential to investigate crystallization of liquid Au because the calculation time of using this potential is less than that of many other ones.

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Models of Some Nano Device Based on Carbon Nanotubes and DNA

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Simple physical models of two new nano devices based on carbon nanotubes and DNA are investigated: an optical bio-sensor by wrapping a piece of DNA around the surface of a single-walled carbon nanotube, and a nano gripper by attaching two carbon nanotubes on the ends of two strands of DNA. The physical mechanisms of those nano devices are: exciton absorption in carbon nanotubes and B-Z structure phase transition in DNA for the case of optical bio sensor, and melting phase transition of DNA for the case of nano gripper. Using above simple models, we studied the working principles of that nano devices and found qualitative agreements with other obtained results.

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Binding Energy Estimation of Hydrogen Storage Materials
by All-Electron Mixed-Basis Program TOMBO

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In 2004, for automobile onboard storage system, the U.S. Department of Energy (DOE) set the target that hydrogen storage capacity should be higher than 6 wt% (45 kg/m^3). Metal-Organic Frameworks (MOFs) are one of the promising candidates for hydrogen storage materials [1].

In the present study, we propose a simple model of MOFs that can expand hydrogen storage capacity by lithium cation doping and clarify the mechanisms of enhancing hydrogen adsorption energy. We use TOhoku Mixed-Basis Orbitals *ab initio* simulation package TOMBO [2, 3] developed by our research group, which enables us to study based on "all-electron mixed-basis approach" with smaller number of plane waves.

We found that the adsorption of Li atoms on benzene unit of MOF-5 improves hydrogen storage function properties of these systems by 1.74 wt% and makes binding energy much higher than the systems without lithium doping.

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Simulation of Mechanical and Electrical Properties of Quartz Crystal Microbalance

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This paper presents a combination of two computational methods for the determination of typical characteristics of quartz crystal microbalance (QCM). FEM-based ANSYS software is used to simulate the mechanical behaviours providing the natural resonant frequency and thickness-shear mode of circular QCM using 3D-SOLID98 element. A MATLAB code-based program is employed to find out the frequency-dependent electrical properties such as the electrical admittance, the phase angles, and the magnitude of normalized impedance in case of being deposited or without a coverage layer on electrode for QCM 5 MHz. The simulation results are agreed well with the theoretical values and experimental study cases.

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Theoretical Investigation of the Hydrogen Storage Ability of a Carbon Nanohorn

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Much attention was put on studying the hydrogen storage ability of carbon-related materials, metal organic framework materials (MOF), clathrate materials, metal hydride materials, and metal-polymer complexes, *etc.*, no proper material could be used for the on-board storage medium of hydrogen for the practical usage till now. Thoug much work still needs to chemically engineer such materials to improve the storage ability, some efforts should be put on searching new materials which may meet the requirement for the practical usage for on-board purpose. We follow such direction to search the potential hydrogen storage medium by first-principles method. The experiment has shown that the binding energy of H_2 molecule on such carbon nanohorn is much stronger than that on its counterpart pure carbon nanotube indicating its potential storage ability for hydrogen gas. Our calculated results show a comparable binding energy for hydrogen molecule sitting on the wall of the horn with those on the nanotube, while the adsorption close to the top section of the horn is enhanced greatly. However, due to the small portion of the top section in the whole carbon nanorhorn, such material may not be enhanced too much for the hydrogen storage compared to it counterpart pure carbon nanotube. The storage of hydrogen in molecule form inside the carbon nanohorn is limited to be below 3wt% for the studied horn model. The outside and the inside walls of the horn could bind H_2 by the weak van deer Walls force, which is too weak to be used at the room temperature. The light metal atom adsorption on it could enhance the binding strength. The adsorption of H_2 molecule on both the inside and the outside walls of carbon nanohorn makes it attractive to store hydrogen in molecule form for the on-board usage.

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First Principles Calculations on Grain Boundary Impurities in Polycrystalline Silicon

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Currently, over half of all solar cells produced worldwide are made from polycrystalline silicon (pc-Si). While these devices have comparatively lower efficiencies mainly due to transition metal impurities (10^{14}–10^{16} cm^{-3}) in most of the pc-Si materials[1]. In the present study we used DFT method to understand relationship between sigma value and impurity precipitation. First we study the dopant position and the nature of interaction between the GB of Σ 5 and transition metal. Finally we have studied the electronic changes that occurred up on doping the transition metal impurities in the GB region. Grain boundary of pc-silicon was constructed using GB studio[2]. We used VASP code[3] for geometrical optimization. To validate our studies we used one Copper, Iron, Nickel and Chromium atom as dopants and compared our findings with the experimental results[4].

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Atomistic Modelling of Artificially Controlled Grain Boundaries in Multicrystalline Silicon

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Multicrystalline silicon (mc-Si) is widely used as a solar cell material because of its low production cost, even though the energy conversion efficiency of mc-Si solar cells is lower than that of single-crystalline Si solar cells due to the random orientations of the crystal grains in the former. Optimization of the grain-boundary structures of mc-Si is a key issue to achieving high efficiency, because these regions act as recombination centers for carriers in solar cell materials. Multicrystalline Si with artificially-controlled grain orientations has been proposed as a means of reducing the number of electrically-active grain boundaries that lead to undesirable carrier recombination.[1] In the present study, we evaluate the 'grain-boundary-energies' at the grain boundaries between <100>, <110>, <111> and <112>-oriented grains by using the Tersoff potential.[2] First, we prepare two silicon crystals which have the same crystal orientations. Then, we independently rotate each crystal about the same direction, such as the <110>-oriented direction. Finally, we combine both crystals to form a grain boundary in a spherical sample, in which one hemisphere of the sphere model corresponds to the first crystal and the other hemisphere corresponds to the second crystal. Figure 1 illustrates a snapshot of a <110>-oriented grain boundary in a spherical sample such as we used in this research. This work was partially supported by New Energy and Industrial Technology Development Organization (NEDO) of Japan.
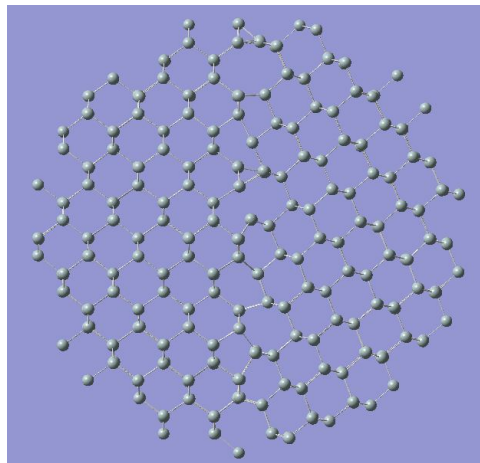
Figure 1 Snapshot of <110>-oriented grain boundary

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Molecular Dynamic Simulation and Extended X-Ray Absorption Fine Structure (EXAFS) Spectroscopy Studies of Cation Local Structure of Tetraglyme/Potassium Thiocyanate Electrolytes

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Solid polymer electrolytes (SPEs) are of great interest in the context of developing a variety of modern electrochemical applications. The wide range of technological applications of SPEs has spurred attempts to understand the mechanism of ionic transport in polymer electrolytes. The local structures around the potassium species of tetraglyme [$CH_3O(CH_2CH_2O)_4CH_3$, a 4-mers model compound for poly(ethylene oxide)] were characterized using a combination of Extended X-Ray Absorption Fine Structure (EXAFS), acquired on BL-8 at Synchrotron Light Research Institute (Public Organization), and Molecular Dynamic (MD) simulation which are give informations such as coordination number and distance of neighbours around potassium species. MD simulations with an empirical potential (COMPASS forcefield) were used to calculate the RDFs and local coordination. Those structural properties obtained from the MD simulations are found to be in very good agreement with other works. The simulated solvation structures were used to compute the MD-EXAFS spectra. MD-EXAFS spectra generated from MD simulations were then compared with the measured spectra. Comparison shows the consistence between the EXAFS spectra from MD simulations and those from the experiments.

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High-Capacity Hydrogen Storage of Al Adsorbed Graphene: Ab Initio Investigation

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The safe and efficient storage of hydrogen is essential technological for a hydrogen-based energy economy [1]. Since current storage technology using cryogenics or high pressure cannot meet the industrial requirements, there is substantial research and development activity in the use of novel hydrogen storage materials. Carbon based nanostructures such as nanotube, fullerenes, and graphene have received continuous interest as potential hydrogen storage material. However, the quantity of hydrogen storage in carbon materials cannot come up to the desirable target of hydrogen storage of 6.5 wt % [2]. Lochan and Head-Gordon reported that ionic atoms such as Li^+, Na^+ and Al^{3+} can bind hydrogen molecules quite strongly [3]. While many studies have performed with metal adsorbed graphene for hydrogen storage, the detailed mechanism and practical implication of Al adsorbed graphene are still not fully understood. In this paper, the structural and electronic characteristic of Al adsorbed graphene for hydrogen storage material was investigated by using ab inito method. It was found that Al atoms can be adsorbed on the (2x2) graphene without clustering and can bind up to four hydrogen molecules with a storage capacity of 6.5 wt%.

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Complex Permeability Model for
Efficient Proximity Losses Computation in Electric Conductors

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Power electronics facilities has become more and more popular. Deep understanding of power loss management in power electronics components is crucial for this industry. One of the most important power electronics component is the high frequency transformer. This is a combination of low loss magnetic material and conductors. These conducting parts working in high frequencies are object of power loss. Proximity losses are predominant in these conductors due to their structure.

Classical calculation methods in finite elements including h-method and p-method are unable to take into account these losses correctly. This is due princicaplly to high number of elements and limited
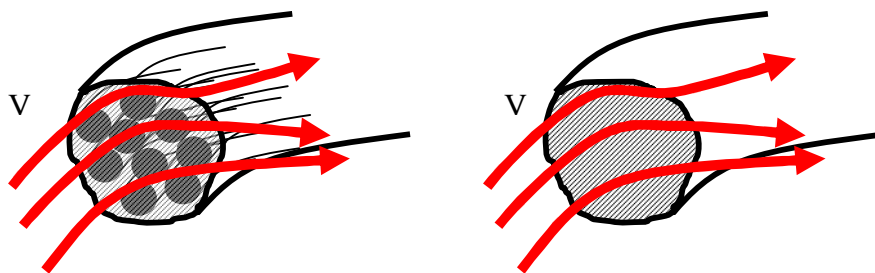
memory capacity of PC. In this paper, we present a novel method to calculate these losses precisely with a limited computation resources by using complex permeability concept. A test case will be presented to confirm the proposed method.

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First-principles Calculations on
Hydrogen Storage Properties of CS-4 clathrate Hydrate

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Clathrate hydrates are crystalline solids composed of water and gas. The gas molecules (guests) are trapped in water cavities (host) that are composed of hydrogen-bonded water molecules. Typical natural gas molecules include methane, ethane, propane and carbon dioxide. While sI, sII, sH are the most common clathrate hydrates, a few other clathrate hydrates have been identified. These other clathrate hydrates include the cubic structure 4 (CS-4) which can reach the hydrogen storage capacity of 6.8% considering 6 H_2 /cage. Only one type of cage/cavity $4^6 6^8$ forms the CS-4 clathrate unit structure including 12 H_2O molecules. This work was investigated using VASP code with Gamma point calculation (k=0). The interaction between ions and electrons was described by the projector-augmented wave (PAW) method with GGA basis set. The main focus of this study is to stabilize the CS-4 structure so that different lattice constants were taken into account to optimize the structure. Finally, we used the most stable volume to calculate the total energy and different distances and angles between hydrogen and Oxygen atoms.
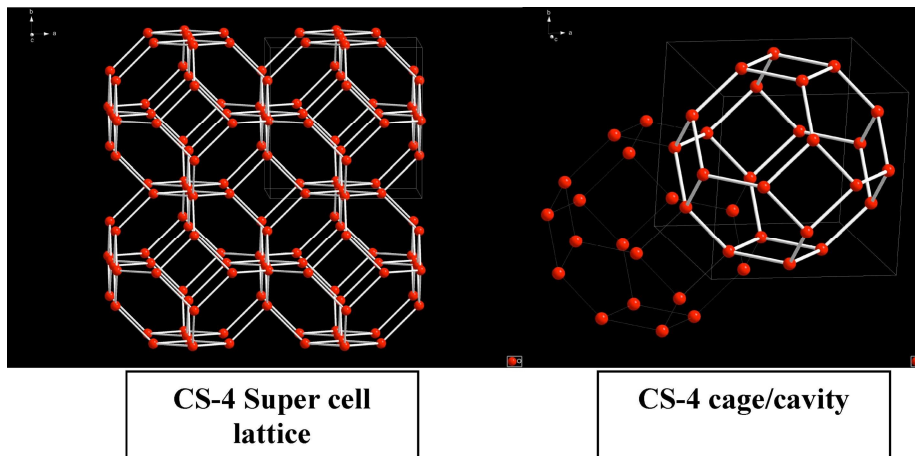
| **CS-4 Super cell lattice** | **CS-4 cage/cavity** |

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Density Functional Study on the Alkali Atom Doped Calix[4]arene as Hydrogen Storage Material

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The search for an ideal material for hydrogen storage is dictated by need to simultaneously satisfy several criteria, such as high gravimetric density, near-ambient temperature, pressure of operation and fast recharge/discharge kinetics. For attaining high gravimentric density, the storage materials should posses only light weight materials. Organic material such as calix[4]arene have high stability due to the existing hydrogen bond and are porous. We carried out at DFT study on alkali functionalized MOF's and *p*-tert-butylcalix[4]arene (TBC)[1] . On reduced models such as Benzene-alakali system, we found that Li doping can hold up to 3 hydrogen molecules in molecular form and Na doping can hold up to 8 hydrogen atoms in quasi molecular form. Our prelimanry studies shows that on calix[4]arene up to 5 Na atoms can be doped.
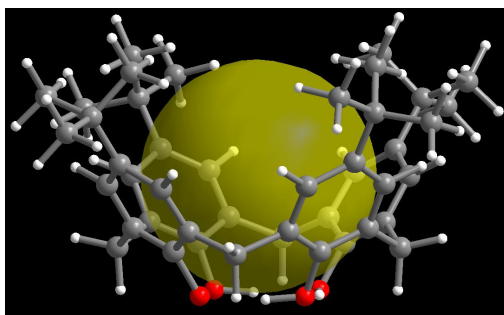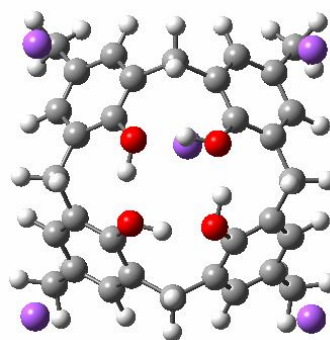
p-tert-butylcalix[4]arene (TBC)   Na-decorated calix[4]arene

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Atomistic Simulation of the Structure, Interaction and Dynamics of Poly(lactic acid) Melt and Graphite Interface

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The interfacial structure and interaction between poly(lactic acid), PLA melt and graphite sheet, was studied by simulations of fully atomistic models. A model for the interface of PLA/Graphite was constructed as thin films of nanoscale thickness (40Å) on a (001) surface of graphite substrate on the one side and exposed to vacuum on the other. Molecular dynamics (MD) simulations were carried out with model, strictly monodisperse PLA samples of chain length up to 20 monomer units with 30 chains in the NVT statistical ensemble at 460 K for the running time up to 2 ns. The interface was formed by moving two surfaces from PLA and graphite sheet close together and then running molecular dynamics and molecular mechanics simulations in a pseudo-two-dimensional periodic cell. MD simulations revealed that the PLA density is significantly perturbed by graphite surfaces, forming layers of highly dense polymer (compared to the bulk melt) that persisted up to 15 Å from the surface. The interaction energy between PLA and graphite was calculated and found that the main contribution of the interfacial energy was from the non-bonded energy terms. Conformational and structural relaxations of the interfacial PLA were found to be slower than those of bulk PLA. The surface structure and electrostatic interactions between PEO and graphite, rather than the increased polymer density at the graphite surface, determine the nature of PLA local dynamic at the graphite interface.

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Effect of Film Thickness on the Phase Transition in Thin Magnetic Films

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The Ising FCC antiferromagnet is fully frustrated and is known to have a very strong first-order transition in the bulk state. In this work, we study the nature of this phase transition in the case of a thin film, as a function of the film thickness. Using Monte Carlo (MC) simulations, we show that the transition remains first order down to a thickness of four FCC cells (eight atomic layers). It becomes clearly second order at a thickness of two FCC cells, i.e. four atomic layers.

It is also interesting to note that the presence of the surface reduces the ground state (GS) degeneracy found in the bulk. For the two-cell thickness, the surface magnetization is larger than the interior one. It undergoes a second-order phase transition at a temperature T_C while interior spins become disordered at a lower temperature T_D. This loss of order is characterized by a peak of the interior spins susceptibility and a peak of the specific heat which do not depend on the lattice size suggesting that either it is not a real transition or it is a Kosterlitz-Thouless nature. The surface transition, on the other hand, is shown to be of second order with critical exponents deviated from those of pure 2D Ising universality class. We also show results obtained from the Green's function method. Discussion is given.

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Fracture Toughness of an Interface between a Submicron-Thick Film and a Substrate

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In microelectronic and micromechanical devices, there are many bi-material interfaces between thin films. It is well known that the free edge of an interface in a bi-material is the place where stress concentrates due to deformation mismatch, and thus becomes the most favorable site of crack initiation. Since the crack initiation strength is of critical importance for the reliability of the devices, evaluation of the mechanical criteria of interface cracking between thin films is a necessary task

The focus of this study was to evaluate the fracture initiation criteria of the Sn/Si interface by Bogy's[1], Kitamura's[2] and Griffth's methods. Experimental data performed by Hirakara et al [3] were used in this study. The critical stress intensity parameter K_{ijC} in Bogy's method and the concentrated stress parameter σ_{ijC} in Kitamura's method were calculated based on the singular stress field near the interface edge, while the work of separation per unit area Γ_o in Griffth's method was calculated based on the work of fracture process. Based on the calculation processes and obtained results, the advantages and disadvantages of the criteria were explored.

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A First Principles Calculation on
the Polythiophene/Graphene Hybrid Nanocomposite

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Graphene, constructed by a single layer of graphite, has been developed in recent years. This two-dimension material is promising in photovoltaic heterojuction with polythiophene since its good conducting properties. Recently reported that pure graphene is prepared from graphite oxide through reduction process [1-2]. Incomplete reaction leaves residual oxygen in the graphene layer, which influences the electrical properties.

In this work, a density functional theory calculation is employed to investigate the interface properties in the polythiophene/graphene hybrid system. The optimized electronic structure is used to calculate the charge transfer between organic and graphene layer. The detail of band alignment at polythiophene/graphene interface is calculated by the band structure and orbital calculation.

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Modelling Fullerenes on Si (100)

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Fullerenes on Si (100) are of great interest both from a fundamental science point of view and due to their potential for the creation of devices. They are one of a number of systems to have been proposed as a possible building block for a solid-state quantum computer. A number of experimental studies have studied fullerenes on Si surfaces, mainly focusing on the position of the fullerenes on the surface and the nanomanipulation of the fullerenes. Nanomanipulation in these systems has proven to be very successful in that it has shown to be reproducible and can be carried out at room temperature.

We will describe ab-initio work using the PLATO code on the simulation of both the C60 and the C82 fullerenes on a Si (100) surface. In this work we have studied the stability of these molecules on the surface to help elucidate the experimental results for this system. We will show that the smaller and higher symmetry C60 molecules appear to bind more strongly to the surface. We will also show that the orientation of the C82 molecule can have a large influence on its binding energy. Analysis of these systems has been performed through the use of the ideas in Bader's atoms in molecules and utilising a new grid based algorithm.

We will also present a study of the interaction between two C60 molecules on a Si surface. The interaction between multiple fullerenes on a surface is essential if we are to create devices from these systems. This work will show that when placed a short distance apart two C60 molecules can interact very strongly causing significant changes to the bonding within the fullerene cage.

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Molecular Dynamics Study of Sputter-induced Composition Modulation in Co-Cu alloy

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Sputtering has been regarded as a novel process to generate periodic nano-scale ripple patterns or quantum dots on the sputtered surface. V. B. Shenoy *et al.* further suggested that, in the case of alloy surfaces, the differences in the sputtering yields and surface diffusivities of the alloy components will lead to a lateral surface composition modulation [1]. In the present work, the classical molecular dynamics simulation was employed to understand the sputter-induced composition modulations in alloy system. During Ar ion bombardment on $Co_{0.5}Cu_{0.5}$ alloy system, layer-by-layer composition modulation was observed without the lateral variation of the composition. The composition of Cu atoms in the top most layer increased while that of the 2nd layer decreased with the Ar bombardment. The difference in the rearrangement yield between Co and Cu turned out to significant for the layer-by-layer composition modulation. Mechanism of the composition modulation was elucidated quantitatively by an analytic model considering both the rearrangement and sputtering in the composition change of each layer.

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Molecular Dynamics Study of Tetrahedral Amorphous Carbon Film Growth

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A three dimensional molecular dynamics is carried out to understand structure and stress evolution during growth of tetrahedral amorphous carbon (ta-C) film. Energetic carbon atoms ranging form 1 eV to 100 eV are deposited onto/into (001) diamond substrate at normal incidence. A modified Brenner potential is used for interatomic interaction of carbon atoms [1, 2]. We investigate structural properties such as sp^3/sp^2 fraction, number of defects (e.g. highly distorted atoms such as fivefold coordinated C atom), and local density with various ion energies. Role of those structural change on the stress generation is studied. Effective ways to control (residual) stress during (after) film growth will be discussed.

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First Principles Calculations of Electronic Structures of F4-TCNQ molecule on Graphene

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Based on density functional theory, we have systematically investigated the electronic structure of fluorine-tetracyanoquinodimethane (F4-TCNQ) molecule on graphene [1, 2]. Several possible adsorption sites and orientations are considered. It is found that F4-TCNQ molecule as a prototypical organic acceptor forms strong interaction with inert graphene. Through detailed analysis of interfacial electronic structures for combined systems, we found that F4-TCNQ molecule attracts electrons from graphene substrate through the hybridization between the lowest unoccupied molecular orbital (LUMO) of F4-TCNQ and π orbitals of graphene, which makes p-doped graphene. The most striking feature of charge transfer at the interface is the charge back-donation from the σ orbital of F4-TCNQ molecule to graphene. This provides an easy and feasible way of functionalizing graphene.

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Local Elastic, Viscoelastic and Geological properties of the Thin polymer layers by means of Scanning Force Probe Microscopy

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Recently, the local physic-mechanical properties of the thin film have been studied by using Scanning Force Probe Microscopy (SFPM). It is a unique method to study the properties of the polymers and biomaterials in Nanometer scale. This paper will shows the theoretical basic of the method to define the Elastic, Viscoelastic and the Rheological properties of the polymer surface in nanoscale using Scanning Force Probe Spectroscopy. Using the Force Spectroscopy by Atomic Force Microscope, we have studied the Elastic modulus tip-sample interactions of the thin film Polivinilpiridina (PVP) prepared by Langmuir-Blodgett technology. The influences of the temperature and pressure on the properties of film have been discussed.

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Spatial Distribution of Transferred Charges at the Interface of TTF and TCNQ Organic Crystals

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Surface or interface properties often exhibit drastic deviations from the bulk properties. For example, it is well known that $SrTiO_3$-$LaAlO_3$ interface becomes conducting even though both $SrTiO_3$ and $LaAlO_3$ are insulators in their bulk forms. [1] Recently it was reported that a mechanical contact between two organic insulators, TTF and TCNQ, can result in the conducting layers. [2] In this presentation, we investigate the electronic structure of the two-dimensional TTF-TCNQ interface by employing the first-principles methods. Transferred charges are localized at the interface layers, and their characteristics can be understood in terms of frontier molecular orbitals with additional surface polarisation.

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Scattering Potentials at Impurity Dimers and Atomic Switch Design on Ge(001) and Si(001): First-principles Study

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On the Si/Ge (001) surface, Si/Ge atoms form buckled dimers with π and σ bonds. The dimers line up and make a dimer row. The π^* band lies in the bulk gap and localizes at the lower atom of the dimer. It behaves as a 1D conduction channel along the dimer row. By controlling the conduction of π^* electrons using the buckled Sn-Ge dimer on Ge(001), Tomatsu *et al.* have fabricated an atomic switch using STM (Science 315 (2007) 1696). Collaborated with Tomatsu *et al.*, we investigated the *ON/OFF* mechanism of the atomic switches. Using first-principles method we calculated the scattering potentials induced by different impurity dimers and obtained good agreement with STM phase shift measurements. We further studied the switch mechanism related with dimer flip motion by electron injection from STM tip. We propose that the flip motion is caused by a resonant scattering of the π^* electrons with localized electronic states. On the other hand, we studied theoretically the scattering by impurity dimers on Si(001) and proposed that it is possible to fabricate good atomic switches using X-Si (X=Ge, Sn and Pb) impurity dimers.

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A Comparative Study on the Optical Properties of Indenofluorene and Indenopyrazine

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As a core structure to design a new functional dye which can be used as materials for electronic devices such as field-effect transistors or light-emitting diodes, indenofluorene and indenopyrazine have been studied. Their UV/Vis absorption and PL emission spectra were predicted by time-dependent density functional theory (TDDFT) method at B3LYP/6-31G* level and CIS/6-31G* level was applied to optimize the geometry of the first excited state used to calculate the emission spctrum. The influence of THF solvent was considered using polarized continuum model TDDFT (PCM-TDDFT) method as well. PCM-TDDFT results are red-shifted by about 10 nm in comparison to the corresponding predicted absorption and emission maximum in vacuum phase. In PCM-TDDFT results, the absorption maxima of indenopyrazine were red-shifted by about 25 nm compared to those of indenofluorene. These spectral shift induced by the nitrogen atoms in the pyrazine ring of indenopyrazine are explained by the analysis of electronic structures of indenofluorene and indenopyrazine and the atomic contributions of the pyrazine nitrogen atoms to the frontier molecular orbital of indenopyrazine.

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Modelling of Thermal Oxidation in Porous Silicon

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Thermal oxidation effects on the nanostructured porous silicon are studied from both theoretical and experimental approaches. The atomic-scale modelling is performed by using the CASTEP of Materials Studio within the density functional theory. Starting from a crystalline silicon supercell of 32 atoms, columnar pores of 13 silicon atoms are removed along the [001] direction and the dangling bonds are firstly saturated with hydrogen atoms [1]. An increase of the supercell volume is observed after performing a geometry optimization. This observation is in agreement with high-resolution X-ray diffraction data. However, when these hydrogen atoms are gradually replaced by oxygen ones, a contraction of the supercell and a reduction of the electronic band gap are found. Nevertheless, this band gap increases when oxygen atoms are additionally introduced into the bulk of porous silicon. In a parallel way, free-standing porous-silicon samples were fabricated by using a standard electrochemical etching procedure [2] and they were thermally oxidized through a wide range of temperatures. The measured transmittance spectra reveal a band gap variation consistent with the ab-initio predictions.

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Atomic Relaxation and Electronic Structure Investigation of Eu2+ doped β-SiAlON: Ab Initio Calculations

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White light-emitting diodes (LEDs), the so-called next-generation solid-state lighting, offer benefits in terms of reliability, energy-saving, maintenance, safety, lead-free, and eco-friendly. Recently, rare-earth-doped oxynitride or nitride compounds have attracted a great deal of interest as a photoluminescent material because of their unique luminescent property, especially for white LEDs applications. Eu^{2+} doped β-SiAlON has been studied as a wavelength conversion phosphor in white LEDs thanks to its high absorption rates, high quantum efficiency, and excellent thermal stability [1]. Previously researches were not enough to understand the detail mechanism and characteristics of β-SiALON. The position of a dopant is unclear even in an X-ray diffraction due to its low density. It is reported that the direct observation of interstitial dopant in phosphor materials by advanced STEM [2]. In this study, to elucidate the Eu^{2+} doping effect on the SiAlON system, the structural properties and electronic structure of the Eu^{2+} doped β-SiAlON was intensively investigated using density functional theory calculations [3]. We have found a single Eu atom site in 1x1x2 β-SiAlON super cell. Furthermore, the density of state, band structure and lattice constant were intensively investigated.

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Combination of Molecular Dynamic Simulation and the Extended X-ray Absorption Fine Structure (EXAFS) Spectroscopy to Probe the Solvation Structure of Calcium ion in Alcohol and Polyvinyl alcohol

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Molecular Dynamics (MD) simulation and the Extended X-ray Absorption Fine Structure (EXAFS) spectroscopy, performed at Synchroton Light Research Institute, Thailand, were employed to obtain the atomistic solvation structure of calcium ion dissolved in ethyl alcohol, iso-propyl alcohol and poly(vinyl alcohol) (PVA). Sets of atomic position of surrounded molecules with different configurations from the MD simulation were used to generate a separate Ca K-edge EXAFS oscillation for each individual atomic configuration by mean of the theoretical XAS modeling package *i.e.* FEFF6 for the analysis of the experimental EXAFS spectra. The simulated EXAFS spectra were compared well with the experimental spectra. From the computing result, it is obvious that there is only one dominant shell from oxygen atoms around calcium ion in alcohol and PVA.

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First-Principles Analysis of Photoabsorption Spectra of $(CdSe)_{34}$ Clusters in Pearl-Necklace Geometry

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CdSe clusters are known to have a strong size dependence of the energy gap and their applications such as a florescence agent are expected. We calculated the photoabsorption spectra of isolated and pearl-necklace geometries of a magic number cluster $(CdSe)_{34}$ within the random phase approximation [1]. We used the all-electron mixed basis approach on the basis of the local density approximation within the density functional theory. A double-peak structure was obtained for pearl-necklace geometry in an orientation that keeps intermolecular distance 3Å, in contrast to a single-peak structure obtained for isolated geometry. The result is consistent with the experimental photoabsorption spectra [2-4]. We checked the wave functions of the two systems to investigate whether the electronic dipole transition is forbidden or not. We suggest that the adjacency of each clusters brought about symmetry breaking of wave function and in turn the double-peak structure. Results for smaller CdSe clusters in more sophisticated method, *GW*+Bethe-Salpeter method with the two-particle Green's function, is also in progress.

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Finite Difference Time Domain Method Optimized for Full Analyses of Photonic Crystal Fibers

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We present an effective finite-difference time-domain method for the analyses of photonic crystal fibers. Basic schemes, important issues, and applications of the method are presented to explore its potentials and limitations regarding the simulation of photonic crystal fibers. Anisotropic resolution and periodic boundary condition are adopted to effectively reduce 3D simulation to 2D, while retaining the original 3D algorithm for flexible switching between 2D and 3D simulations. The optimization of various simulation parameters is discussed to achieve high accuracy with reasonable computation loads. In addition to the intrinsic functions of FDTD, we demonstrate the calculation of bending loss and the simulation based on fiber images, which show the great potential of the method for various applications.

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The Photocatalysis of H_2O Absorption on TiO_2 Rutile (110) Studied by DFT Calculations

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Our calculations based on density functional theory and the pseudopotential method have been used to investigate the energy of H_2O absorption on the (110) surface of TiO_2. Full relaxation of atomic positions is performed on slab system with periodic boundary conditions and the full coverage are studied. Both molecular and dissociative absorption are treated. Our results show that for molecular absorption, the Ti_{5f}-O_{water} bond lengh is $2.255A^0$ agreement with experimental and there is a favourable when H_2O dissociative on the TiO_2(110) surface.

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Positively Charged Excitons in Quantum Dots

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We study positively charged exctions in two-dimensional parabolic quantum dots containing holes with low concentration (up to $N = 12$) by means of an unrestricted Hartree-Fock method. The shell structures for ground states of hole occupations are shown, both in the absence and in the presence of magnetic field. We consider the effect of excess holes in energy shifts of interband transitions by excitons. The numerical simulation results on the absorption by positively charged excitons show new features in comparison with the absorption by negatively charged excitons and give more insight on the electrons and holes interactions and its relationship in quantum dots. The fine tructure of interband absorption spectra due to both magnetic fields and the asymmetry between electrons and holes and the effects of polarization of lights are predicted, which can be detected in experiments on single dots.

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Tracking Acetylene/Vinylidene Isomerization Process by Ultrashort Laser Pulses using High Harmonic Generation

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We simulate the Acetylene/Vinylidene isomerization by the Born-Oppenheimer molecular dynamics method implemented in the GAUSSIAN 3.0 package. Furthermore, by using the Lewenstein model we then calculate the high-order harmonic generation (HHG) spectra emitted by C_2H_2 molecule during the chemical reaction path of isomerization due to interacting with the 10 fs pulse of the 800nm intense laser. We identify the intensity peaks of HHG spectra nearby the stable, meta-stable and transition states of the C2H2 molecule that can be useful for tracking the Acetylene/Vinylidene isomerization process.

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The Investigation of the Effects of Ga-doping on the Electronic Structure and the Optical Properties of ZnO under the Density Functional Theory

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The effects of Ga doping on the electronic structure and optical properties of ZnO are studied using the plane-wave pseudopotential method based on the density functional theory (DFT) within the Perdew-Wang 91 generalized gradient approximation (GGA-PW91). The calculated results reveal that due to electron doping, there are lots of carriers in the bottom of conduction band and the Fermi level shifts into conduction bands. Concurrently, the density of states (DOS) shifts towards low energies and the optical band gap is broadened. A sharp resonance attributed to the Ga 4s orbital shows up just below the low-lying Zn 3d valence bands. The width of this peak becomes broader as the amount of the Ga dopant is increased, reflecting an increased interaction with the 2p orbitals of the surrounding O atoms. The calculated result reproduces the pronounced Burstein- Moss shift and the shrinkage of the fundamental band gap. Furthermore, an increase of the Ga content leads the volume of the unit cell to be amplified. The optical properties including the electric function, refractive index, extinction coefficient, absorption coefficient, reflectivity and plasma frequency are also investigated in detailed. The obtained results show that doping concentration strongly affects the optical parameters. The optical parameters shifted to higher energy as increasing doping concentration. The Materials Studio 3.2 software is used for calculating in this work.

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Opto-electronic and Magnetic Properties of the Mn-doped Indium in Oxide: A First-principles Study

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The indium tin-oxide (ITO) has been widely investigated due to its excellent electrical and optical properties. It is one of the most widely used as transparent conducting materials in various optoelectronic devices. At present, major component of ITO is indium which is expensive and scarce so it is required to develop material with reduced amount of it. Recently[1-4], it is reported that low doping of Mn ions in ITO films provides remarkable magnetic property without significant degradation in optical transparency. The electronic, optical and magnetic properties of manganese doped indium tin oxide (ITO) were calculated by using the density functional theory (DFT). Our spin polarized calculations for opto-electronic and magnetic properties are in good agreement with the experimental observations.
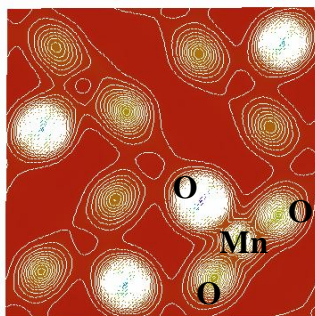
Charge density plot for Mn-doped oxidized Indium tin oxide (ITO)

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Vibration Signatures of O_{Te} and O_{Te}-V_{Cd} in CdTe: A First Principles Study

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Chen *et al*. [1] experimentally observed vibration signatures related to defects in oxygen-doped CdTe using an ultrahigh resolution Fourier transform infrared (FTIR) spectrometer. At a low temperature, they observed an absorption peak at 350 cm^{-1}. In addition, under certain growth conditions they observed two peaks at higher frequencies at 1097 and 1108 cm^{-1} that are merged into one at room temperature. They attributed the low frequency peak (350 cm^{-1}) to the vibration of O_{Te} and the two higher frequencies (1097 and 1108 cm^{-1}) to the vibration modes of O_{Te}-V_{Cd} complex. Later, they observed the similar modes around 1100 cm^{-1} in O-doped CdSe [2] that they attributed to O_{Se}-V_{Cd} complex. We employed first principles DFT calculations to calculate the vibration modes of these defects in CdTe. While our calculations show that the 350 cm^{-1} mode is consistent with O_{Te}, the modes around 1100 cm^{-1} are more than twice of the expected frequencies of O_{Te}-V_{Cd} complex or O_{Se}-V_{Cd} in CdSe, which we published a comment on their work [3]. In this presentation, we will describe the computation approaches used for calculating the vibration frequencies of O_{Te} and O_{Te}-V_{Cd} complex.

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DFT Study on Elastic and Piezoelectric Properties of BaTiO$_3$ Crystals

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Based on the theoretical formalism built by P. Ravindran et al. [1], we calculate the elastic constants employing the electronic density-functional theory (DFT) and the generalized gradient approximation (GGA). Bulk modulus, and Debye temperature are also calculated and found to be in good agreement with experimental results. Furthermore, we present an efficient scheme for studying the mechanism of the piezoelectric effects of BaTiO$_3$ crystals. The calculated piezoelectric properties compare favorably with experimental values. According to our model, the changes of dipole moment in different directions of the BaTiO$_3$ single crystal are calculated. We find that the variations of dipole moment are in direct proportion to the piezoelectric tensors, which can successfully explained the differences in piezoelectric behavior along different crystallographic axes in BaTiO$_3$. We hope that our results will be beneficial for the design and search for other good piezoelectric crystals.
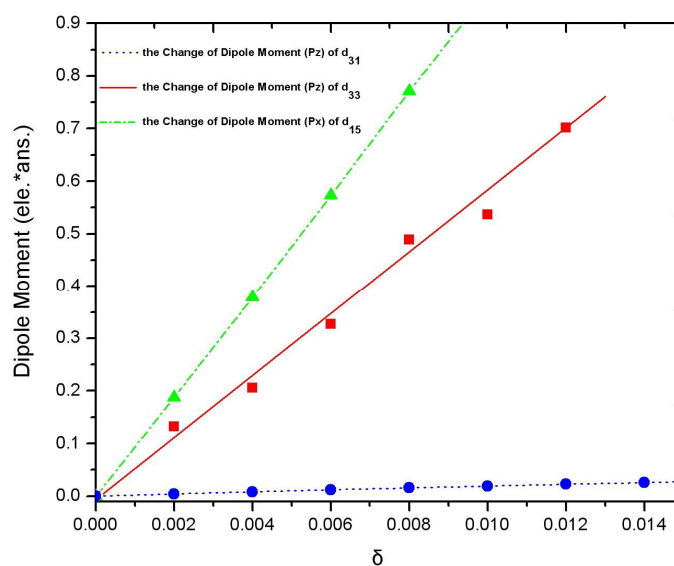
Figure 1. The changes of dipole moment in different directions with lattice distortion of BaTiO$_3$

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Parametric Study of Left-Handed Combined Metamaterial

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Recently, the naturally available range of the matter-wave interaction is extended by the appearance of an artificial-class material, the so-called left-handed metamaterial (LHM), with novel properties, such as negative refraction, resulting from the simultaneously negative permittivity and permeability [1]. In this report, we numerically studied the effect of parametric properties of combined metamaterial (CM), which consits of cut-wire pairs (CWP) and continous wires, on the LH behavior. The transmission properties of CM were calculated by the transfer-matrix method [2] and using a commercial code, CST Microwave Studio. The corresponding effective permittivity and permeability were extracted from the complex scattering parameters utilizing the standard retrieval method. By examining the lattice constants, the width and the length of CWP and continuous wire, the impact of embedding medium, and the thickness and the dielectric constant of spacer, it is elucidated that the LH behavior is rigorously affected by these parameters. Our detailed numerical results are useful for the theoretical understanding and the fabrication of LHM as well as the investigation on the feasibility of various applications.

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Gaint Moment Reduction of Fe Impurity in Dilute Pd-V Alloys

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Electronic structure calculations based on density functional theory using LSDA+U method are performed in order to investigate the local magnetic behaviour of isolated Fe impurity in dilute Pd-V alloys. The calculations performed for different near neighbor configurations and V concentrations reveal that the giant magnetic moment of Fe in Pd is drastically suppressed in Pd-V mainly due to reduction of the induced ferromagnetic polarization of the host Pd atoms and the development of a negative spin moment on the V atoms. The results are compared with experimental data obtained from γ-ray perturbed angular distribution measurements.

Direct Enumeration Studies of Band-Gap Properties of $Al_xGa_yIn_{1-x-y}P$ Alloys

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The advantage of alloying is that the alloy properties, such as band gap, can be tuned by varying the alloy composition to meet the specific requirements of modern device applications. The direct enumeration approach is used to study the properties of AlGaInP alloys [1]. First, a good representative set of alloy configurations is generated (~5000 configurations). Then, the band gap properties of each configuration in the set are calculated using the empirical pseudopotential method. Our results show that the band gap of this alloy system depends strongly on the cation arrangement in addition to the alloy composition. However, the band gap type (direct/indirect), which has an important implication on the optical properties, is found to depend strongly on the composition and only weakly on the cation arrangements. The range of possible band gaps vs. compositions is presented. The direct and indirect band gap domain in the composition space is identified. Overall, the calculated band gaps are lower than those predicted by Vegard's rule. This band gap reduction is attributed to the ordering effects. Our computational results are in good agreement with available experimental results.

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Electron Diffraction and High Resolution Electron Microscopy Techniques Study on the Microstructure of NdFeCoAl-(B,C) Based Alloys

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Magnetic materials on basis of the NdFeAl alloys have been intensively studied because of their interesting physical properties and application potential. The magnetic measurements reveal that the samples exhibit hard-magnetic characteristics quite good at room temperature [1-4]. However, the relationship between hard magnetic properties and microstructure in these alloys are still not well understood.

We present here the results of studies on the microstructure of some NdFeAl-(B,C) alloy system by the electron microscopy techniques as TEM, HRTEM, SEM, SAED, EDX and EBSD. Rods and ribbons of the NdFeCoAl-(B,C) alloys were prepared from the pure elements Nd, Fe, Al, B and C by rapid-quenching methods. We used a Philips CM20-FEG TEM and a FEI NovaNanoSEM 200 SEM to characterize the microstructure of these alloys.

We found the different crystalline phases in the alloys. In the NdFeCoAlB samples, the tetr. $Nd_2(Fe,Co)_{14}B$ (2:14:1), fcc Nd rich, hcp Nd, alpha-Fe and in the NdFeCoAlC samples, the tetr. $Nd_6(Fe,Al,Co)_{14}$ (delta), μ phase and hex. $Nd_2Fe_{15}Al_2$ (2:15:2) crystalline phases embedded in an amorphous matrix were identified. The grain size of the crystallites is ranging from 3 nm to 250 nm. The 2:14:1 phase is supposed the high coercivities up to 1202 kA/m at room temperature of the NdFeCoAlB alloys. Other antiferromagetic phases as the 2:15:2, delta phase can be played an important role in hard magnetic properties of alloys at low temperature ranges. The amorphous phase with high fraction was found in all of these alloys have also good hard magnetic properties (higher than 3 kOe). In the NdFeCoAlC alloys, we did not find the crystalline phase 2:14:1 but still obtained higher 7 kOe in coercivity.

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Structural Elements for Modelling the Elastic Properties of Graphene

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Plain symmetric structural elements
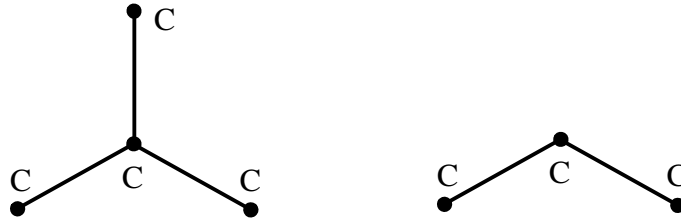
are considered. It is shown that the full number of independent stiffness constants for each system is equal 4. Stiffness matrixes are presented in the form of the sum of matrixes

$$[K] = [K]_{bs} + [K]_{bab} + [K]_{add}$$

where $[K]_{bs}$ – matrix proportional to bond stretching constant [1]; $[K]_{bab}$ – matrix proportional to bond angle bending constant [1]; $[K]_{add}$ – a matrix containing two additional constants. Last matrix does not correspond for any elementary physical model of mechanics and molecular spectroscopy.

The finite-element model of a rectangular plate of graphene is builded. Tests for a stretching are simulated. Estimation of influence of additional stiffness constants on value of the Young's modulus and Poisson's ratio of graphene is made.

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Synthesis, Characterization and Luminescence Properties of Schiff bases-Zn(II) complex: Experimental and Theoretical Study to towards Application as Organic Light Emitting Diodes

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Schiff bases complexes have been studied for their wide applications in various fields such as catalysis, corrosion and sensors in addition to their biological activity towards cancer, tumer, antituberculous, antimalarial… etc. We have been interested in preparing Schiff bases and its zinc complexes in an effort to study and develop the understanding on the luminescence properties of these compounds. This work deals with the synthesis, characterization and photophysical properties of Schiff bases-Zn(II) complex, for possible application as organic light emitting diodes and sensor. This complex was synthesized and characterized by FTIR, elemental analysis, and single crystal X-ray crystallography. Electronic spectra and fluorescence properties of this compound were investigated using UV/Vis and fluorescence spectroscopy in both solid state and in solution. Computational methods were employed to study its molecular properties such as absorption, molecular orbital and molecular orbital energy for this compound. The calculated results correlate well with the experimental findings and provide good understanding of the structural and electronic behaviors associated with this molecule.

Keywords: Zinc, Schiff base, Luminescence and OLED.

First-principles Study of Hydrogen Storage Using Ca Atom with Functional Group

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Using first - principles calculations based on the density functional theory, we study the application of the hydroxyl group-Ca complex for hydrogen storage. The Ca atom is bound to the hydroxyl group with a binding energy comparable to the cohesive energy of bulk Ca and then the Ca atom can bind up to $7H_2$ molecules in molecular form, which can give a very high weight percent storage (example, 15.2 wt% for propane-1,3-diol). However, the average binding energy is about 0.1 eV per hydrogen molecule, which is somewhat smaller than the requirement for the room temperature application (≥ 0.2 eV/H_2). We also show that polarizations of H_2 molecules induced by the ionized Ca atom play an important role to the binding of H_2 molecules to Ca atom. This result shows a possibility of organic materials functionalized with the hydroxyl group for hydrogen storage media at near ambient temperature and pressure. Dipole interaction contributes significantly to the bonding of H_2 molecules on Ca atom.

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The Motion Behavior of Li Atom in LiBH4 Low temperature Phase, High temperature Phase, and the Intermediate State Structures

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We have studied the reason why titanium atom can not enhance the motion of lithium atom in $LiBH_4$ high temperature (HT) phase structure. Diffusion process and corresponding energy barrier of Li atom in low temperature (LT), high temperature (HT) phases of $LiBH_4$, and the intermediate state (IS) structure have been studied and compared through nudged elastic band (NEB) method. The role of the titanium atom in the destabilizing process and the role of the anion unit $[B_{12}H_{12}]^{2-}$ in stabilizing the intermediate state structure : $Li_2B_{12}H_{12}$ has been has been studied.

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Stability of Polymoph in ZnO Under Different Loading Conditions

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In this work, homogeneous phase transformations of ZnO from wurtzite (WZ) to three other different crystalline structures; unbuckled wurtzite (HX), rocksalt (RS), and BCT-4 under different loading conditions are studied by using first-principle calculations method. The stability of each crystal structure is determined by analyzing enthalpy of the structures under distortions. Under different loading conditions, the lowest enthalpy configuration is identified. By gradually increase the pressure (or stress) the homogeneous transformation path can be described. Under hydrostatic pressure, transformation into a six-fold coordinated rocksalt (RS) structure occurs. This is consistent with available experimental and theoretical results in the literatures. For the uniaxial stress conditions, we found that (1) under the uniaxial compression along the [0001] direction or the uniaxial tension along the [01$\overline{1}$0] direction, a transformation into a five-fold coordinated unbuckled wurtzite structure (HX) is observed;(2) under the uniaxial tension along the [0001] direction, a transformation into a body-centered-tetragonal structure (BCT-4) is observed.

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Aggregation of Metal Adatoms on Si(001) in the Presence of C-defects

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We present the results of our theoretical study of the aggregation of metal adatoms diffusing on Si(001) substrate. We have analysed the influence of the C-defects on the formation of the ordered low-dimensional structures by different kinds of metal adatoms such as metals from III group (Al,In), carbon group (Pb, Sn), and transition metals (Ag). Our theoretical study has been performed using *ab initio* calculations based on the density functional theory (DFT).

C-defects are commonly observed on Si(001) surface, however their origin and physical nature are still source of controversy. The recent STM measurements and also theoretical considerations strongly support the opinion that C-defect originates from the dissociative adsorption of single water molecule - in our consideration we have applied the model of C-defect based on such mechanism.

The room temperature (RT) STM measurements indicate that C-defects on Si(001) act as unique nucleation centres for metal atoms diffusing on this substrate. Metal adatoms deposited on this substrate tend to form chains pinned to C-defect and oriented perpendicular to dimmer rows. The experimental results strongly suggest that C-defect increases considerably the local chemical reactivity of the silicon substrate. The aim of our present theoretical study is to determine the mechanism responsible for the strong reactivity of C-defect and to analyse the formation, by the diffusing adatoms, of one-dimensional structures in the front of C-defects. The obtained results let us to understand the energy conditions associated with the growth of such structures and to determine their structural and electronic properties – theoretical results provided by our *ab initio* calculations will be analysed and discussed in the context of existing STM/STS data.

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A Potential Model for Protonated Hydrogen Fluoride H+(HF)n Clusters

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In this work, a potential model has been developed in order to simulate protonated hydrogen fluoride clusters. The potential is based on OSS2 functional form which was formerly designed for protonated water clusters by Ojamae et al.[1] It inherits the characteristics from OSS2 model such as polarizability and disassociation. Nevertheless, several modifications have been introduced to adapt to H+(HF)n clusters: the three-body-term interaction is simplified and the dipole constant is adjusted to the experimental result. The potential was then derived by fitting with the electronic surface of small-sized H+(HF)n (n=1-5) isomers at ab initio MP2 calculation. It reproduces well ground-state structures and binding energies at MP2 calculation and describes correctly the interaction in proton transfer reactions of protonated hydrogen fluoride dimers. The good results open a possibility to extend the model to be capable to simulate other hydrogen bonding systems and the mixed clusters of hydrogen fluoride and water in the future.

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Electronic Structure of $In_xGa_{1-x}As_ySb_{1-y}$ Alloys

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The quaternary semiconducting III-V alloys system $In_xGa_{1-x}As_ySb_{1-y}$ provides basis for devices operating over the spectral range of 2-4 µm. Its application in injection lasers has enhanced its technological applications further. The system has large miscibility gap with high critical temperature. Electronic band gap and the electronic structure are essential prerequisites for alloy semiconductors like $In_xGa_{1-x}As_ySb_{1-y}$ to analyse the physical phenomenon underlying optoelectronic applications. Empirical pseudopotential method is one of the suitable and widely used electronic structure method specially for semiconductor alloys. The alloying disorder in this method can be treated employing modified virtual crystal approximation. We present the electronic band structures of four compositions of $In_xGa_{1-x}As_ySb_{1-y}$ alloys with x,y=0.25 and 0.75. The band gap, ionicity and the refractive index are also presented and compared with the available experimental data for the alloys. Calculations are also performed to report the electronic density of states.

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Electronic and Structural Properties of g-Be3N2 by LCAO Method

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First principle calculations are performed to report electronic and structural properties of γ-Be$_3$N$_2$ following the linear combination of atomic orbital method within the generalized gradient approximation in the framework of density functional theory. The total energy calculations are performed to estimate equilibrium lattice constant, bulk modulus and B'. The electronic band structure, X-ray Structure factors and the Compton profiles are also reported. The derived quantities are compared with the corresponding experimental observables wherever available. The possibilities of pressure induced phase transitions to the α-Be$_3$N$_2$ are explored.

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