ACCMS-5 SCIENTIFIC PROGRAM

Location: Melia Hotel

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 Fibril Formation of Peptides and Related Structural Diseases: from Lattice to All-Atom Simulations

Mai Suan Li

Institute of Physics, Polish Academy of Sciences, Al. Lotnikow 32/46, 02-668 Warsaw, Poland

15:05-15:30 I3 - 3 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

15:30-15:45 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

15:45-16:00 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

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

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 CaCu3Ti4O12 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 **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

P - 7 **First Principles Calculations of SrHfO3**

A. Yangthaisong and S. J. Clark

Department of Physics Ubonrajathanee University Ubonratchathani THAILAND 34190

P - 8 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 - 9 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 - 10 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 - 11 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 - 12 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 UniversitÃ¤t Bremen Am Fallturm 1 28359 Bremen, Germany

P - 13 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 - 14 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 - 15 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 - 16 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 - 17 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 - 18 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 - 19 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 - 20 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

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P - 21 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

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P - 22 Calculation of the Field Emission Current from Carbon Nanotubes Using the Bardeen Transfer Hamiltonian Method

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P - 23 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

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P - 24 An Efficient Tool for Modeling and Prediction of Fluid Flow in Nanochannels

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P - 25 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

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P - 26 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 - 27 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

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P - 28 Computation of Chemical Equilibrium in Multi-component Zzirconium Alloys for Biomaterials Applications

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P - 29 Samdwich Microstructure of Tumblebug Cuticle

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

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P - 30 Spiry Microstructure of Aragonite Sheets of Chamidae Shell

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P - 31 Anisotropic Diffusion in Disordered Fractals

Do Hoang Ngoc Anh, Steffen Seeger and Karl Heinz Hoffmann

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P - 32 Study of Thermodynamic Properties of Cerium Dioxide under High Pressures

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

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P - 33 Electrophonon Resonance in Square Quantum Wells of n-GaAs Materials

Tran Cong Phong, Vo Thanh Lam, Luong Van Tung

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P - 34 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

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P - 35 Complex Characterization of the Nanostructured Materials by Using the Scanning Probe Microscopy Methods

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P - 36 Another SP3 Bonded Carbon Crystal

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P - 37 Mesoscale Simulation on Phase Behaviour of Triblock Copolymers with Different Chain Architecture in Aqueous Solution

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P - 38 Challenges in Modelling TCP Phase Formation in Ni-based Superalloys

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

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P - 39 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

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P - 40 Scanning Probe Microscopy Methods in the Complex Characterization Nanostructured Material and Surface

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

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P - 41 Effect of Stereochemical Composition on Dynamic Properties of Polypropylene Melts: A Multiscale Molecular Simulation

Tanissara Pinijmontree and Visit Vao-soongnern

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P - 42 Finite Element Analysis of Magnetic-Mechanical Structures for AFM

Dung C.T.P, Tan T.D, Long N.T, Thuy N.P

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P - 43 **Multiscale Modelling of Nanoindentation**

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P - 44 **Spherical Indentation On Ceramic Coatings**

Le Thuong Hien, Tran Ich Thinh, Bui Van Binh, Nguyen Van Duong

235- Hoangquocviet str., Hanoi, Vietnam Electric Power University

P - 45 **A new Stiffened Element Using to Analyse the Mechanical Behaviour of Stiffened Laminated Plates under Free Vibration**

Tran Ich Thinh, Ngo Nhu Khoa, Do Tien Dung

Thai Nguyen University - VietNam

P - 46 **Nonlinear Analysis of Stability for Functionally Graded Cylindrical Shells under Mechanical Loads**

Nguyen Dinh Duc, Hoang Van Tung

Vietnam National University, Hanoi

P - 47 **Numerical Simulation of Heat Stresses and Durability of the Combustor Wall**

Nguyen Phu Khanh, Nguyen Viet Hung, Hoang Thanh Tung

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P - 48 **Study on Mechanical and Thermodynamic Property of Some Cryocrystals**

Nguyen Quang Hoc and Dinh Quang Vinh

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P - 49 **Effect of Current Crowding on Electromigration Lifetime Investiganted by Simulation and Experiment**

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P - 50 **Numerical Simulation of the CUA DAT Dam**

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P - 51 An Application of the Meshfree Radial Point Interpolation Method in Solving the Two-Dimensional Node-To-Node Contact Problems

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P - 52 Finite Element Modeling and Experimental Study on Bending and Vibration of Laminated Stiffened Glass Fiber/polyester Composite Plates

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P - 53 Finite Element Modeling for Bending and Vibration Analysis of Laminated and Sandwich Composite Plates Based on Higher-order Theory

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P - 54 Evolution of Void and Constitutive Descriptions of Casting Magnesium Alloy

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

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P - 55 Atomic Structures and the Magnetism of fcc Fe/Cu(111) Films: First-principles Calculations

Heechae Choi and Yong-Chae Chung

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P - 56 Modelling Gadolinium Doped Gallium Nitride

B. Hourahine, S. Sanna, T. Frauenheim

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P - 57 Tailoring Intramolecular Exchange Coupling of Mn4 Single-Molecule Magnets: A Wway to Develop Single-Molecule Magnets

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P - 58 NMR in Nanoscale One-dimensional Spin Chain

Hoang Nam Nhat, Pham The Tan and Nguyen Duc Tho

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P - 59 Density Functional Study of Electronic Properties of Perovskite Systems La_1-xSr_xFeO_3

Nguyen Duy Huy, Nguyen Thuy Trang, Nguyen Hoang Linh, Nguyen Tien Cuong,Pham Huong Thao, and Bach Thanh Cong

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P - 60 Influence of Doped Rare-Earth Elements on Electronic Properties of RxCa1-xMnO3 Systems

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

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P - 61 Ground State of Spin Chain System by Density Functional Theory

Nguyen Thuy Trang, Nguyen Duc Tho and Hoang Nam Nhat

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P - 62 Structural Stability, Magnetism and Hyperfine Interactions of Hydrogen Monomer, Dimers, Trimers and Tetramers on Graphene

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P - 63 The Monte Carlo Simulation of Magnetic Nanoparticle Systems

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P - 64 Atomistic Simulation of the Interlayer Structures and Dynamics of the Hydrated Potassium-Montmorillonite

Chinnawut Pipatpanukul, Supagorn Rugmai and Visit Vao-soongnern

School of Chemistry Inst. of science Suranaree University of Technology Nakhon Ratchasima 30000

P - 65 Kinetic Monte Carlo Simulations of Diffusion-Limited Nucleation

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

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P - 66 Investigation of the Solidification Process of Monatomic Lennard-Jones Systems.

Le Nguyen Tue Minh and Vo Van Hoang

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P - 67 Structure and Dynamical Properties in Noblemetal Halide Mixture Include Two Kinds Cations, Ag+ and Cu+

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P - 68 Modeling of the Phase Transformation sII – sH in Ar Hydrates at High Pressure

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P - 69 Thermodynamic Prediction of Structural Transitions in Binary Methane-Ethane Hydrates at Low Temperatures

T.P. Adamova, O.S. Subbotin, A. A. Pomeransky, V.R. Belosludov

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P - 70 Influence of Methane Content on Clathrate Hydrate Structure Transformation sI – sII

O. S. Subbotin, V. R. Belosludov, R. V. Belosludov , H. Mizuseki and Y. Kawazoe

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P - 71 Analysis of Protein Hydration Water by Means of Data Mining Method

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

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P - 72 Molecular Dynamics Simulation of Structural and Thermodynamics Properties of Amorphous GeO2 Nanoparticles

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P - 73 Structure and Diffusion in Simulated Liquid GaAs

Tran Thi Thu Hanh and Vo Van Hoang

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P - 74 Molecular Dynamic Simulation Study of Gold Structure in Amorphous and Liquid States

Truong Nguyen Duy Ly, Ngo Huynh Buu Trong and Vo Van Hoang

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P - 75 First-principles Molecular Dynamics Study on the Structure of Amorphous Ge2Sb2Te5

Eunae Cho, Jino Im, Jisoon Ihm, and Seougwu Han

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P - 76 Models of Some Nano Device Based on Carbon Nanotubes and DNA

N. N. Hieu, N. A. Poklonski , N. V. Thanh and N. A. Viet

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P - 77 Binding Energy Estimation of Hydrogen Storage Materials by All-Electron Mixed-Basis Program TOMBO

Ryoji Sahara, Hiroshi Mizuseki, Kaoru Ohno, Marcel Sluiter, and Yoshiyuki Kawazoe

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P - 78 **Simulation of Mechanical and Electrical Properties of Quartz Crystal Microbalance**

Vu Ngoc Hung, Nguyen Van Dinh, and Trinh Quang Thong

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P - 79 **Theoretical Investigation of the Hydrogen Storage Ability of a Carbon Nanohorn**

G. Chen, Q. Peng, H. Mizuseki, and Y. Kawazoe

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P - 80 **First Principles Calculations on Grain Boundary Impurities in Polycrystalline Silicon**

Ambigapathy Suvitha, N. S. Venkataramanan, Ryoji Sahara, Hiroshi Mizuseki and Yoshiyuki Kawazoe

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P - 81 **Atomistic Modelling of Artificially Controlled Grain Boundaries in Multicrystalline Silicon**

Hiroshi Mizuseki, Ambigapathy Suvitha, Ryoji Sahara, and Yoshiyuki Kawazoe

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P - 82 **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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P - 83 **High-Capacity Hydrogen Storage of Al Adsorbed Graphene: Ab Initio Investigation**

Hong-Lae Park, Byung-Hyun Kim and Yong-Chae Chung

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P - 84 **Complex Permeability Model for Efficient Proximity Losses Computation in Electric Conductors**

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P - 85 First-principles Calculations on Hydrogen Storage Properties of CS-4 clathrate Hydrate

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P - 86 Density Functional Study on the Alkali Atom Doped Calix[4]arene as Hydrogen Storage Material

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P - 87 Atomistic Simulation of the Structure, Interaction and Dynamics of Poly(lactic acid) Melt and Graphite Interface

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P - 88 Effect of Film Thickness on the Phase Transition in Thin Magnetic Films

V. Thanh Ngo, D.Tien Hoang, X. T. Pham-Phu and H. T. Diep

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P - 89 Fracture Toughness of an Interface between a Submicron-Thick Film and a Substrate

Do Van Truong, Vuong Van Thanh, Trinh Dong Tinh

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P - 90 A First Principles Calculation on the Polythiophene/Graphene Hybrid Nanocomposite

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P - 91 Modelling Fullerenes on Si (100)

Paul C Frangou, David J King, Steven D Kenny and Ed Sanville

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P - 92 Molecular Dynamics Study of Sputter-induced Composition Modulation in Co-Cu alloy

Byung-Hyun Kim, Sang-Pil Kim, Kwang-Ryeol Lee, Yong-Chae Chung

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P - 93 First-principles Study of the Preferential Atomic Sites for Hydrogen incorporated in the Epitaxial Graphene on SiC

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P - 94 Molecular Dynamics Study of Tetrahedral Amorphous Carbon Film Growth

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P - 95 First-principles Study on the Electronic Properties of Graphene Nnanoribbons

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P - 96 First Principles Calculations of Electronic Structures of F4-TCNQ Molecule on Graphene

Jiatao Sun, Wei Chen, Yuanping Feng, Andrew T. S. Wee

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P - 97 Local Elastic, Viscoelastic and Geological properties of the Thin polymer layers by means of Scanning Force Probe Microscopy

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P - 98 Spatial Distribution of Transferred Charges at the Interface of TTF and TCNQ Organic Crystals

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P - 99 Scattering Potentials at Impurity Dimers and Atomic Switch Design on Ge(001) and Si(001): First-principles Study

Binghai Yan, Chenchen Wang, Bing, Huang, Gang Zhou, Wenhui Duan, Binglin Gu, Kota Tomatsu, Fumio Komori, Andreia Luisa da Rosa, Thomas Frauenheim

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P - 100 A Comparative Study on the Optical Properties of Indenofluorene and Indenopyrazine

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P - 101 Modelling of Thermal Oxidation in Porous Silicon

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P - 102 Atomic Relaxation and Electronic Structure Investigation of Eu2+ doped β-SiAlON: Ab Initio Calculations

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P - 103 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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P - 104 First-Principles Analysis of Photoabsorption Spectra of (CdSe)34 Clusters in Pearl-Necklace Geometry

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P - 105 Finite Difference Time Domain Method Optimized for Full Analyses of Photonic Crystal Fibers

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P - 106 The Photocatalysis of H2O Absorption on TiO2 Rutile (110) Studied by DFT Calculations

Dinh Son Thach, Nguyen Doan Thanh Vinh

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P - 107 Positively Charged Excitons in Quantum Dots

Nguyen Hong Quang, Duong Xuan Long, Vu Duc Tho

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P - 108 Tracking Acetylene/Vinylidene Isomerization Process by Ultrashort Laser Pulses using High Harmonic Generation

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P - 109 The Investigation of the Effects of Ga-doping on the Electronic Structure and the Optical Properties of ZnO under the Density Functional Theory

Đinh Son Thach, Tran Nguyen Quynh Nhu

12P, Thu Khoa Huan, Phuong 1, My Tho, Tien Giang

P - 110 Opto-electronic and Magnetic Properties of the Mn-doped Indium in Oxide: A First-principles Study

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P - 111 Vibration Signatures of OTe and OTe-VCd in CdTe: A First Principles Study

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P - 112 DFT Study on Elastic and Piezoelectric Properties of BaTiO3 Crystals

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P - 113 Parametric Study of Left-Handed Combined Metamaterial

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P - 114 Gaint Moment Reduction of Fe Impurity in Dilute Pd-V Alloys

M. S. Bahramy, S. N. Mishra, G. P. Das and Y. Kawazoe

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P - 115 Discrimination of Individual Molecules from Other Molecules One by One by Restricting the Light Emitting Space

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P - 116 Direct Enumeration Studies of Band-Gap Properties of AlxGayIn1−x−yP Alloys

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P - 117 Electron Diffraction and High Resolution Electron Microscopy Techniques Study on the Microstructure of NdFeCoAl-(B,C) Based Alloys

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P - 118 Structural Elements for Modelling the Elastic Properties of Graphene

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P - 119 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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P - 120 First-principles Study of Hydrogen Storage Using Ca Atom with Functional Group

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P - 121 The Motion Behavior of Li Atom in LiBH4 Low temperature Phase, High temperature Phase, and the Intermediate State Structures

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P - 122 Stability of Polymoph in ZnO Under Different Loading Conditions

K. Sarasamak, A. J. Kulkani, M. Zhou, F. J. Ke, J. Wang, S. Limpijumnong

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P - 123 Aggregation of Metal Adatoms on Si(001) in the Presence of C-defects

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P - 124 A Potential Model for Protonated Hydrogen Fluoride H+(HF)n Clusters

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P - 125 Electronic Structure of $In_xGa_{1-x}As_ySb_{1-y}$ Alloys

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P - 126 Electronic and Structural Properties of g-Be3N2 by LCAO Method

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