The 14th Asian Workshop on First-Principles Electronic Structure Calculations (ASIAN-14)

October 30 − November 2, 2011
Takeda-Hall
The University of Tokyo
Japan

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- Asia Pacific Center for Theoretical Physics (APCTP)
- Computational Materials Science Initiative (CMSI)
- Scientific Research on Innovative Areas, 'Materials Design through Computics: Complex Correlation and Non-equilibrium Dynamics'

Timetable

Oct. 30 (Sun)			
18:00	Registration (18:00-20:00)		
Oct. 31 (Mon)			
9:30	Opening		
9:45	A-15	H. Ishii	Transport
10:15	A-16	T. Tada	
10:45	Break (20min)		
11:05	A-1	S. Han	Materials
11:35	A-2	Y.-S Kim	
12:05	A-3	M. Zhao	
12:35	Lunch (100min) [Get-together lunch for invited speakers and committee members]		
14:15	S-2	S. Goedecker	Structure
15:00	A-4	C.M. Chang	
15:30	A-5	S. Ogata	
16:00	Break (20min)		
16:20	A-6	M.-Y Chou	Topology
16:50	A-7	S.-H Jhi	
17:20	A-8	H. Weng	

Timetable was revised on Oct. 31, 2011

Nov. 1 (Tue)			
9:30	S-3	M. Sprik	Reactions and dynamics
10:15	A-9	W. Y. Kim	
10:45	Break (20min)		
11:05	A-10	K. Yabana	
11:35	A-11	H.J. Xiang	Multiferroics
12:05	A-12	K. Yamauchi	
12:35	Lunch (85min) [International Organizing Committee Meeting]		
14:00	A-13	T. Miyake	Superconductors
14:30	A-14	H.J. Choi	
15:00	S-4	M. Gillan	Methodology
15:45	Conference Photo		
16:00	Poster		
18:20	Banquet		

Nov. 2 (Wed)			
9:30	S-1	R. Car	
10:15	A-17	L. He	Methodology
10:45	Break (20min)		
11:05	A-18	Y.-C Chang	
11:35	A-19	T. Ozaki	
12:05	Closing		

General Information

Program

Oct. 30 (Sun)

18:00 Registration and get-together (18:00-20:00)

Oct. 31 (Mon)

9:30 Opening

TRANSPORT

9:45 A-15 H. Ishii

"Order-N electron transport calculations for ballistic, diffusive and polaron transport regimes"

10:15 A-16 T. Tada

"Quantum transport and quantum information processing on single molecular junctions from first principles"

MATERIALS

10:45 Break (20min)

11:05 A-1 S. Han

"Universal features in band structures of crystalline and amorphous transparent conducting oxide"

11:35 A-2 Y.-S. Kim

"Cation composition effects on the electronic structure of amorphous oxide semiconductors"

12:05 A-3 M. Zhao

"Spin-polarizaion and magnetism in cubic silicon carbide"

12:35 Lunch (100min)

STRUCTURE

14:15 S-2 S. Goedecker

"Structure prediction of clusters and solids by the minima hopping global geometry optimization method"

15:00 A-4 C.M. Chang

"Ab-initio random structure search for metallic clusters"

15:30 A-5 S. Ogata

"First-principles modeling of deformation and diffusion"

16:00 Break (20min)

TOPOLOGY

16:20 A-6 M.-Y. Chou

"Electronic structure of twisted multilayers of epitaxial graphene"

16:50 A-7 S.-H. Jhi

"Topological phase in Dirac fermionic heterostructures"

17:20 A-8 H. Weng

"Half-metallic surface states and topological superconductivity in $NaCoO_2$"

Nov. 1 (Tue)

REACTIONS AND DYNAMICS

9:30 S-3 M. Sprik

"Reactivity of valence band holes at the rutile TiO2/water interface"

10:15 A-9 W. Y. Kim

"Time-dependent density functional method for studying electron transfer at solid-molecule interfaces"

10:45 Break (20min)

11:05 A-10 K. Yabana

"Time-dependent density functional theory for femtosecond electron dynamics in dielectrics"

MULTIFERROICS

11:35 A-11 H.J. Xiang

"General theory for the ferroelectric polarization induced by spin-spiral order"

12:05 A-12 K. Yamauchi

"Novel mechanisms for multiferroicity and magnetoelectric effects in transition metal oxides"

12:35 Lunch (85min)

[International Organizing Committee Meeting]

SUPERCONDUCTORS

14:00 A-13 T. Miyake

"Electronic structure and correlation effects in iron-based superconductors"

14:30 14:30 A-14 H.J. Choi

"Orbital features in electronic and magnetic properties of iron pnictides and chalcogenides"

METHODOTOGY

15:00 S-4 M. Gillan

"Beyond DFT with quantum Monte Carlo and wavefunction-based quantum chemistry"

15:45 Conference Photo

16:00 **Poster** (16:00-18:00)

18:20 **Banquet** (Sanjo Conference Hall in the Univ. Tokyo)

Nov. 2 (Wed)

9:30 S-1 R. Car

"Recent progress in first-principles simulations of water"

METHODOLOGY

10:15 A-17 L. He

"Systematically improvable optimized atomic basis sets for ab inito calculations"

10:45 Break (20min)

11:05 A-18 Y.-C Chang

"First-principles calculations of large super cells and nanoclusters based on symmetrized basis"

11:35 A-19 T. Ozaki

"Low-Order Scaling Density Functional Methods Based on Quantum Nearsightedness"

12:05 Closing

Posters

Posters are put up during the conference at the lobby in front of the conference room. The size of the board for each poster presentation is **90cm(W) x 150cm(H)**.

1 Sirichok Jungthawan
"Effects of strain on gas separation properties of porous graphene"

2 Shiow-Fon Tsay
"Pt induced nanowires on Ge(001) surface"

3 Chung-Huai Chang
"First-principle studies of molecule adsorption on graphene: The adsorption-induced band"

4 Yoshihiro Gohda
"Structure and electronic properties of nitride interfaces"

5 Meng Hsiung Weng
"Density function theory study of the oxidation of CO on W(111) surface"

6 Yosuke Harashima
"Effect of Disorder and Electron-Electron Interaction near Metal-Insulator Transition in Doped Semiconductors using Density Functional Theory"

7 Jeongwoo Kim
"The band insulator – topological insulator transition in chalcogenide heterostructure"

8 Ming-Hsien Lee
"Bond-Type Labeling for First-Principle Computed Core-Leve Spectra"

9 Kyung-Hwan Jin
"Epitaxy of graphene on the surface of Sb_2Te_3 topological insulator"

10 Jung-Hoon Lee
"First-Principles Study of the Origin of Ferroelectricity in Orthorhombic $YMnO_3$"

11 Jinwoong Kim
"Topological insulating phase of GeTe induced by atomic disorder"

12 Tay-Rong Chang
"Electronic Structure and Orbital Ordering of Superconductor $HgxReO_3$"

13 Yun-Wen Chen
"Finding the Reaction Pathways of Water Splitting on Polar and Non-Polar GaN Surfaces via Simulations"

14 Dorj Odkhuu
"A first-principles study of the electronic structures and magnetic properties of magnetite and ulvospinel"

15 Kim Jae Nyeong
Control of Multiple CDW Phase in $SmNiC_2$ by Magnetism & Pressure"

16 Ten-Ming Wu
"Revisiting anomalous structures in liquid Ga"

17 Jeng-Da Chai
"Density Functional Theory with Fractional Occupations"

18 Ken-Ming Lin
"Strain effects on band gap of SWCNTs"

19 Ji-Hui Yang

“First-principles study of defect properties of zinc-blende MgTe”

20 Savas Berber

“Modifying the physical properties of carbon nanotubes: Chemistry on defects”

21 Jen-Hsien Wong

“Electronic properties of graphene/nanoribbon superlattices”

22 Jhih-Rong Huang

“MnFe2O4 in Single-Valence State”

23 Shao-Hua Chen

"Investigation of possible half-metal material on double perovskites $Sr_2BB'O_6$ (B, B' = 3d transition metal) by first-principle calculations."

24 Mitsuaki Kawamura

"Ab initio prediction of superconducting transition temperature based on density functional theory for superconductors"

25 Hanhim Kang

“Non-Stoner Itinerant Ferromagnetism in Low-Dimension System”

26 Sheng-Chieh Huang

“Gapless Band Structure of $PbPdO_2$: A Combined First Principles Calculation and Experimental Study”

27 Yoshiyuki Miyamoto

“One-side dehydrogenation of graphane by asymmetric laser pulse”

28 Bo Xiao

“Theoretical investigation on the interaction between carbon monoxide and carbon nanotubes with single vacancy defect”

29 Maximilian Amsler

“Crystal structure prediction: a novel approach based on minima hopping”

30 Ji-Sang Park

“Stability and electronic structure of donor-pair defects in $Si_{1-x}Ge_x$ alloy nanowires”

31 Young Jun Oh

“Boron segregation and effect of point defects in Si/SiO_2 interface”

32 Hyeon-Kyun Noh

“Schottky barriers and work functions of Ni/HfO_2 and Ni/SiO_2 gate stacks”

33 Bharat Sharma

“Magnetism during adsorption of O_2 on Pt segregated Pt_3Ni (111): Density Functional Study”

34 Alex Lee

“Electrical conductance and Anderson localization in carbon nanotubes with vacancy defects”

35 Seung Ill Hyun

“Magnetic Interactions in Fe-doped TiX_2 (X=S, Se)”

36 Adisak Boonchun

“Critical Evaluation of the LDA + U Approach for Band Gap Corrections in Point Defect Calculations: The Oxygen Vacancy in ZnO Case Study”

37 Masato Morita

"Origin of huge difference in the vibrational spectra between $OH-(H_2O)_3$ and $OH-(H_2O)_4$ clusters”

38 Tetsuta Nagata

"First-principles calculation of transport properties of Al/GaN interface"

39 Jyh-Pin Chou

“New structural model for Na_6Si_3 magic cluster on Si(111)-7x7 surface”

40 ZhufengHou

“Interaction between Nitrogen Dopants and Native Point Defects in Graphene”

41 Shigeru Tsukamoto

“Electron transport through molecular junctions with thiloate–Au and carboxylate–Cu anchoring bonds”

42 Chih-Huan Chen

“Ab initio studies of structural and electronics properties, spin waves and exchange interaction, and Curie temperature in bulk Gadolinium”

43 Ching Cheng

“Structural and Magnetic Phase Transition of Fe, Co and Ni under Anisotropic Compression”

44 Hung-Lung Huang

“Ab Initio Studies of Electronic Structure, Magnetism and Ferroelectricity in $BiMnO_3$”

45 Naoto Umezawa

"Revisiting the mechanism of photocatalytic activities in N-doped TiO_2"

46 Hideo Sekino

“Time Evolution of Wavefunction by Quantum Walk”

47 Chunping Hu

“Multiple conical intersections in time-dependent density functional theory”

48 Taichi Kosugi

"Slab Thickness Dependence of Rashba Splitting on Au(111) Surface: First-Principles and Model Analyses”

49 Sathya Subramanian

“First principle study of doping $HoMnO_3$ with lone pair cations”

50 Jae Won Yang

“Gap Opening of Bilayer Graphene by Dual Doping Method”

51 Masayuki Ochi

“Optimization of the Jastrow factor based on pseudo-variance minimization by the transcorrelated method for solids”

52 Shinya Nishino

"Li ion dynamics in Li_4GeS_4 and Li_3PS_4: First Principle Electronic Structure Calculation and Long Time Tight Binding Molecular Dynamics Simulation"

53 Chang-Youn Moon

“Anisotropic Dirac-cone on the side surface of topological insulator Bi_2Se_3”

54 Yu Takano

“Coordination effects on the electronic structures of the CuA site in cytochrome c oxidase”

55 Xianlong Wang

“Study of the NMR chemical shifts of graphene clusters doped with nitrogen”

56 Michiaki Arita

"Theoretical studies on a gramicidin A channel using a linear-scaling DFT technique"

57 Ayako Nakata

“Long-range corrected spin-orbit TDDFT calculations”

58 Pakpoom Reunchan

“Theory of Chromium-doped $SrTiO_3$ photocatalyst”

59 Yasuteru Shigeta

“Structural feature of entrance at a proton transfer pathway”

60 Giacomo Giorgi

“Excitons at the (001) surface of anatase: Spatial behavior and optical signatures”

61 Masato Sumita

“Water Contamination Effect on Liquid Acetonitrile / TiO_2 Anatase (101) Interface for Durable Dye-sensitized Solar Cell“

62 Takao Tsumuraya

“First-principles study on structural and electronic properties of $Pd(dmit)_2$ salts under high pressure”

63 Ryosuke Akashi

"Unconventionality of High-Tc Superconductivity in Layered Nitrides MNCl (M=Ti, Zr, Hf): A Study based on Density-Functional Theory for Superconductivity"

64 Muhammad Farhan

“First principle calculations of Pressure driven Insulator to Metal Transition in $SrMnSb_2$”

65 Tatsuhiko Ohto

“Bias Dependent Switching Rate of STM-Induced Melamine/Cu(001) Switch”

66 Linh Nguyen

"Electronic Structure and Magnetic Properties of Undoped Fe Pnictide Materials - LaFeAsO"

67 Jun Haruyama

"Time-Dependent Density Functional Calculation of the Excited State Nuclear Forces"

68 Terumasa Tadano

"Thermal conductivity calculations of semiconductors from first-principles anharmonic lattice model"

69 Tomoki Kobori

"Electronic Structure Analysis of FKBP-ligands system based on FMO-LCMO"

70 Hyungjun Lee

“The Role of d-Orbitals in Rashba-Type Spin-Splitting in Noble Metal Surfaces”

71 Katsumasa Kamiya

“First-Principles Molecular Dynamics Study on Reaction Mechanisms of Nylon-6 Byproduct-Degrading Enzyme”

72 Takeru Sugiyama

“Development of First-Principles Maxwell+TDDFT Multi-Scale Simulator for Propagation of High-Intensity Laser Pulse”

73 Mohammad Alam

“First-principles calculations of mono-hydrogen and di-hydrogen in Graphene and Carbon Nanotubes”

74 Sergiu Arapan

“Recent Progress in a linear-scaling DFT code CONQUEST: parallel efficiency and optimization of local orbitals”

75 Tatsuya Shishidou

“Fermi surface and spin texture of the noncentrosymmetric superconductors Li_2Pd_3B and Li_2Pd_3B”

76 Hiromasa Ohnishi

“Weak ferromagnetism in the lightly electron-doped $CaMnO_3$”

77 Shinichi Motonaka

"First-principles study of the orbital state in antiferromagnetic FeO"

78 Hideyuki Kamisaka

“DFT-based First Principle Study of the Carrier Compensation Mechanism in Nb-doped Rutile TiO_2”

79 Masayuki Toyoda

“Order-N method for calculating orbital-dependent exchange”

80 Guan-De Li

“Long-range corrected meta-generalized gradient approximation density functional with dispersion corrections”

81 Hao Wang

“LDA+U study of PuO_2 on ground state with spin-orbital coupling”

82 Ying-Cheng Li

“Effect of messenger on small protonated water cluster”

83 Hsin-An Chen

“A First Principles Calculation on Graphene-based Heterojunctions”

84 Yusuke Nomura

“Ab initio Derivation of Low-energy Models for Aromatic and C_{60} Superconductors”

85 Tsuyoshi Miyazaki

"Recent progress in a linear-scaling DFT code CONQUEST: parallel efficiency and optimisation of local orbitals"

86 Yoshinobu Akinaga

“Methanethiol on noble metal surfaces: Determination of reaction paths”

87 Kazuaki Kobayashi

“First-Principles Study of Various SiC polytypes”

88 Takao Otsuka

“Interaction energy and large-scale DFT calculations of DNA with unnatural base pair systems”

89 Cuong Nguyen

“Origin of the n-type Transport Behavior of $C_{59}N$ Encapsulated Semiconducting Single-Walled Carbon Nanotube”

90 Sho Iwasaki

“Electronic structure and magnetic properties of YMn_2”

91 Fumiyuki Ishii

"Spin-Polarized Electronic States and Rashba Effect in the Graphene on Ni(111)"

92 Keitaro Sodeyama

"Protonated carboxyl anchor for stable adsorption of N749 Ru dye (black dye) on TiO_2 anatase (101) surface”

93 Hee Jung Kim

“The role of van der Waals interaction in FeSe superconductor”

94 Shusuke Kasamatsu

"Ab-initio study of the capacitance density of high-k nanocapacitors"

95 Sora Park

“Computational Study on the Transport Properties of Rigidly Interconnected Carbon Nano Foam”

96 Hyung-June Lee

“Ab Initio Study on H_2S Sensing Mechanism of Functionalized Carbon Nanotube-based Sensors”

97 Jian-Hao Li

“Size and Lattice Effects of Plasmonic Properties of Na Spheres Investigated by Real-Time TDDFT Simulations”

98 Shotaro Doi

“Development of first-principles electronic structure calculation code by using real space screened KKR method”

99 Toshiaki Iitaka

"Low temperature structure of filled ice hydrogen hydrate: an ab initio molecular dynamics study"

100 Jer-Lai Kuo

“Low-temperature Phase Transitions in Ice by First-Principles Methods”

101 Seoung-Hun Kang

“First-Principles Study on Doping and Electric Field Effects of Carbon Nanotubes on Hexagonal Boron Nitride Substrate”

102 Chang-sun Lee

“Modeling of Punctured Nanotube Device Channels for Device Performance Enhancement”

103 Bon-Gil Koo

“Geometrical and Electronic Structures of Self-Assembled One-Dimensional Metal-Molecule Hybrid Chains: First Principle Study.”

104 Liang Li

“Stable structures of adsorption Tl on the clean Tl/Si(111)”

105 Marcus Heide

"Convergence of DFT Calculations: Rotated Magnetic Moments, Total Energy, and Forces"

106 Tetsuya Nagata

"First-principles calculation of transport properties of Al/GaN interface"

107 Masako Ogura

“Enhancement of magnetism of Fe by Cr and V”

108-1 Yu-ichiro Matsushita

"Analyses of relationships between stacking structures of sp^3 network materials and their band gaps”

108-2 Yu-ichiro Matsushita

“Comparative study of hybrid functionals applied to condensed matters: structural and electronic properties"

109 Yasunobu Ando

“First-principles study of the electric double-layer capacitance at water-graphene interfaces”

110 Keisuke Sawada

"Magnetism and Transport Property of Graphene on Substrates"

111 Yoshiteru Takagi

"Band-Gap Engineering of Hydrogen-Potassium Graphite Ternary Intercalation Compound Thin films"

112 Bailey Hsu

"Current Streamline Flow on Current-Induced Effects in Highly Asymmetric Molecular Junctions"

113 Jaehoon Jung

"Controlling chemical reactivity of ultrathin oxide film by interface manipulation"

114 Hiroki Kotaka

"Fully relativistic calculation of Bi (001) films without inversion symmetry"

115 Hu Sung Kim

"Origin of Multiple Conductance Peaks in Single-Molecule Junction Experiments"

117 Koun Shirai

“Material design for superconductivity on semiconducting boron”

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Exhibitions are presented nearby the posters.

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