International Symposium on Computics: Quantum Simulation and Design

ISC-QSD2014

Supported by Grant-in-Aid for Scientific Research on Innovation Area “Materials Design through Computics: Complex Correlation and Non-equilibrium Dynamics” and Computational Materials Science Initiative (CMSI) in the HPCI Strategic Program from the Ministry of Education, Culture, Sports, Science and Technology of Japan

December 1 – December 3, 2014
Koshiba Hall, University of Tokyo
Hongo, Tokyo, Japan
Organizing Committee
Masatoshi Imada (Tokyo)
Mary Inaba (Tokyo)
Hiroshi Nakanishi (Osaka)
Atsushi Oshiyama (Tokyo) Chair
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Oral presentations
Invited talks: 35 minutes including discussion
Contributed talks: 20 minutes including discussion

LCD projectors will be available in the auditorium. If you wish to give your presentation from your laptop, you are requested to be present before the start of the session to connect your laptop. You can also bring your presentation (in PowerPoint or PDF) on a memory stick and load it onto a PC in the symposium room. In this case also, you should be present before the start of the session and contact a stage operator to set up your presentation.

Poster presentations
Poster sessions will be held in the Foyer of the Koshiba Hall. A poster board will be available for each poster. The poster session will be held on Tuesday afternoon (13:40~16:40). The posters can be put up as soon as the boards are ready on the first day of the Symposium. Authors will stand by their posters during the session. The posters should be removed before the end of the Symposium. The authors are responsible to put up and remove their posters. Posters not removed by the indicated time will be discarded.
Monday, December 1

9:50 – 10:10  Opening  
Chair: Satoshi Watanabe
Opening Address
Atsushi Oshiyama (Symposium Chair)
Shinji Tsuneyuki (Computational Materials Science Initiative: CMSI)

10:10 – 12:05  Oral Session I  
Chair: Shinji Tsuneyuki
10:10  Theoretical and Computational Studies of Quasi Two-Dimensional Materials
Steven G. Louie  (invited)
10:45  *Ab initio* GW analysis on low-energy plasmaron states
Kazuma Nakamura
11:05  Isotope effect on the band structure of graphene
Takashi Koretsune
11:25  Surface as a Foundation to Realizing Designer Materials
Hideaki Kasai
11:45  Underscreened Kondo state of collective molecular spin in Mn-Phthalocyanine on Pb(111)
Emi Minamitani

Symposium Photo
Lunch

13:30 – 15:05  Oral Session II  
Chair: Kazuhiro Yabana
13:30  Ultrafast laser-induced demagnetization of ferromagnetic solids: Identifying the mechanism with real-time TDDFT
Eberhard Gross  (invited)
14:05  Application of time-dependent density functional theory to electron emission and scattering at nano scale
Kazuyuki Watanabe
14:25  Photo-Enhancement of Cohesion; Cases of Noble Atoms and Layered Materials
Yoshiyuki Miyamoto
14:45  Exact nuclear potential and exact electronic potential in coupled electron-ion dynamics
Yasumitsu Suzuki

Coffee Break

15:30 – 17:55  Oral Session III  
Chair: Hiroshi Nakanishi
15:30  Experimental and theoretical study of electron transport through single π-stacked systems and ionic wires
Manabu Kiguchi  (invited)
16:05  First-principles study on tantalum oxide based resistive switching devices
       Satoshi Watanabe

16:25  Magnetic anisotropy induced by itinerant electrons in Y2Fe14B
       Yoshihiro Gohda

16:45  Clustering tendency and change in band structure of GaMnAs and InMnAs
       Van An Dinh

17:05  Robust flat bands in RCo5 (R: rare earth) compounds
       Masayuki Ochi

17:25  Topological Effects in Tellurium and Selenium
       Motoaki Hirayama

18:30  Symposium Dinner (Banquet)
Tuesday, December 2

9:30 – 10:40 Oral Session IV  
Chair: Mary Inaba

9:30  Scientific Simulation on Zetta-Scale computing systems  
Kei Hiraki  (invited)

10:05  Variational Principles and Computation of Linear Response Eigenvalue Problems with Application to Excited State Calculations  
Zhaojun Bai  (invited)

Coffee Break

11:00 – 12:35 Oral Session V  
Chair: Zhaojun Bai

11:00  Krylov subspace theories and one-hundred-million-atom electronic structure calculations on the K computer  
Takeo Hoshi  (invited)

11:35  Performance of the Block Jacobi Method for the Symmetric Eigenvalue Problem on the K computer  
Yusaku Yamamoto

11:55  Stable and Efficient Linear Scaling First-Principles Molecular Dynamics for 10,000+ atoms  
Tsuyoshi Miyazaki

12:15  Quantum Monte Carlo simulations of molecular crystal polymorphism on the K supercomputer  
Kenta Hongo

Lunch

13:40 – 16:40 Poster Session

16:40 – 18:30 Oral Session VI  
Chair: Eberhard Gross

16:40  Water: from deep undercooling to ultrahigh pressure  
Roberto Car  (invited)

17:15  Novel reaction mechanism of Lithium-ion battery electrolyte by DFT free energy calculation with parallel blue-moon ensemble on K computer  
Yoshitaka Tateyama  (invited)
17:50  Real-space implementation of the Car-Parrinello molecular dynamics for massively-parallel computers
       Jun-ichi Iwata
18:10  Quantum states of positive-muon and proton in materials
       Hiroshi Nakanishi
Wednesday, December 3

9:30 – 11:00    Oral Session VII    Chair: Masatoshi Imada

9:30  “Screened Exchange Dynamical Mean Field Theory” Or How to get rid off the LDA in “LDA+DMFT”
       Silke Biermann  (invited)
10:05 Honeycomb-Lattice Iridates Na$_2$IrO$_3$ under Strong Spin-Orbit Interaction and Electron Correlation Studied by Ab Initio Scheme
       Youhei Yamaji
10:25 Effective Coulomb interaction in solids from constrained random-phase approximation
       Ersoy Sasioglu  (invited)

Coffee Break

11:20 – 12:35    Oral Session VIII    Chair: Yasutami Takada

11:20  Adaptation of Dynamical Mean-Field Theory for Nanoscale Systems
       Talat S. Rahman  (invited)
11:55 Mechanism of superconductivity in iron-based superconductors studied by ab-initio downfolding scheme
       Takahiro Misasa
12:15 Ab initio calculation of superconducting transition temperature for alkali-doped fullerides
       Yusuke Nomura

12:35 – 12:55    Closing
Poster Session
13:40 – 16:40 Tuesday, December 2, 2014

P-01  H. Maeda and D. Takahashi  
(University of Tsukuba)  
Performance Evaluation of Sparse Matrix-Vector Multiplication Using GPU/MIC Cluster

P-02  T. Miyata and K. Nishizawa  
(Nagoya University)  
Multishift QR algorithm with GPU for eigenvalue problems

P-03  Hiori Kino, Takashi Miyake, Koji Hukushima and Masato Okada  
(National Institute for Materials Science)  
Potential energy surface by linear regression, application to Si and SiO2

P-04  A. Nakata, D.R. Bowler, Y. Futamura, T. Sakurai and T. Miyazaki  
(National Institute for Materials Science)  
Efficient optimization of local orbitals and eigenstate calculations in O(N) DFT code CONQUEST

P-05  Mitsuaki Kawamura, Yoshihiro Gohda, and Shinji Tsuneyuki  
(The University of Tokyo)  
Improved tetrahedron method for the Brillouin-zone integration applicable to DFPT calculations

P-06  Eiji Tsuchida  
(National Institute of Advanced Industrial Science and Technology)  
An algorithm for increasing the stability limit of ab initio molecular dynamics simulations

P-07  Y. Yoshimoto  
(The University of Tokyo)  
Multicanonical simulation combined with first-principles calculation: application to the melting of ice

P-08  T. Kawatsu, K. Ishimura and M. Tachikawa  
(The University of Tokyo)  
Hierarchical parallelization of the ab initio path integral molecular dynamics simulation

P-09  T. Udagawa, T. Tsuneda and Masanori Tachikawa  
(Gifu University)  
Development of new Colle-Salvetti type electron-nucleus correlation functional in MC_DFT

P-10  Shigeru Iwase, and Tomoya Ono  
(Osaka University)  
Efficient treatment of the Green’s function for first-principles transport calculation
P-11  T. Ohgoe and M. Imada  
(The University of Tokyo)  
Multi-variable variational Monte Carlo method for electron-phonon coupled systems

P-12  S.A. Sato and K. Yabana  
(University of Tsukuba)  
Ab-initio simulation for initial process of ultrafast laser-processing

P-13  Pham Thi Nu and Kaoru Ohno  
(Yokohama National University)  
Adiabatic and non-adiabatic molecular dynamics in time-dependent density functional theory

P-14  Kaoru Ohno, Shota Ono, Swastibrata Bhattacharyya, Tomoyuki Horikiri, and Hideo Kosaka  
(Yokohama National University)  
Development of a time-dependent T-matrix theory

P-15  Z. Futera, T. Watanabe, Y. Einaga and Y. Tateyama  
(Keio University)  
Semiconductor-water interfaces investigated by first principle-calculations on boron-doped diamond

P-16  Ryo Kishida, Adhitya G. Saputro, Nakanishi Hiroshi, Wilson Agerico Diño and Hideaki Kasai  
(Osaka University)  
Reaction mechanism of dopachrome conversion, a precursor reaction of melanin biosynthesis: implications for effects of pH and metal ions

P-17  K. Akagi  
(Tohoku University)  
Water rings at solid-liquid interfaces

P-18  N. Tsuji  
(The University of Tokyo)  
Nonequilibrium dynamical cluster approximation: non-local correlation and real-time dynamics

P-19  Y. Murakami, P. Werner, N. Tsuji and H. Aoki  
(The University of Tokyo)  
Non-equilibrium DMFT study of thermalization in an electron-phonon system

P-20  Y. Yamada, Y. Yamaji, and M. Imada  
(The University of Tokyo)  
Nonequilibrium dynamics of dissipative excitons in carbon nanotubes

P-21  J. Katayama, K. Maekawa, K. Sat, Y. Minami, K. Yanagi, M. Kitajima and J. Takeda  
(Yokohama National University)  
Fermi Energy Dependence of High-Frequency Coherent Phonons in Metallic Carbon Nanotubes
(Yokohama National University)  
Nonlinear Dynamics of Electrons on Dirac-Like Band  
in Semi-Metal Bismuth Induced by an THz Electric Pulse

P-23  **W. Oba**, I. Katayama, Y. Minami, T. Saiki and J. Takeda  
(Yokohama National University)  
Single-shot visualization of ultrafast amorphization in chalcogenide alloy thin films

P-24  **Y. Kanematsu**, T. Mashiko and M. Tachikawa  
(Yokohama-City University)  
Quantum or thermal fluctuation on molecules in solution

P-25  **Masato Oda**  
(Wakayama University)  
Electronic structure of a Cerasome Model

P-26  **Y. Takano**, A. Kusaka, H. Nakamura  
(Osaka University)  
Computational analysis of the molecular interactions in secondary structures of proteins

P-27  **Ayori Mitsutake** and Hiroshi Takano  
(Keio University)  
Dynamics of 10-Residue Peptide, Chignolin, Studied by Relaxation Mode Analysis

(University of Nagoya)  
Theoretical Study of the electron transfer reaction by DNA photolyase

P-29  **Keitaro Sodeyama**, Yuki Yamada, Atsuo Yamada, and Yoshitaka Tateyama  
(Kyoto University)  
Sacrificial anion reduction mechanism for electrochemical stability improvement in highly concentrated Li-salt electrolyte

P-30  **J. Haruyama**, K. Sodeyama, K. Takada* and Y. Tateyama  
(National Institute for Materials Science)  
DFT+U investigation of oxide cathode/sulfide electrolyte interface for all-solid-state Li-ion batteries

P-31  **Y. Ootani**, K. Sodeyama, L. Han, and Y. Tateyama  
(National Institute for Materials Science)  
Ru Dye–Organic Dye Interaction on TiO2 in Co-Sensitized Dye-Sensitized Solar Cell:  
DFT investigation
P-32  L. Szabova, V. Matolin, S. Fabris and Y. Tateyama  
(National Institute for Materials Science)  
Water adsorption and dissociation at metal-supported ceria thin films: Thickness and interface-proximity effects studied with DFT+U calculations

P-33  S. Hagiwara, C. Hu and K. Watanabe  
(Tokyo University of Science)  
Two-component density functional theory of positron state at lithium adsorbed Al(100) surface

P-34  J. Lin, T. Yamasaki and M. Saito  
(International Center for Materials Nanoarchitectonics)  
First-principles study of spin-polarized positron lifetimes in ferromagnets

P-35  Y. Kita, T. Oyamada, and M. Tachikawa  
(Yokohama City University)  
First-principle calculations of positron-attached polyatomic molecules

P-36  T. Ono  
(University of Tsukuba)  
DFT calculations for oxidation of SiC

P-37  Y. Tatetsu, S. Tsuneyuki and Y. Gohda  
(The University of Tokyo)  
Theoretical analysis of Fe/Cu(001) ultrathin films by density functional theory

P-38  K. Sawada, J.-I. Iwata and A. Oshiyama  
(The University of Tokyo)  
First-Principles Calculations on Electronic and Magnetic Properties in Nanofacet on SiC(0001) Surface

P-39  Christopher Kirkham and Tomoya Ono  
(Osaka University)  
Effect of SiC stacking on the electronic properties of the SiC/SiO2 interface

P-40  S. Arapan, D. Bowler and T. Miyazaki  
(National Institute for Materials Science)  
The role of surface reconstruction in determining the growth path of the \{105\} facet of a Ge hut

P-41  Miho Nishida, Fumiyuki Ishii, Hiroki Kotaka and Mineo Saito  
(Kanazawa University)  
First-principles study of Rashba effect in artificial superlattice (LaAlO3)n/(SrTiO3)n

P-42  H. Kotaka, F. Ishii, and M. Saito  
(Kanazawa University)  
Surface states of Bi (001) multi-layer nano film: spin distribution in the real space and momentum space
M. Rahaman, S. Watanabe and J. Iwata  
(The University of Tokyo)  
Stacking-faults and anti-phase boundary energies in Ni3X (X = Si, Ga, Ge) alloys: An ab initio study

S. Nakamura, Y. Ando, E. Minamitani, R. Shimizu, K. Iwaya, T. Ohsawa, T. Hitosugi, S. Watanabe  
(The University of Tokyo)  
Ab-initio calculation of structure and electronic properties of a La0.75Ca0.25MnO3 surface

T. Kato, H. Kotaka and F. Ishii  
(Kanazawa University)  
First-principles study of strain-induced topological phase transitions in bismuth chalcogenides

E.F. Arguelles, S. Amino, S. Aspera, H. Nakanishi and H. Kasai  
(Osaka University)  
Surface magnetism induced by interstitial impurities in α-PbO

K. Shimizu, W.A. Diño and H. Kasai  
(Osaka University)  
Rotational Effects on the Dissociative Adsorption and Abstraction Dynamics of O2/Al(111)

Moh Adhib Ulil Absor, Fumiyuki Ishii, Hiroki Kotaka, and Mineo Saito  
(Kanazawa University)  
Spin-orbit coupling on wurtzite ZnO (1010) surface: first-principles density functional study

(The University of Tokyo)  
Two-dimensional Valley Electrons and Excitons in 3R MoS2 Multilayers

R. Akashi and R. Arita  
(The University of Tokyo)  
Hopping Selection Rule of Electrons in Stacked Multilayers and Emergent Flat Band Dispersion

Yoshitaka Fujimoto and Susumu Saito  
(Tokyo Institute of Technology)  
Electronic Structures and Stabilities of Defects and Impurities in Hexagonal Boron-Nitride Atomistic Layers

Sholihun and Mineo Saito  
(Kanazawa University)  
First-principles Calculation of the Free Energy of Silicon Monovacancy
P-53  J. Yamauchi and N. Matsushima  
(Keio University)  
Relaxation effect of X-ray photoelectron spectroscopy for defects in semiconductors: 
a first-principles study

P-54  Kanako Yoshizawa, Yoshiki Iwazaki, Yoshihiro Gohda, and Shinji Tsuneyuki  
(The University of Tokyo)  
Charge states of impurity hydrogen in rutile oxide semiconductors MO2 (M=Si, Ge, Sn, Pb, Ti, 
Zr, Hf)

P-55  M. Alaydrus, M. Sakaue and H. Kasai  
(Osaka University)  
A DFT+U study on oxygen ion migration in strained Sm-doped ceria

P-56  T. Tsumuraya, H. Seo, R. Kato and T. Miyazaki  
(RIKEN)  
First-principles study of hydrogen-bonded molecular conductor, κ-H3(Cat-EDT-TTF/ST)2

P-57  Y. Kawashiri, D. Hirai, K. Sasaoka, A. Tawara, and S Watanabe  
(The University of Tokyo)  
Ab-initio calculation for AC transport properties of single molecule bridging between metallic 
electrodes

P-58  Teppei Kato, Shinji Usui and Takahiro Yamamoto  
(Tokyo University of Science)  
Thermoelectric Property of Carbon Nanotube Buckypaper

P-59  K. Takashima, T. Yamamoto  
(Tokyo University of Science)  
Quantum Transport Simulation of Edge-Disordered Graphene Nanoribbons

P-60  S. Konabe and S. Okada  
(University of Tsukuba)  
Exciton many-body physics in carbon nanotubes

P-61  A. Yamanaka and S. Okada  
(University of Tsukuba)  
Electronic Properties of Graphene under an Electric Field

P-62  M. Maruyama and S. Okada  
(University of Tsukuba)  
Electronic Structures of Two-dimensional sp2 Carbon Networks of Fused Pentagon Trimers

P-63  K. Uchida, J.-I. Iwata and A. Oshiyama  
(The University of Tokyo)  
Atomic and Electronic Structure Calculations for Twisted Bilayer of h-BN Sheets
P-64 Y. Sakai and A. Oshiyama  
(The University of Tokyo)  
Electronic properties and stacking geometries of bilayer silicone

P-65 T. Tadano and S. Tsuneyuki  
(The University of Tokyo)  
First-principles calculation of high-temperature phonon: Applications to cubic SrTiO3

P-66 M. Geshi  
(Osaka University)  
First-principles calculation of elastic constants for metallic hydrides under high-pressure

P-67 T. Nishimoto, T. Tadano, Y. Gohda, and S. Tsuneyuki  
(The University of Tokyo)  
Development of a first-principles model with long-range interactions for ferroelectrics

P-68 F. Ishii, and H. Kotaka, T. Ohnishi, M. Nishida, M. Saito  
(Kanazawa University)  
Ferroelectric tuning of spin-orbit field in ATiO3(A=Sr,Ba, and Pb)

P-69 D. Hirai, S. Tsuneyuki, and Y. Gohda  
(The University of Tokyo)  
Theoretical Analysis of Magnetic Properties of ε-Fe2O3

P-70 M. Callsen, V. Caciuc, N. Atodiresei, N. Kiselev and S. Blügel  
(National Institute for Materials Science)  
Magnetic hardening induced by nonmagnetic organic molecules

P-71 A. Masago, T. Fukushima, K. Sato and H. Katayama-Yoshida  
(Osaka University)  
Circular polarization in Eu, Mg, and O codoped GaN

P-72 T. Domon, Y. Sugimura, K. Kanazawa, R. Akiyama, S. Kuroda  
(University of Tsukuba)  
Interaction between different kinds of transition-metal elements in quaternary magnetic semiconductors

P-73 M.-T. Suzuki  
(RIKEN)  
First-principles study of multipole ordered states

P-74 W. Sano, T. Koretsune, and R. Arita  
(The University of Tokyo)  
Crystal orientation dependence of the carrier type in IrO2: A first-principles study
(Osaka University)  
First-principles calculation of Hubbard $U$ parameter for gap states in dilute magnetic semiconductors

P-76  Kazuma Nakamura, Shiro Sakai, Yoshiro Nohara, Yoshihide Yoshimoto  
(Kyushu Institute of Technology)  
Ab initio derivation of low-energy effective model based on constrained many-body perturbation theory

P-77  Hiroaki Matsui and Hitsohi Tabata  
(The University of Tokyo)  
Material designs of plasmonic nanomaterials on oxides

P-78  K. Miwa, H. Imada, M. Sakaue, H. Kasai and Y. Kim  
(RIKEN)  
Quantum interference between the dynamics of molecular exciton and interface plasmons in scanning tunneling microscope-induced light emission

(Nagasaki University)  
Interaction between L-alanine and plasma generated in hydrogen peroxide water

(University of Tsukuba)  
Topological surface state in topological crystalline insulator SnTe thin films

P-81  Shota Ono, Kousei Tanikawa, Riichi Kuwahara, and Kaoru Ohno  
(Yokohama National Univ)  
End-cap geometry dependence of power conversion efficiency of solar cells based on capped-carbon nanotubes

(Osaka University)  
Computational design of chalcogenide- and pnictogenidebased photovoltaic solar cell materials

P-83  K. Shirai, K. Sakuma, and N. Uemura  
(Osaka University)  
Survey of high $Tc$ materials in hard semiconducting boron crystals

P-84  R. Akashi and R. Arita  
(The University of Tokyo)  
Density Functional Theory for Plasmon-Assisted Superconductivity
P-85  **Masahiro Sakurai** and **Yasutami Takada**  
(The University of Tokyo)  
Superconductivity in Pseudoferroelectric Crystals: Case of $n$-doped SrTiO3

P-86  **T. Koretsune**, R. Akashi, S. Sato, H. Isobe and R. Arita  
(RIKEN)  
Possible superconductivity in naphthalene-based organic molecular crystal

P-87  **Motoharu Kitatani**, Naoto Tsuji, and Hideo Aoki  
(The University of Tokyo)  
DMFT+FLEX approach to unconventional superconductivity

P-88  **S. Kitamura**, N. Tsuji and H. Aoki  
(The University of Tokyo)  
A density functional design of an interaction-driven topological insulator in cold atoms on an optical lattice