International Symposium on Computics: Quantum Simulation and Design ISC-QSD2014

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"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

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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.

Time Table


December 1 (Mon)
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December 3 (Wed)
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Oral Session V
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Oral Session VII
Coffee Break
Oral Session VIII
Closing
Lunch
Adjourn

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_2IrO_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 vartiational 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 I. 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

P-22 Y. Minami, K. Araki, T. D. Dao, T. Nagao, J. Takeda, M. Kitajima, and I. Katayama
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Nonlinear Dynamics of Electrons on Dirac-Like Band
in Semi-Metal Bismuth Induced by an THz Electric Pulse

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Single-shot visualization of ultrafast amorphization in chalcogenide alloy thin films

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Quantum or thermal fluctuation on molecules in solution

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Electronic structure of a Cerasome Model

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Computational analysis of the molecular interactions in secondary structures of proteins

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

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(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
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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
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Ru Dye–Organic Dye Interaction on TiO2 in Co-Sensitized Dye-Sensitized Solar Cell: DFT investigation

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Water adsorption and dissociation at metal-supported ceria thin films:
Thickness and interface-proximity effects studied with DFT+U calculations

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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

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First-princile calculations of positron-attached polyatomic molecules

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DFT calculations for oxidation of SiC

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(The University of Tokyo)
Theoretical analysis of Fe/Cu(001) ultrathin films by density functional theory

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First-Principles Calculations on Electronic and Magnetic Properties in Nanofacet on SiC(0001) Surface

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Effect of SiC stacking on the electronic properties of the SiC/SiO2 interface

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The role of surface reconstruction in determining the growth path of the {105} facet of a Ge hut

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Surface states of Bi (001) multi-layer nano film: spin distribution in the real space and momentum space

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Topological surface state in topological crystalline insulator SnTe thin films

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End-cap geometry dependence of power conversion efficiency of solar cells based on capped-carbon nanotubes

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Superconductivity in Pseudoferroelectric Crystals: Case of *n*-doped SrTiO3

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DMFT+FLEX approach to unconventional superconductivity

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A density functional design of an interaction-driven topological insulator in cold atoms on an optical lattice