4 PUBLICATION LIST

Example:

LASTNAME, Firstname [project class; # points (B), # points (C)] (Page #)
Project title
1. First paper
   Names of Authors, etc.
2. Second paper
   ...

□ ISSP Joint Research Projects

ADACHI, Takahiro [C class; 2500 (B), 300 (C)] (230)
— *Heat Transfer Characteristics of Condensate Film Flow along Vertical Plates with Microscopic Grooves*

AKAGI, Kazuto [B,C class; 4600 (B), 0 (C)] (91)
— *Local structure analysis around impurity atoms in a metal oxide*
— *Exploration of structure motifs characterizing the behavior of metal oxides*
1. The chemistry of simple alkene molecules on Si(100)c(4 × 2): The mechanism of cycloaddition and their selectivities
   K. Akagi and J. Yoshinobu: Surf. Sci. in press
2. Theoretical investigation on oxidation of lithium peroxide by tetrathiafulvalene in non-aqueous Li-O_2 battery
   S. Jung and K. Akagi: submitted to J. Phys. Chem. Lett.

AKAI, Hisazumi [B class; 300 (B), 700 (C)] (121)
— *Electronic structure of rare earth magnets*
1. Role of N in the Permanent Magnet Materials $Sm_2Fe_{17}N_x$
   M. Ogura and H. Akai: J. Phys. Soc. Jpn. **84** (2015) 084702.
2. Near-field correction in the first-principles calculations by the exact two-center expansion for the inverse of the distance
   M. Ogura, C. Zecha, M. Offenberger, H. Ebert, and H. Akai: J. Phys: Condens. Matter. **27** (2015) 485201
3. Schottky junctions studied by KKR non-equilibrium Green's function method
   M. Ogura and H. Akai: submitted to Phys. Rev. B.

AKASHI, Ryosuke [C class; 1500 (B), 200 (C)] (107)
— *Ab initio calculation of superconducting pairing interactions in materials with complex Fermi surface*

ANDO, Yasunobu [C class; 2000 (B), 2200 (C)] (95)
— *Theoretical analysis of electrochemical interfaces by first-principles calculation and statistical approach*
1. First-principles study of metal–insulator control by ion adsorption on Ti_2C MXene dioxide monolayers
   Y. Ando, and S. Watanabe: Appl. Phys. Express **9**, (2016) 015001.

AOKI, Hideo [C class; 4000 (B), 2400 (C)] (149)
— *Photoinduced phase transitions in strongly correlated superconductors*
1. FLEX+DMFT approach to the d-wave superconducting phase diagram of the two-dimensional Hubbard model

M. Kitatani, N. Tsuji, H. Aoki: Phys. Rev. B **92**, 085104 (2015).
2. Theory of Anderson pseudospin resonance with Higgs mode in a superconductor
Naoto Tsuji and Hideo Aoki: Phys. Rev. B **92**, 064508 (2015).
3. Multiple amplitude modes in strongly coupled phonon-mediated superconductors
Yuta Murakami, Philipp Werner, Naoto Tsuji and Hideo Aoki: Phys. Rev. B **93**, 094509 (2016).

AOYAMA, Kazushi [B class; 700 (B), 0 (C)] (249)
— *Spin-lattice coupling effects in Heisenberg antiferromagnets on breathing pyrochlore lattices*

ARAIDAI, Masaaki [C class; 2500 (B), 800 (C)] (99)
— *First-Principles Study on Device Properties of Emerging Phase-Change Memory Devices*

ARAKAWA, Naoya [B class; 400 (B), 0 (C)] (174)
— *Theoretical study of many-body effects on spin transports in a multiorbital system*

1. Spin-orbital-coupled vector chirality in a non-frustrated Mott insulator with the strong spin-orbit coupling without *ab*-plane's inversion symmetry
N. Arakawa: arXiv:1604.05867.
2. Microscropic theory on charge transports of a correlated multiorbital system
N. Arakawa: arXiv:1505.05274.
3. Many-body effects on the resistivity of a multiorbital system beyond Landau's Fermi-liquid theory
N. Arakawa: Mod. Phys. Lett. B **29** (2015) 1530005.
4. Interaction-driven temperature dependence and spin-Coulomb-drag-induced correction in intrinsis anomalous-Hall and spin-Hall effects on multiorbital metals
N. Arakawa: arXiv:1510.03988
5. Controlling spin Hall effect by using a band anticrossing and nonmagnetic impurity scattering
T. Mizoguchi and N. Arakawa: Phys. Rev. B **93** (2016) 041304(R).

ARAKI, Takeaki [B class; 700 (B), 0 (C)] (248)
— *Self-propelled motion of a Janus particle in periodically phase separating mixtures*

1. Controlled motion of Janus particles in periodically phase-separating binary fluids
T. Araki and S. Fukai: Soft Matter **11** (2015), 3470.

ARITA, Ryotaro [C class; 3500 (B), 0 (C)] (159)
— *First-principles study of multi-orbital correlated materials*

1. Ab initio downfolding study of the iron-based ladder superconductor $BaFe_2S_3$
R. Arita, H. Ikeda, S. Sakai and M-T. Suzuki, Phys. Rev. B **92**, (2015) 054515.
2. First-Principles study of magnetic properties in Fe-ladder compounds $BaFe_2S_3$
M-T. Suzuki, R. Arita and H. Ikeda: Phys. Rev. B **92**, (2015) 085116.

DEKURA, Haruhiko [C class; 2000 (B), 0 (C)] (106)
— *First-principles calculations of iron solid solution effects on the lattice thermal conductivity of lower mantle minerals*

EGAMI, Yoshiyuki [C class; 2500 (B), 3300 (C)] (74)
— *Development and application of first-principles electron-transport simulator based on time-dependent density functional theory*

1. First-principles calculation method for electron transport based on grid Lippmann-Schwinger equation
Y. Egami, S. Iwase, S. Tsukamoto, T. Ono and K. Hirose: Phys. Rev. E **92** (2015) 033301.

FUCHIZAKI, Kazuhiro [C class; 2500 (B), 0 (C)] (234)
— *Melting phenomena and polyamorphism*

1. Accurate Equation of State for the Modified Lennard-Jones Solid
K. Fuchizaki, K. Okamoto, and S. Doi: J. Phys. Soc. Jpn. **84** (2015) 085002.
2. Nonequilibrium Effects on Macromolecules Immersed in a Solvent

K. Fuchizaki: JPSJ News and Comments 12 (2015) 13.
3. Determination of a melting curve using the one-phase approach
K. Fuchizaki and K. Okamoto: Phys. Lett. A **380** (2016) 293.
4. ヨウ化錫系に期待される第二臨界現象
渕崎員弘: 日本結晶学会誌 **58** (2016) 42.

FUJIMOTO, Yoshitaka [C class; 1000 (B), 0 (C)] (119)
— *Stabilities, structures, and electronic properties of atomic-layered materials*
1. Electronic structures and stabilities of bilayer graphene doped with boron and nitrogen
Y. Fujimoto and S. Saito: Surface Science **634**, 57 (2015).
2. Atomic geometries and electronic structures of hexagonal boron-nitride bilayers under strain
Y. Fujimoto and S. Saito: Journal of the Ceramic Society of Japan **123**, 576 (2015).
3. Formation, energetics, and electronic properties of graphene monolayer and bilayer doped with boron and nitrogen
Y. Fujimoto: Advances in Condensed Matter Physics **2015**, 571490 (2015).
4. First-Principles Computational Design of Graphene for Gas Detection
Y. Fujimoto: Smart Materials for Waste Water Application, Wiley-Scrivener Publishers, Chapter 6 (2016).
5. Effects of strain on Carbon Donors and Acceptors in Hexagonal Boron-Nitride Monoalyers
Y. Fujimoto and S. Saito: Physical Review B **93**, 045402 (2016).
6. Energetics and scanning tunneling microscopy images of B and N defects in graphene bilayer
Y. Fujimoto and S. Saito: submitted.
7. Gas adsorption, energetics and electronic properties of boron- and nitrogen-doped bilayer graphenes
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8. Interlayer distances and band-gap tuning of hexagonal boron-nitride bilayers
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FUJIWARA, Susumu [B class; 600 (B), 0 (C)] (251)
— *Molecular Simulation Study of Micellar Shape Transition in Amphiphilic Solution*
1. Molecular Dynamics Simulation of Phase Behavior in a Bolaamphiphilic Solution
S. Fujiwara, T. Miyata, M. Hashimoto, Y. Tamura, H. Nakamura and R. Horiuchi: Plasma Fusion Res. **10** (2015) 3401029.
2. Melt memory of a spherulite nucleus formed through a seeding process in the crystal growth of isotactic polystyrene
M. Hashimoto, J. O'ishi, S. Moriya and S. Fujiwara: Polymer J. **47** (2015) 481-486.
3. Dissipative Particle Dynamics Simulation of Self-Assembly in a Bolaamphiphilic Solution
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Y. Tamura, H. Nakamura and S. Fujiwara: Plasma Fusion Res. in press.

FUKUI, Ken-Ichi [C class; 5500 (B), 3800 (C)] (64)
— *Microscopic Investigations of Solid / Liquid Interfaces Using First-Principles and Classical Molecular Dynamics*
— *First-Principles and Classical Molecular Dynamics Investigations of Electrolyte Solution / Electrode Interfaces: Potential Dependence*
1. Density Functional Theory Investigations of Ferrocene-Terminated Self-Assembled Monolayers: Electronic State Changes Induced by Electric Dipole Field of Coadsorbed Species
Y. Yokota, S. Akiyama, Y. Kaneda, A. Imanishi, K. Inagaki, Y. Morikawa and K. Fukui:J. Phys. Chem. C, in press.

FURUKAWA, Akira [C class; 5000 (B), 0 (C)] (217)
— *Rheology of Glassy Materials*
1. Probing colloidal gels at multiple length scales: The role of hydrodynamics
C. P. Royall, J. Eggers, A. Furukawa, and H. Tanaka: Physical Review Letters

2. Essential Difference in the Dynamics between Strong and Fragile Glass-formers
   A. Furukawa and H. Tanka: submitted

GOHDA, Yoshihiro [C class; 3500 (B), 2200 (C)] ()
— *Doping effects of heavy elements for multiferroic materials*

HAMAMOTO, Yuji [C class; 3500 (B), 2900 (C)] (72)
— *First principles study of catalytic properties of Pt cluster supported on graphene*

HARADA, Kenji [C class; 7500 (B), 0 (C)] (205)
— *Tensor network calculation on two-dimensional quantum spin models*
1. SU(N) Heisenberg model with multicolumn representations
   T. Okubo, K. Harada, J. Lou, and N. Kawashima: Phys Rev B **92**, 134404 (2015).
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HASHIMOTO, Tamotsu [C class; 2000 (B), 0 (C)] (238)
— *Molecular dynamics simulation of ferroelectrics using a shell model*
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   T. Hashimoto and H. Moriwake: Mol. Simul. **41** (2015) 1074.
2. Electrical Susceptibilities of $KNbO_3$ by Molecular Dynamics Simulations Using a Shell Model
   T. Hashimoto and H. Moriwake: Physica B **485** (2016) 110.
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   T. Hashimoto and H. Moriwake: J. Phys. Soc. Jpn. **85** (2016) 034702.

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— *Variety of bulk-edge correspondence by numerical methods*
1. Entanglement Chern Number of the Kane-Mele Model with Ferromagnetism
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2. Hannay Angle: Yet Another Symmetry-Protected Topological Order Parameter in Classical Mechanics
   Toshikaze Kariyado, Yasuhiro Hatsugai, Journal of the Physical Society of Japan, **85**, 043001 (2016).
3. Topological order parameters of the spin- 1/2 dimerized Heisenberg ladder in magnetic field
   Toshikaze Kariyado, Yasuhiro Hatsugai, Phys. Rev. B**91** 214410 (2015).
4. Manipulation of Dirac Cones in Mechanical Graphene
   Toshikaze Kariyado, Yasuhiro Hatsugai, Scientific Reports 5, 18107 (2015).

HATTORI, Ken [B class; 600 (B), 500 (C)] (111)
— *Model calculations in Si surfaces with adsorbates*
1. Surface structure and electronic states of epitaxial β-$FeSi_2$(100)/Si(001) thin films: Combined quantitative LEED, *ab initio* DFT, and STM study
   O. Romanyuk, K. Hattori, M. Someta, H. Daimon: Phys. Rev. B **90** (2014) 155305.

HIDA, Kazuo [B class; 400 (B), 0 (C)] (260)
— *Numerical Study of One Dimensional Frustrated Quantum Spin Systems*
1. K. Hida: Characterization of Topological Phases of Spin-1/2 Frustrated Ferromagnetic-Antiferromagnetic Alternating Heisenberg Chains by Entanglement Spectrum
   K. Hida: J. Phys. Soc. Jpn. 85 024705 (2016).

HIRAI, Daisuke [C class; 2500 (B), 1800 (C)] (93)
— *First-Principles Study of Coercivity in Hard Magnetic Materials*

HIRAI, Kunitomo [B class; 100 (B), 50 (C)] (141)
— *Electronic State and Proximity Effects around Interface in Layered Superlattices*

HOSHI, Takeo [C class; 3000 (B), 2000 (C)] (88)
— *Parallelized ultra-large-scale electronic-structure theory based on first principle calculation and novel numerical method*

1. Efficient numerical solver for first-principles transport calculation based on real-space finite-difference method
   S. Iwase, T. Hoshi, T. Ono, Phys. Rev. E 91, 063305, 9pp. (2015)
2. Hybrid numerical solvers for massively parallel eigenvalue computation and their benchmark with electronic structure calculations
   H. Imachi and T. Hoshi, J. Inf. Process. 24, pp. 164 – 172 (2016)
3. One-hundred-nm-scale electronic structure and transport calculations of organic polymers on the K computer
   H. Imachi, S. Yokoyama, T. Kaji, Y. Abe, T. Tada, submitted; Preprint http://arxiv.org/abs/1603.09616

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— *Monte Carlo Study of Itinerant and Localized Chiral Helimagnets*

1. Superconductivity from Emerging Magnetic Moments
   Shintaro Hoshino and Philipp Werner: Phys. Rev. Lett. **115**, 247001 (2015).
2. Anisotropic Magnetic Response in Kondo Lattice with Antiferromagnetic Order
   M. Shinozaki, S. Hoshino, Y. Masaki, J. Kishine and Y. Kato: arXiv1512.00235 (2015).
3. Electronic orders in multi-orbital models with lifted orbital degeneracy
   Shintaro Hoshino and Philipp Werner: Phys. Rev. B **93**, 155161 (2016).

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— *Research for multipole ordering and superconductivity induced by multipole fluctuations in seven-orbital Hubbard model with spin-orbit coupling*

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   Yasuhiro Kondo and Takashi Hotta: Phys. Procedia **75** (2015) 671-678.
2. Quantum Interference of Surface-Induced Friedel Oscillations Enhanced by Fermi-Surface Nesting in Layered Manganites
   Ryosuke Yamamura and Takashi Hotta: Phys. Procedia **75** (2015) 902-910.
3. Effect of Spin-Orbit Coupling on Kondo Phenomena in f^7-Electron Systems
   Takashi Hotta: J. Phys. Soc. Jpn. **84** (2015) 114707-1-12.
4. Fermi-Surface Topology and Pairing Symmetry in BiS_2-Based Layered Superconductors
   Tomoaki Agatsuma and Takashi Hotta: J. Magn. Magn. Mater. **400** (2016) 73-80.
5. Valence Imbalance of Manganese Ions between Surface and Bulk Enhanced by Fermi-Surface Structure in Layered Manganites
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— *First-principles simulation of electrolyte diffusion process on constant-potential electrodes*

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— *Equilibrium and dynamical properties in glassy systems*

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   S.Takabe and K. Hukushima: Phys. Rev. E **89** (2014) 043801/1-4
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   A. Okamoto, T. Kuwatani, T. Omori and K. Hukushima: Phys. Rev. E **92** (2015) 042130/1-9
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   Y. Sakai and K. Hukushima: Phys. Rev. E **93** (2016) 043318/1-13.

IGARASHI, Ryo [C class; 2500 (B), 2000 (C)] (221)
— *Development of parallelized MPS algorithm and its application to various frustrated systems*
— *GPU parallelization of MPS algorithm and its application to various frustrated systems*

IKUHARA, Yuichi [C class; 4500 (B), 2700 (C)] (69)
— *Study of atomic structure and electronic states of interfaces and dislocations*
— *First-Principles Study of Atomic and Electronic Structure of Grain Boundaries*

1. Atomic-Scale Structure and Local Chemistry of CoFeB-MgO Magnetic Tunnel Junctions
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— *Numerical studies on photoinduced superconductivity in two dimensional doped Hubbard model by high-precision variational wave functions*

1. *Ab initio* Studies on Magnetism in the Iron Chalcogenides FeTe and FeSe
   Motoaki Hirayama, Takahiro Misawa, Takashi Miyake, Masatoshi Imada: J. Phys. Soc. Jpn. **84** (2015) 093703.
2. Hidden fermionic excitation in the superconductivity of the strongly attractive Hubbard model
   Shiro Sakai, Marcello Civelli, Yusuke Nomura, and Masatoshi Imada: Phys. Rev. B **92** (2015) 180503.
3. Exciton Lifetime Paradoxically Enhanced by Dissipation and Decoherence: Toward Efficient Energy Conversion of a Solar Cell
   Yasuhiro Yamada, Youhei Yamaji, and Masatoshi Imada: Phys. Rev. Lett. **115** (2015) 197701.
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5. Hidden Fermionic Excitation Boosting High-Temperature Superconductivity in Cuprates
   Shiro Sakai, Marcello Civelli, Yusuke Nomura, and Masatoshi Imada: Phys. Rev. Lett. **116** (2016) 057003.
6. Finite-Temperature Variational Monte Carlo Method for Strongly Correlated Electron Systems
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7. Tensor network algorithm by coarse-graining tensor renormalization on finite periodic lattices
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8. Real-space renormalized dynamical mean field theory
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9. Clues and criteria for designing Kitaev spin liquid revealed by thermal and spin excitations of honeycomb iridates Na_2IrO_3
   Youhei Yamaji, Takafumi Suzuki, Takuto Yamada, Sei-ichiro Suga, Naoki Kawashima, and Masatoshi Imada: submitted to Phys. Rev. B.
10. Modulated Helical Metals at Magnetic Domain Walls of Pyrochlore Iridium Oxides
    Youhei Yamaji, Masatoshi Imada: submitted to Phys. Rev. B.
11. Stabilization of Topological Insulator Emerging from Electron Correlations on Honeycomb Lattice and Its Possible Relevance in Twisted Bilayer Graphene

Moyuru Kurita, Youhei Yamaji, Masatoshi Imada: submitted to Phys. Rev. B.

12. Clues and criteria for designing Kitaev spin liquid revealed by thermal and spin excitations of honeycomb iridates Na_2IrO_3
Youhei Yamaji, Takafumi Suzuki, Takuto Yamada, Sei-ichiro Suga, Naoki Kawashima, and Masatoshi Imada : submitted to Phys. Rev. B.

INAGAKI, Kouji [C class; 8000 (B), 3700 (C)] (54)
— *First-principles meta-dynamics analysis of Catalytic Referred Etching method (Analysis of atom removal process)*

1. Study on the mechanism of platinum-assisted hydrofluoric acid etching of SiC using density functional theory calculations
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— *Novel properties of low-dimensional electron systems at solid surfaces and finite electron systems in nanoparticles*

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— *Novel quantum phase and real time dynamics in correlated electron systems*
— *Numerical analyses of nonequilibrium state in electron-lattice correlated systems*

1. Charge Dynamics in a Correlated Fermion System on a Geometrically Frustrated Lattice
M. Naka and S. Ishihara, J. Phys. Soc. Jpn. **84**, (2015) 023703.
2. Emergence of charge degrees of freedom under high pressure in the organic dimer-Mott insulator β'-(BEDT-TTF)$_2$ICl$_2$
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5. Ultrafast electronic state conversion at room temperature utilizing hidden state in cuprate ladder system
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— *First-Principles Calculation of Spin-Orbit Field and Thermopower*
— *Spin-orbit coupling parameters at surfaces and interfaces of semiconductors: first-principles study*

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2. Spin-split bands of metallic hydrogenated ZnO (10-10) surface: First-principles study

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— *Nonequilibirum phase transition in the large scale dense hard sphere molecular dynamics simulation*

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M. Isobe: Proceedings Book of Berni Alder's 90th Birthday Symposium. in press.

KAGESHIMA, Hiroyuki [C class; 1000 (B), 0 (C)] (117)
— *Study on formation and property mechanism of semiconductor surfaces/interfaces/defects*

KAKEHASHI, Yoshiro [B class; 200 (B), 0 (C)] (140)
— *First-Principles Momentum Dependent Local Ansatz Theory and Its Application to Fe Compounds*

1. First-Principles Theory of Momentum-Dependent Local Ansatz for Correlated Electron System
S. Chandra and Y. Kakehashi : Physics Procedia **75** (2015) 41-48.
2. Molecular Spin Dynamics Analysis of Complex Magnetic Structure on the FCC Lattice in Itinerant Electron System
Y. Kakehashi, S. Chandra, and T. Uchida: Physics Procedia **75** (2015) 625-633.
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— *Theoretical research on dissociation of N2 and H2 for designing new ammonia synthesis catalysts*

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— *Development and Application of the Quantum Monte Carlo Method for Critical Phenomena of Random Bosonic Systems*

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MATSUSHITA, Katsuyoshi [C class; 3000 (B), 0 (C)] (229)
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— *Numerical simulation of ^{4}He adsorbed on substrates*

MURASHIMA, Takahiro [C class; 3500 (B), 2200 (C)] (35)
— *Viscoelastic analysis on soft matter systems (polymer, liquid crystal, micelle) and multiscale simulation*

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OTSUKA, Yuichi [C class; 3500 (B), 1600 (C)] (156)
— *Numerical study of critical phenomena in strongly correlated Dirac electrons*

OZEKI, Yukiyasu [C class; 5000 (B), 0 (C)] (215)
— *Improvement of dynamical scaling and accurate analysis of nonequilibrium relaxation data*

RAEBIGER, Hannes [C class; 3000 (B), 0 (C)] ()
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— *Derivation of effective model in transition metal compounds by first-principles calculation and its analysis from the view point of many body effect*

SAKASHITA, Tatsuya [B class; 700 (B), 0 (C)] (246)
— *Study of Heisenberg-Kitaev model by exact diagonalization package Rokko*

SAKATA, Kaoruho [B class; 400 (B), 300 (C)] (123)
— *Ab-initio DFT Calculations of Photocatalyst Material for Water Splitting*

SANO, Masaki [B class; 500 (B), 0 (C)] (254)
— *Absorbing phase transition and viscoleasticity of Non-Brownian suspension in Low Reynolds number fluid*

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— *Phase transition on scale-free networks*
— *Phase transition on scale-free networks 2*

SHISHIDOU, Tatsuya [D class; 7000 (B), 1500 (C)] ()
— *First-principles study of chiral magnet Cr(NbS2)3*

SUGINO, Osamu [C class; 4000 (B), 1000 (C)] ()
— *Constant-potential simulation of electrode interfaces*

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— *First-Principles Study of the Structure of a-$InGaZnO_4$*

YASUOKA, Kenji [C class; 5000 (B), 0 (C)] (78)
— *The role of the negatively charged oxygen vacancy in the chemisorption process of oxygen molecules on TiO2 (110)*

YOSHIDA, Tsuneya [C class; 6000 (B), 0 (C)] (151)
— *Study of correlation effects on topological phases*

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2. Large and small Fermi-surface spin density waves in the Kondo lattice model
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YOSHIMOTO, Yoshihide [B class; 800 (B), 200 (C)] (112)
— *Development of first-principles electronic structure calculation package xTAPP*

1. X-ray photoelectron spectroscopy analysis of boron defects in silicon crystal: a first-principles study
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ZHONGCHANG, Wang [C class; 2000 (B), 1000 (C)] ()
— *First-principles investigation of functional interfaces in metallic oxides*

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ASAI, Yoshihiro [R class; 10000 (B), 0 (C)] (287)

— *Large scale computational simulations of non-equilibrium transport phenomena*

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— *Superconducting Mechanism Driven by Both Electron-Phonon and Strong Electron Correlations*

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9. Clues and criteria for designing Kitaev spin liquid revealed by thermal and spin excitations of honeycomb iridates Na_2IrO_3
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KAWASHIMA, Naoki [R class; 10000 (B), 10000 (C)] (267)
— *Monte Carlo Study of Novel Quantum Phases and Critical Phenomena*
— *Study of Novel Quantum Phases and Critical Phenomena by Monte Carlo Method and Tensor Network*

1. SU(N) Heisenberg model with multicolumn representations
   Tsuyoshi Okubo, Kenji Harada, Jie Lou, Naoki Kawashima: Phys. Rev. B **92** (2015) 134404/1-5.
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1. Reducing the Cost and Preserving the Reactivity in Noble-Metal-Based Catalysts: Oxidation of CO by Pt and Al–Pt Alloy Clusters Supported on Graphene
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— *Multi-scale simulation of nano-structured materials from electronic to mechanical properties*

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OHNO, Kaoru [R class; 10000 (B), 10000 (C)] (282)
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OTANI, Minoru [R class; 5000 (B), 10000 (C)] (281)
— *First-principles simulations of electrode-electrolyte interfaces in secondary batteries with a bias-control technique*
— *First-principlemolecular dynamics study toward a high performance Li-ion battery*

SAITO, Mineo [R class; 10000 (B), 10000 (C)] (272)
— *Materials design for spintronics/multiferroics applications*

1. Spin-split bands of metallic hydrogenated ZnO ($101^{-}0$) surface: First-principles study
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SUGINO, Osamu [R class; 10000 (B), 5000 (C)] (278)
— *Interface science on energy conversion*
— *Structure and functionality of electrode-electrolyte interface in battery*

TAKATSUKA, Kazuo [R class; 0 (B), 5000 (C)] (263)
— *Nonadiabatic electron dynamics and many-body nuclear dynamics in molecules*

TOHYAMA, Takami [R class; 5000 (B), 5000 (C)] (266)
— *Study of Excitation Dynamics in Strongly Correlated Electron Systems*

1. Magnetization Plateaux by Reconstructed Quasi-spinons in a Frustrated Two-Leg Spin Ladder under a Magnetic Field
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TSUNEYUKI, Shinji [R class; 5000 (B), 10000 (C)] (271)
— *Development and Application of First-Principles Simulations for New Materials Exploration*

YAMASHITA, Koichi [R class; 0 (B), 10000 (C)] (277)
— *Large scale calculations on the fundamental processes of solar cells and their optimization in conversion efficiency*

1. The Mechanism of Slow Hot-Hole Cooling in Lead-Iodide Perovskite: First-Principles Calculation on Carrier Lifetime from Electron–Phonon Interaction
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□ Doctor theses

1. **IIZUKA, Hideyuki**
   Scattering processes of exciton at organic semiconductor interfaces: interface disorder and energy dissipation
   Chiba University, 2016-03

2. **IIZUKA, Shota**
   Electronic structures of impurity complexes and tunneling current properties at Si-p/n interfaces
   Chiba University, 2016-03

3. **KIKKAWA, Nobuaki**
   Theoretical and Computational Study of Ion Transport through Water–Oil Interface
   Tohoku University, 2016-03

4. **MORENO, Joaquin Lorenzo Valmoria**
   Density functional theory-based studies on precious metal-free surfaces as alternative catalysts for green energy applications : Carbon nanotubes and copper oxide
   Osaka University, 2015-09

5. **MUSA, Alaydrus**
   Theoretical investigation of ionic conduction in rare-earth oxide materials
   Osaka University, 2016-03

6. **NGUYEN, Hoang Linh**
   Theoretical Study on The Role of Oxygen Vacancy in The Improvement of Metal Oxides' Reactivity for Green Technology Applications
   Osaka University, 2015-09

7. **OTOMURA, Kotaro**
   Rheology and Structure of Non Brownian Suspension under Large Amplitude Oscillatory Shear Strain
   University of Tokyo, 2015-4

8. **SATO, Shunsuke**
   Time-dependent density functional theory for extremely nonlinear interactions of light with dielectrics
   University of Tsukuba, 2016-03

9. **SHIMIZU, Koji**
   Dissociative AdsorptionEAbsorption and DesorptionEScattering Dynamics of Atoms and Molecules on Solid Surfaces
   Osaka University, 2016-03

10. **SHINJO, Kazuya**
    Density-matirx renormalization group study of quantum spin systems with Kitaev-type anisotropic interaction
    Kyoto University, 2016-03

11. **SHIRAI, Tatsuhiko**
    Long-time asymptotic of periodically driven open quantum systems
    University of Tokyo, 2016-03

12. **TAKEMORI, Nayuta**
Strong electron correlation effects in a quasiperiodic lattice
Tokyo Institute of Technology, 2016-03

13. **WATANABE, Eriko**
First principles study on electrocatalyst/water interfaces for oxygen reduction/evolution reactions
University of Tokyo, 2016-03

14. **YAMAMOTO, Yoshiyuki**
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University of Tokyo, 2016-03

15. **YASUDA, Shinya**
Study of quantum criticality with strong space-time anisotropy by quantum Monte Carlo
University of Tokyo, 2016-03

□ Master Theses

1. **FUJITA, Hiroyuki**
   Chiral Magnetic Effect in Condensed Matter Systems
   University of Tokyo, 2016-03

2. **HATOMURA, Takuya**
   Quantum dynamics of nano-magnets under time-dependent fields
   University of Tokyo, 2016-03

3. **HWANG, Jaekyun**
   Theoretical investigation of the evaluation method for the SOFC cathodes performance by first-principles calculation
   University of Tokyo, 2016-03

4. **IKEUCHI, Hiroki**
   Study of the spectra of Electron-Spin-Resonance from the quantum time time evolution of magnetization
   University of Tokyo, 2016-03

5. **IMOTO, Fumihiro**
   Microscopic mechanisms of initial formation process of graphene on SiC(0001) surfaces based on the density functional theory
   University of Tokyo, 2016-03

6. **KAMBE, Hiroyuki**
   Calculation of solvation free energy using the QM/MM-ER approach which incorporates the first solvation shell in the QM region
   Tohoku University, 2016-03

7. **KAWANABE, Go**
   Theoretical study on the electronic structure of pentacene adsorbed on a graphite surface
   University of the Ryukyus, 2016-03

8. **KAWASAKI, Wataru**
   Theoretical study of negative ion production on solid surfaces
   Osaka University, 2016-03

9. **KITAGAWA, Naohiro**
   Ab initio study on dioxygen coordinated iron porphyrin complex considering hemoglobin environment
   Kanazawa University, 2016-03

10. **KOJIMA, Shoya**
    DMFT analysis for $BiNiO_3$
    Tokyo Institute of Technology, 2016-03

11. **KUROKAWA, Daiichi**
    Spin-Dependent O2 Binding to Hemoglobin
    Osaka University, 2016-03

12. **KUWABARA, Yuki**
    Time-Space analysis of nonlinear polarization by time-dependent density functional theory
    University of Tsukuba, 2016-03

13. **MASUGATA, Yoshimitsu**
Scattering processes of exciton polarons at organic semiconductor interfaces
Chiba University, 2015-03

14. **MIMURA, Takaaki**
Analysis of spin models with deterministic Monte Carlo methods
University of Tokyo, 2016-03

15. **MIYARA, Shota**
Study of bond-randomness-induced magnetic moment in quantum spin systems with the degree of freedom of the lattice
University of the Ryukyus, 2016-03

16. **MURAYAMA, Kaori**
Ortho-para conversion of H2 on alpha-Fe2O3(0001) surface
Osaka University, 2016-03

17. **NAKANO, Hiroto**
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Kanazawa University, 2016-03

18. **OHBA, Koji**
Calculation of thermal conductivity of silicon nanowires by density functional theory
University of Tokyo, 2016-03

19. **ONDA, Yukiko**
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Chiba University, 2015-03

20. **OSUGA, Yuki**
First-principles study of impurity, surface, and interface of BaSi2
Chiba University, 2015-03

21. **SAKAGAWA, Yasuaki**
Improvement of continuous-space path-integral Monte Carlo and search for novel quantum phase of He4
University of Tokyo, 2016-03

22. **SASAKI, Shogo**
Defects and Schottky barrier at metal/Ge interfaces; first-principles study
Chiba University, 2015-03

23. **SHINOHARA, Yurie**
Calculation of light absorption properties in nanoscale structures
Ochanomizu University, 2016-03

24. **TANAKA, Shogo**
Molecular dynamics study of the water bending mode in sum frequency generation spectroscopy
Tohoku University, 2016-03

25. **UMINO, Satoru**
Construction of the exchange repulsion in QM/MM system based on the exchange hole function and its application to condensed phase
Tohoku University, 2016-03

26. **WANG, Lingjian**
Effects of hydration on ion transfer through liquid-liquid interface
Tohoku University, 2015-09

27. **YAMADA, Takuto**
Magnetic excitations of Kitaev-Heisenberg models
University of Hyogo, 2015-03

28. **YANATORI, Hiromasa**
Ordered phases of multi-component fermion systems in optical lattices
Tokyo Institute of Technology, 2016-03

29. **YOSHIKAWA, Daiki**
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Kanazawa University, 2015-09