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

AKAGI, Kazuto [C class; 4000 (B), 0 (C)] (105)

— *Topological Analysis and Order Parameter of the System*

1. Local chemical ordering within the incubation period as a trigger for nanocrystallization of a highly supercooled Ti-based liquid
   Z. Wang, C. L. Chen, S. V. Ketov, K. Akagi, A. A. Tsarkov, Y. Ikuhara and D. V. Louzguine-Luzgin: Materials and Design **156** (2018) 504-513.

AKAI, Hisazumi [B class; 1300 (B), 50 (C)] (139,140)

— *Stability and magnetic properties of rare earth mixed crystal magnet materials*

1. First-principles study of spin-wave dispersion in $Sm(Fe_{1-x}Co)_{12}$
   T. Fukazawa, H. Akai. Y. Harashima, and T. Miyake : J. Magn, Magn. Mater. **469**, 296 (2019).
2. Ab initio Study of High-field NMR Shift of ^{59}Co in the Ferromagnetic Heusler Alloy C_2TiGa
   H. Nishihara, H. Akai, K. Sato, T. Kanomata, M. Geshi, T. Sakon, and T. Wada: J. Phys. Soc. Jpn. **88**, 034712 (2019).

AKASHI, Ryosuke [C class; 6500 (B), 0 (C)] (70)

— *First-principles quantitative approach to the interplay of charge and spin fluctuations in superconductors*

AOYAMA, Kazushi [B class; 1300 (B), 90 (C)] (282)

— *Theoretical study of dynamical spin correlations in Heisenberg antiferromagnets on the triangular lattice*

— *Transport properties of the classical antiferromagnetic Heisenberg model in two dimension*

1. Spin ordering induced by lattice distortions in classical Heisenberg antiferromagnets on the breathing pyrochlore lattice
   K. Aoyama and H. Kawamura: Phys. Rev. B **99** (2019) 144406.

ARAI, Munehito [C class; 5000 (B), 0 (C)] ()

— *Theoretical analysis and design of proteins for industrial and pharmaceutical applications*

ARAIDAI, Masaaki [C class; 2500 (B), 800 (C)] (117)

— *First-principles study on two-dimensional crystals of germanium*

ASANO, Yuta [C,E class; 22000 (B), 3300 (C)] (205)

— *A Molecular Dynamics Study of the Cavitation*

— *Molecular Dynamics Simulation of a Karman-Vortex Cavitation*

1. Polymer effects on Karman vortex: Molecular dynamics study

Y. Asano, H. Watanabe, and H. Noguchi: J. Chem. Phys. **148**,(2018) 144901.

BUI, PHO VAN [C class; 4000 (B), 1300 (C)] (88)
— *Study on removal mechanism in catalyst referred etching of single crystalline SiC with pure water*

1. Catalyzed Chemical Polishing of SiO2 Glasses in Pure Water
   D. Toh, P.V. Bui, A. Isohashi, N. Kidadi. S. Matsuyama, Y. Sano, Y. Morikawa, K. Yamauchi: Rev. Sci. Instru. **90** (2019) accepted
2. High-efficiency SiC polishing using a thin film catalyst in pure water
   P.V. Bui, D. Toh, S. Matsuyama, Y. Sano, K. Yamauchi: euspen's 19th Internation Conference and Exhibition (2019)

EGAMI, Yoshiyuki [C class; 3500 (B), 350 (C)] (107)
— *Development of a time-dependent electron-transport simulator and its application to atomic-layered materials*

1. Efficient calculation of the self-energy matrices for electron-transport simulations
   Y. Egami, S. Tsukamoto and T. Ono: submitted to Phys. Rev. B.

FUCHIZAKI, Kazuhiro [C class; 4500 (B), 0 (C)] (252)
— *Phase equilibria and polyamorphism*

1. Liquid–Gas Spinodal of the Modified Lennard-Jones Fluid
   K. Fuchizaki and K. Watanabe: J. Phys. Soc. Jpn. **87** (2018) 114006.
2. Pressure-induced local symmetry breaking upon liquid–liquid transition of GeI_4 and SnI_4
   K. Fuchizaki, T. Sakagami, and H. Iwayama: J. Chem. Phys. **150** (2019) 114501.
3. A polymerization scenario of the liquid–liquid transition of GeI_4
   K. Fuchizaki, H. Naruta, and T. Sakagami: J. Phys.: Condens. Matter **31** (2019) 225101.

FUJIMOTO, Yoshitaka [C class; 2000 (B), 0 (C)] (128)
— *First-principles study of electronic properties of graphene layers*

1. Gas adsorption effects on the stabilities, electronic structures and scanning tunneling microscopy of graphene monolayers doped with B or N
   Y. Fujimoto and S. Saito: Jpn. J. Appl. Phys. **58**, 015005 (2019).
2. STM visualization of carbon impurities in sandwich structures consisting of hexagonal boron nitride and graphene
   T. Haga, Y. Fujimoto, and S. Saito: Jpn. J. Appl. Phys., Accepted.
3. Electronic structures and scanning tunneling microscopy images of graphene/carbon-doped hexagonal boron nitride heterostructures
   T. Haga, Y. Fujimoto, and S. Saito: Phys. Rev. B, submitted.
4. Design and Analysis of Carbon-Based Nanomaterials for Removal of Environmental Contaminants
   Y. Fujimoto: Nanotechnology for Sustainable Water Remediation (Wiley-Scrivener Publishers 2018) Chapter 9, p.277.

FUJISHIRO, Hiroki [C class; 1500 (B), 0 (C)] (137)
— *Strained Band-Structure Engineering for Antimonide-Based Terahertz Transistors*

FUKUDA, Jun-ichi [B class; 1500 (B), 0 (C)] (279)
— *Calculation of ordered structures and their optical properties of soft materials*

1. Liquid-crystalline half-Skyrmion lattice spotted by Kossel diagrams
   J. Fukuda, A. Nych, U. Ognysta, S. Žumer and I. Muševič: Scientific Reports **8** (2018) 17234.
2. Theoretical study on optical properties of liquid crystalline Skyrmion lattice
   J. Fukuda and S. Žumer: Proc. SPIE **10941** (2019) 1094108.

FUKUI, Ken-ichi [C class; 2000 (B), 0 (C)] (271)
— *Analysis on Structuring and Dynamics of Ionic Liquid Forming Electric Double Layer at Electrode Interfaces*

1. Microscopic properties of ionic liquid / organic semiconductor interfaces revealed by molecular

dynamics simulations
Y. Yokota, H. Miyamoto, A. Imanishi, J. Takeya, K. Inagaki, Y. Morikawa, and K. Fukui: Phys. Chem. Chem. Phys. **20** (2018) 13075.

2. Potential dependent changes of structural and dynamical properties of 1-butyl-3-methylimidazolium bis(trifluoromethanesulfonyl)imide on graphite electrode revealed by molecular dynamics simulation
H. Miyamoto, Y. Yokota, A. Imanishi, K. Inagaki, Y. Morikawa, K. Fukui: Phys. Chem. Chem. Phys.**20** (2018) 19408.

FUKUMOTO, Yoshiyuki [B class; 500 (B), 0 (C)] (305)
— *Theoretical studies on kagome antiferromagnets and related systems*

1. Impact of Dzyaloshinsky-Moriya Interactions and Tilts of the g Tensors on the Magnetization Process of a Spherical Kagomé Cluster in $\{W_{72}V_{30}\}$
Y.Fukumoto, Y. Yokoyama, and H. Nakano: J. Phys. Soc. Jpn. 87, 124710, 2018
2. Canonical-Ensemble Calculations of the Magnetic Susceptibility for a Spin-1/2 Spherical Kagome Cluster With DzyaloshinskiiMoriya Interactions by Using Microcanonical Thermal Pure Quantum States
K. Inoue, Y. Maeda, H. Nakano, Y. Fukumoto: IEEE TRANSACTIONS ON MAGNETICS 55, 2019

GESHI, Masaaki [C class; 3500 (B), 700 (C)] (100)
— *Development of new structural search method and search for new functional materials*

GOHDA, Yoshihiro [C class; 4500 (B), 800 (C)] (87)
— *Rashba effects in surface-Bi nanostructures*

1. First-principles study of magnetoelectric coupling at $Fe/BiFeO_3(001)$ interfaces
K. Fujita and Y. Gohda: Phys. Rev. Appl. **11**, 024006 (2019).
2. First-principles prediction of one-dimensional giant Rashba splittings in Bi-adsorbed In atomic chains
T. Tanaka and Y. Gohda: Phys. Rev. B **98**, 241409(R) (2018).
3. First-principles study on substitution effects in $Nd_2(Fe, X)_{14}B$
Y. Tatetsu, S. Tsuneyuki, and Y. Gohda: Mater. **4**, 388 (2018).
4. Hidden order in amorphous structures: extraction of nearest neighbor networks of amorphous Nd-Fe alloys with Gabriel graph analyses
A. Terasawa and Y. Gohda: J. Chem. Phys. **149**, 154502 (2018).
5. Role of typical elements in $Nd_2Fe_{14}X$ (X=B, C, N, O, F)
Y. Tatetsu, Y. Harashima, T. Miyake, and Y. Gohda: Phys. Rev. Mater. **2**, 074410 (2018).

HAGITA, Katsumi [C class; 3500 (B), 700 (C)] (254)
— *Coarse grained MD simulation for fracture and reinforcement of polymer materials*

1. Super resolution for asymmetric resolution of FIB-SEM 3D imaging of silica nanoparticles in SBR
K. Hagita, T. Higuchi and H. Jinnai: Scientific reports, 8 (2018) 5877.
2. Molecular dynamics simulations of cross-linked phenolic resins using a united-atom model
A. Izumi, Y. Shudo, K. Hagita and M. Shibayama: Macromolecular Theory and Simulations, 27 (2018) 1700103.
3. Two-dimensional scattering patterns of polymers in elongated polymer networks and composites
K. Hagita: Polymer, 147 (2018) 247-259.
4. Diffusion Behavior of Methanol Molecules Confined in Cross-Linked Phenolic Resins Studied Using Neutron Scattering and Molecular Dynamics Simulations
Y. Shudo, A. Izumi, K. Hagita, T. Yamada, K. Shibata and M. Shibayama: Macromolecules, 51 (2018) 6334-6343.
5. Multipoint segmental repulsive potential for entangled polymer simulations with dissipative particle dynamics
N. Iwaoka, K. Hagita and H. Takano: J. Chem. Phys., 149 (2018) 114901.
6. Two-dimensional scattering patterns and stress-strain relation of elongated clay nano composite

gels: Molecular dynamics simulation analysis
K. Hagita, Y. Shudo and M. Shibayama: Polymer, 154 (2018) 62-79.

7. Thinning Approximation for Calculating Two-Dimensional Scattering Patterns in Dissipative Particle Dynamics Simulations under Shear Flow
K. Hagita, T. Murashima and N. Iwaoka: Polymers, 10 (2018) 1224.
8. Structure formation of a quenched single polyethylene chain with different force fields in united atom molecular dynamics simulations
K. Hagita, S. Fujiwara and N. Iwaoka: AIP Advances, 8 (2018) 115108.
9. Molecular Dynamics Studies on Pressure-Induced Structural Change of Poly(4-methyl-1-pentene) Melts
K. Hagita and Y. Senda: J. Phys. Soc. Jpn., 87 (2018) 114803.
10. Elongational viscosity of weakly entangled polymer melt via coarse-grained molecular dynamics simulation
T. Murashima, K. Hagita and T. Kawakatsu: J. Soc. Rheol. Jpn. (Nihon Reoroji Gakkaishi), 46 (2018) 207-220.
11. Effect of diameter distribution on two-dimensional scattering patterns of a rubber model filled with carbon black and silica NPs
K. Hagita: Polymer, 160 (2019) 65-72.
12. Scattering Patterns and Stress-Strain Relations on Phase-separated ABA Block Copolymers under Uniaxial Elongating Simulations
K. Hagita, T. Tominaga, K. Akutagawa and H. Jinnai: Soft Matter, 15 (2019) 926-936.
13. Study of Commodity VR for Computational Material Sciences
K. Hagita, S. Matsumoto and K. Ohta: ACS Omega, 4 (2019) 3990-3999.
14. An Accelerated United-Atom Molecular Dynamics Simulation on the Fast Crystallization of Ring Polyethylene Melts
K. Hagita, S. Fujiwara and N. Iwaoka: J. Chem. Phys., 4 (2019) 3990-3999.
15. Two-dimensional scattering patterns of coarse-grained molecular dynamics model of filled polymer gels during uniaxial expansion
K. Hagita: Polymer, 166 (2019) 155-168.
16. Applications of aesthetic pentagon-shaped stereo tiling employing pentagraphene carbon - star walls and embossment design
K. Hagita, Y. Kawazoe and M. Ogino: AIP Advances, 9 (2019) 035001.
17. Nanovoids in Uniaxially Elongated Polymer Network Filled with Polydisperse Nanoparticles via Coarse-Grained Molecular Dynamics Simulation and Two-Dimensional Scattering Patterns
K. Hagita: Polymer, (2019) in press.

HAGIWARA, Satoshi [B class; 700 (B), 90 (C)] (149)
— *First-principles study on positron states in d0 ferromagnetics and at solid surfaces*

HAMADA, Ikutaro [C class; 4500 (B), 800 (C)] (86)
— *van der Waals density functional study of molecular adsorption on metal surfaces*

HAMAMOTO, Yuji [C class; 2000 (B), 0 (C)] (126)
— *van der Waals density functional study of organic-metal interfaces*

HARADA, KENJI [C class; 5000 (B), 0 (C)] (248)
— *Numerical study of phase transition in non-equilibrium systems*

1. Entropy governed by the absorbing state of directed percolation
Kenji Harada and Naoki Kawashima, arXiv:1902.10479.

HASHIMOTO, Tamotsu [C class; 3000 (B), 0 (C)] (262)
— *Molecular dynamics simulation of ferroelectrics using a shell model IV*

1. Structure of Amorphous $BaTiO_3$ by Molecular Dynamics Simulations Using a Shell Model
T. Hashimoto and H. Moriwake: submitted.

HASHMI, Arqum [C class; 1500 (B), 0 (C)] ()
— *Spin-valley polarization & quantum anomalous Hall conductivity in Transition metal dichalcogenides*

HATANO, Naomichi [B class; 0 (B), 90 (C)] ()
— *Fractality of the Anderson localization with binary randomness*

HATSUGAI, Yasuhiro [C class; 4000 (B), 750 (C)] (249)
— *Numerical studies of topological phases and bulk-edge correspondence*

1. Weyl points of mechanical diamond
   Y. Takahashi, T. Kariyado and Y. Hatsugai: Phys. Rev. B 99, 024102 (2019).
2. Z_N Berry Phases in Symmetry Protected Topological Phases
   Toshikaze Kariyado, Takahiro Morimoto, and Yasuhiro Hatsugai: Phys. Rev. Lett. 120, 247203 (1-5) (2018).
3. Fractional Quantum Hall Effect in n = 0 Landau Band of Graphene with Chern Number Matrix
   K. Kudo and Y. Hatsugai: J. Phys. Soc. Jpn. 87, 063701 (1-5) (2018).
4. Many-Body Chern Number without Integration
   Koji Kudo, Haruki Watanabe, Toshikaze Kariyado, and Yasuhiro Hatsugai: Phys. Rev. Lett. 122, 146601 (1-5) (2019), (Editors' Suggestion).
5. Phase diagram of a disordered higher-order topological insulator: A machine learning study
   H. Araki, T. Mizoguchi and Y. Hatsugai: Phys. Rev. B 99, 085406 (1-8) (2018).
6. Symmetry-protected exceptional rings in two-dimensional correlated systems with chiral symmetry
   Tsuneya Yoshida, Robert Peters, Norio Kawakami, and Yasuhiro Hatsugai: Phys. Rev. B 99, 121101(R)(1-5) (2019).

HATTORI, Ken [C class; 3000 (B), 650 (C)] (110)
— *Atomic structure and electronic states for Si surfaces with adsorbates*

HAYAMI, Satoru [C class; 6000 (B), 0 (C)] (183)
— *Effect of magnetic anisotropy on skyrmion crystal in the Kondo lattice model*

1. Néel- and Bloch-Type Magnetic Vortices in Rashba Metals
   S. Hayami and Y. Motome: Phys. Rev. Lett. **121**, 137202 (2018).
2. Classification of atomic-scale multipoles under crystallographic point groups and application to linear response tensors
   S. Hayami, M. Yatsushiro, Y. Yanagi, and H. Kusunose: Phys. Rev. B **98** (2018) 165110.
3. Effect of magnetic anisotropy on Skyrmions with a high topological number in itinerant magnets
   S. Hayami and Y. Motome: Phys. Rev. B **99**, 094420 (2019).
4. Multiple-Q Magnetic States in Spin-Orbit Coupled Metals
   S. Hayami and Y. Motome: IEEE Trans. Magn. **55**, 1500107 (2018).

HIDA, Kazuo [B class; 300 (B), 90 (C)] (308)
— *Numerical Study of One Dimensional Frustrated Quantum Spin Systems*

HIGUCHI, Yuji [C class; 4500 (B), 0 (C)] (251)
— *Assembly process and mechanical properties of crystalline polymers by large-scale coarse-grained molecular dynamics simulation*

HINOKIHARA, Taichi [C class; 4000 (B), 0 (C)] (258)
— *Construction of coarse-graining spin model and analysis of the coercivity*

HINUMA, Yoyo [B class; 600 (B), 80 (C)] (154)
— *Calculation of oxide surface properties for catalyst informatics*

1. Density Functional Theory Calculations of Oxygen Vacancy Formation and Subsequent Molecular Adsorption on Oxide Surfaces
   Y. Hinuma, T. Toyao, T. Kamachi, Z. Maeno, S. Takakusagi, S. Furukawa, I. Takigawa, and K. Shimizu: J. Phys. Chem. C, **122** (2018) 29435.

2. Effects of composition, crystal structure, and surface orientation on band alignment of divalent metal oxides: A first-principles study
   Y. Hinuma, Y. Kumagai, and I. Tanaka, F Oba: Phys. Rev. Mater., **2** (2018) 124603.
3. Temperature coefficient of redox potential of LixFePO4
   Y. Fukuzumi, Y. Hinuma, and Y. Moritomo: AIP Advances, **8** (2018) 065021.

HIRATSUKA, Masaki [B class; 1300 (B), 170 (C)] ()
— *ab initio calculations to determine the phase equilibrium conditions of TBAB semiclathrate hydrates*
— *ab initio molecular dynamics study on the vibrational spectra of semi-clathrate hydrates*

HIYAMA, Miyabi [B class; 600 (B), 80 (C)] (153)
— *Elucidation of electronic states for caged compounds in aqueous solution*

HOSHI, Takeo [C class; 5000 (B), 850 (C)] (80)
— *Large-scale device-material research by massively parallel electronic structure calculation and data-driven science*

1. Solution of the k-th eigenvalue problem in large-scale electronic structure calculations
   Dongjin Lee, Takeo Hoshi, Tomohiro Sogabe, Yuto Miyatake, Shao-Liang Zhang, submitted; Preprint (arXiv.1710.05134)

HOSHINO, Shintaro [C class; 2500 (B), 0 (C)] (192)
— *Numerical approach to unconventional electronic orderings in strongly correlated systems*

1. Spontaneously orbital selective superconductivity in a three-orbital Hubbard model
   K. Ishigaki, J. Nasu, A. Koga, S. Hoshino and P. Werner: Phys. Rev. 98, 235120 (2018)a
2. Staggered ordered phases in the three-orbital Hubbard model
   K. Ishigaki, J. Nasu, A. Koga, S. Hoshino and P. Werner: Phys. Rev. 99, 085131 (2019)a
3. Unconventional orbital ordering and emergent dimensional reduction in fulleride superconductors
   S. Hoshino, P. Werner and R. Arita, arXiv:1902.09053 (2019)
4. Nature of superconducting fluctuation in photo-excited systems
   R. Iwazaki, N. Tsuji and S. Hoshino, arXiv:1904.05820 (2019)
5. Unconventional full-gap superconductivity in Kondo lattice with semi-metallic conduction bands
   S. Iimura, M. Hirayama and S. Hoshino, arXiv:1904.06240 (2019)

HOTTA, Chisa [D class; 2000 (B), 0 (C)] (195)
— *Study on the bond random transverse Ising model*

HOTTA, Takashi [C class; 5500 (B), 0 (C)] (187)
— *Multi-channel Kondo Effect in Rare-Earth Systems*

1. Impurity Effects in Nodal Extended s- and Nodeless d-Wave Superconductors: Gap Symmetry of BiS_2-Based Layered Superconductors
   Akihiro Ichikawa and Takashi Hotta, J. Phys. Soc. Jpn. **87**, 114706 (2018).
2. Microscopic Theory of Γ_3 Quadrupole Ordering in Pr Compounds on the Basis of a j-j Coupling Scheme
   Ryosuke Yamamura and Takashi Hotta, J. Phys. Soc. Jpn. **88**, 034715 (2019).

HUKUSHIMA, Koji [C class; 6500 (B), 0 (C)] (228)
— *Data-driven science for material science*
— *Statistical-mechanical study for chiral magnets*

1. Phase transitions in quantum annealing of an NP-hard problem detected by fidelity susceptibility
   J Takahashi, K Hukushima: Journal of Statistical Mechanics: Theory and Experiment (2019) 043102a
2. Solid-liquid transition of skyrmions in a two-dimensional chiral magnet
   Y Nishikawa, K Hukushima, W Krauth: Physical Review B **99** (2019) 064435/1-10
3. Power-law decay in the nonadiabatic photodissociation dynamics of alkali halides due to quantum wavepacket interference

Y Mizuno, K Hukushima: J. Chem. Phys. **149** (2018) 174313/1-6
4. Data-driven diagnosis for compressed sensing with cross validation
Y Nakanishi-Ohno, K Hukushima: Physical Review E **98** (2018) 052120/1-6

IGARASHI, Ryo [C class; 500 (B), 150 (C)] ()
— *Full diagonalization using low-rank approximation to Hamiltonian matrices and its application to quantum spin models*

IKEDA, Hiroaki [B class; 1100 (B), 70 (C)] (142)
— *Development of the first-principles approach and analysis of superconductivity*
— *Electronic structure and superconductivity based on a first-principles approach*

IKUHARA, Yuichi [C class; 6000 (B), 0 (C)] (79)
— *Ab initio study on atomic and electronic structure of functional materials*
— *Atomic structure and properties of functional materials*

1. Ceramic phases with one-dimensional long-range order
D. Yin, C. Chen, M. Saito, K. Inoue, Y. Ikuhara: Nat. Mat. **18** (2019) 19-23.
2. Atomic-scale valence state distribution inside ultrafine CeO_2 nanocubes and its size dependence
X. Hao, A. Yoko, C. Chen, K. Inoue, M. Saito, G. Seong, S. Takami, T. Adschiri, Y. Ikuhara: SMALL **14** (2018) 1802915.

IMADA, Masatoshi [D,E class; 52000 (B), 6700 (C)] (168,171)
— *Highly accurate analysis of an effective Hamiltonian for high Tc cuprates by the many-variable variational Monte Carlo method combined with tensor network*
— *Mechanism of pseudogap and superconductivity with low-energy fermionic excitations in high-Tc cuprates*
— *Study on frustrated quantum spin systems using machine-learning solvers*

1. Competition among various charge-inhomogeneous states and d-wave superconducting state in Hubbard models on square lattices
Kota Ido, Takahiro Ohgoe, and Masatoshi Imada: Phys. Rev. B **97** (2018) 045138.
2. Quantum spin liquid signatures in Kitaev-like frustrated magnets
Matthias Gohlke, Gideon Wachtel, Youhei Yamaji, Frank Pollmann, and Yong Baek Kim: Phys. Rev. B **97**, (2018) 075126.
3. Ab initio effective Hamiltonians for cuprate superconductors
Motoaki Hirayama, Youhei Yamaji, Takahiro Misawa, and Masatoshi Imada: Phys. Rev. B. **98** (2018) 134501.
4. Direct connection between Mott insulators and d-wave high-temperature superconductors revealed by continuous evolution of self-energy poles
Shiro Sakai, Marcello Civelli, and Masatoshi Imada : Phys. Rev. B.**98** (2018) 195109
5. Stripe and superconducting order competing in the Hubbard model on a square lattice studied by a combined variational Monte Carlo and tensor network method
Andrew S. Darmawan, Yusuke Nomura, Youhei Yamaji, and Masatoshi Imada: Phys. Rev. B 98,**98** (2018) 205132.
6. Resummation of diagrammatic series with zero convergence radius for strongly correlated fermions
Riccardo Rossi, Takahiro Ohgoe, Kris Van Houcke, and Felix Werner: Phys. Rev. Lett. **121** (2018) 130405.
7. Contact and Momentum distribution of the Unitary Fermi Gas
Riccardo Rossi, Takahiro Ohgoe, Kris Van Houcke, and Felix Werner: Phys. Rev. Lett. **121** (2018) 130406.
8. mVMC-Open-source software for many-variable variational Monte Carlo method
Takahiro Misawa, Satoshi Morita, Kazuyoshi Yoshimi, Mitsuaki Kawamura, Yuichi Motoyama, Kota Ido, Takahiro Ohgoe, Masatoshi Imada, Takeo Kato: Compt. Phys. Commun.,**235** (2019) 447.
9. Excitons and Dark Fermions as Origins of Mott Gap, Pseudogap and Superconductivity in Cuprate Superconductors — General Idea and Basic Concept Based on Gap Physics

Takafumi J. Suzuki, Masatoshi Imada: J. Phys. Soc. Jpn. **88** (2019) 024701.

INAGAKI, Kouji [C class; 4000 (B), 400 (C)] (166)
— *First-principles meta-dynamics analysis of Catalyst Referred Etching method -Analysis of surface roughness formed by etching-*

1. Platinum-catalyzed hydrolysis etching of SiC in water: A density functional theory study
   P. V. Bui, D. Toh, A. Isohashi, S. Matsuyama, K. Inagaki, Y. Sano, K. Yamauchi, and Y. Morikawa: Jpn. J. Appl. Phys. **57** (2018) 055703.

INAOKA, Takeshi [C class; 500 (B), 150 (C)] (155)
— *Search and realization of novel electronic properties of solid surfaces and interfaces and of small particles*

1. Vibration-induced structures in scanning tunneling microscope light emission spectra of Ni(110)-(2x1)O
   Y. Uehara, T. Inaoka, T. Nishio, and S. Katano: J. Appl. Phys. **123** (2018) 224302 (8 pages).

ISHIBASHI, Shoji [C class; 4000 (B), 0 (C)] (104)
— *Prediction of properties of organic ferroelectrics and piezoelectrics by first-principles calculation*

1. Computational findings of metastable ferroelectric phases of squaric acid
   S. Ishibashi, S. Horiuchi, and R. Kumai: **97** (2018) 184102.

ISHIDA, Kunio [B class; 1300 (B), 90 (C)] (280)
— *Ultrafast nonadiabatic dynamics of electron-phonon-photon system*
— *Ultrafast nonadiabatic dynamics of electron-phonon-photon systems*

1. Interplay of electron-phonon nonadiabaticity and Raman scattering in the wavepacket dynamics of electron-phonon-photon systems
   Kunio Ishida: Eur. Phys. J. D, doi:10.1140/epjd/e2019-09485-5

ISHIHARA, Sumio [B class; 1600 (B), 0 (C)] (196)
— *Complexed quantum dynamics in strongly interacting systems*
— *Opto-spintronics in correlated magnets*

1. Photocontrol of magnetic structure in an itinerant magnet
   Atsushi Ono and Sumio Ishihara: Phys. Rev. B **98**, 214408 (2018).
2. Photoinduced topological spin texture in a metallic ferromagnet
   Atsushi Ono and Sumio Ishihara: J. Phys. Soc. Jpn. **88**, 023703 (2019).
3. Photoinduced collective mode, inhomogeneity, and melting in a charge-order system
   Hitoshi Seo, Yasuhiro Tanaka, and Sumio Ishihara: Phys. Rev. B **98**, 235150 (2018).
4. Quantum Paramagnet Near Spin-State Transition
   K. Tomiyasu, N. Ito, R. Okazaki, Y. Takahashi, M. Onodera, K. Iwasa, T. Nojima, T. Aoyama, K. Ohgushi, Y. Ishikawa, T. Kamiyama, S. Ohira-Kawamura, M. Kofu, and S. Ishihara: Advanced Quantum Technologies, 1800057 (2018).
5. Probing ultrafast spin-relaxation and precession dynamics in a cuprate Mott insulator with seven-femtosecond optical pulses
   T. Miyamoto, Y. Matsui, T. Terashige, T. Morimoto, N. Sono, H. Yada, S. Ishihara, Y. Watanabe, S. Adachi, T. Ito, K. Oka, A. Sawa, and H. Okamoto: Nature Communications **9**, 3948 (2018).

ISHII, Fumiyuki [C class; 13500 (B), 0 (C)] (27)
— *First-principles study of spin conversion materials*
— *First-principles study of topological thermoelectric materials*

1. Clear variation of spin splitting by changing electron distribution at non-magnetic metal/Bi_2O_3 interfaces
   H. Tsai, S. Karube, K. Kondou, N. Yamaguchi, F. Ishii, Y. Otani: Sci. Rep. **8** (2018) 5564.
2. Strong Rashba effect in the localized impurity states of halogen-doped monolayer $PtSe_2$
   M. A. U. Absor, I. Santoso, Harsojo, K. Abraha, H. Kotaka, F. Ishii, and M. Saito: Phys. Rev. B **97**, (2018) 205138.

3. First-principles study on thermoelectric properties of half-Heusler compounds CoMSb(M=Sc, Ti, V, Cr, and Mn)
   S. Minami, F. Ishii, Y. P. Mizuta, and M. Saito: Appl. Phys. Lett. **113** (2018) 032403.
4. First-principles Study of Rashba Spin Splitting at Strained SrTiO3(001) Surfaces
   N. Yamaguchi and F. Ishii: e-J. Surf. Sci. Nanotechnol. **16** (2018) 360.
5. Implementation of Generalized Bloch Theorem Using Linear Combination of Pseudo-Atomic Orbitals
   T. B. Prayitno and F. Ishii: J. Phys. Soc. Jpn. **87** (2018) 114709.
6. Large Anomalous Nernst Coefficient in an oxide Skyrmion Crystal Chern Insulator
   Y. P. Mizuta, H. Sawahata, and F. Ishii: Phys. Rev. B **98** (2018) 205125.
7. Electric field dependence of topological edge states in one-bilayer Bi(111) : A first-principles study
   H. Sawahata, N. Yamaguchi, H. Kotaka, and F. Ishii : e-J. Surf. Sci. Nanotechnol. **16** (2018) 427.
8. Anisotropic thermoelectric effect on phosphorene and bismuthene: first-principles calculations based on nonequilibrium Green's function theory
   Y. Tanaka, M. Saito, and F. Ishii: Jpn. J. App. Phys. **57** (2018) 125201.
9. First-principles design of the spinel iridate Ir_2O_4 for high-temperature quantum spin ice
   S. Onoda and F. Ishii: Phys. Rev. Lett. **122** (2019) 067201.
10. Doping-induced persistent spin helix with a large spin splitting in monolayer SnSe
    M.A.U. Absor and F. Ishii: Phys. Rev. B. **99** (2019) 075136.
11. First-principles Study of Spin-wave Excitations of 3d Transition Metals with Linear Combination of Pseudo-atomic Orbitals
    T.B. Prayitno and F. Ishii: J. Phys. Soc. Jpn. **88** (2019) 054701.

ISHIZUKA, Ryosuke [E class; 12000 (B), 1950 (C)] ()
— *Seeking of catalytic reaction with the MD/order-N DFT self-consistent scheme*

ISOBE, Masaharu [B class; 700 (B), 0 (C)] (295)
— *Nonequilibrium phase transition and slow dynamics in the dense hard sphere systems*
1. 粉体乱流ーマクロとミクロをつなぐ架け橋へ
   礒部雅晴，齊藤国靖：日本物理学会誌, **73** (2018) 469-474.

IYODA, Eiki [C class; 2500 (B), 0 (C)] (267)
— *Numerical study of eigenstate thermalization hypothesis in phase transition*

JESCHKE, Harald [C class; 6500 (B), 0 (C)] (226)
— *Doping effect on electronic structure and superconductivity in two-dimensional layered materials*
— *Effects of pressure in iron chalcogenide superconductors*
1. Two-dome superconductivity in FeS induced by a Lifshitz transition
   M. Shimizu, N. Takemori, D. Guterding, H. O. Jeschke: Phys. Rev. Lett. **121**, 137001 (2018)
2. Quantum and classical phases of the pyrochlore Heisenberg model with competing interactions
   Y. Iqbal, T. Mller, P. Ghosh, M. J. P. Gingras, H. O. Jeschke, S. Rachel, J. Reuther, R. Thomale: Phys. Rev. X **9**, 011005 (2019)

KAGESHIMA, Hiroyuki [C class; 1500 (B), 0 (C)] (136)
— *Study on physical properties of structural elementary excitations of semiconductor surfaces and interfaces*
1. Oxygen concentration dependence of silicon oxide dynamical properties
   Yuji Yajima, Kenji Shiraishi, Tetsuo Endoh, and Hiroyuki Kageshima: Jpn. J. Appl. Phys. **57** (2018) 06KD01.
2. First-principles Study on Charged Vacancies in MoS_2
   S. Urasaki and H. Kageshima, Jpn. J. Appl. Phys. **57** (2018) 125202.

KAMACHI, Takashi [B class; 600 (B), 80 (C)] ()
— *Database construction for activation and reaction of small molecules on solid surfaces*

KARIYADO, Toshikaze [B class; 600 (B), 90 (C)] (300)

— Realization and Manipulation of Topological States by Nanostructures

1. Z_N Berry Phases in Symmetry Protected Topological Phases
   T. Kariyado, T. Morimoto, and Y. Hatsugai: Phys. Rev. Lett. **120** (2018) 247202.
2. Counterpropagating topological interface states in graphene patchwork structures with regular arrays of nanoholes
   T. Kariyado, Y.-C. Jiang, H. Yang, and X. Hu: Phys. Rev. B **98** (2018) 195416.
3. Weyl points of mechanical diamond
   Y. Takahashi, T. Kariyado, and Y. Hatsugai: Phys. Rev. B **99** (2019) 024102.

KASAMATSU, Shusuke [C class; 6000 (B), 950 (C)] (69)

— Development of Structure/Property Prediction Framework Based on Replica Exchange Method Combined with Ab Initio Calculations

1. Direct coupling of first-principles calculations with replica exchange Monte Carlo sampling of ion disorder in solids
   S. Kasamatsu and O. Sugino: J. Phys.: Condens. Matter **31** (2019) 085901.

KATO, Takeo [D class; 1000 (B), 0 (C)] (287)

— Transport properties of one-dimensional interacting electron systems by a quantum Monte Carlo method

KAWAKAMI, Norio [C class; 11500 (B), 1900 (C)] (177)

— Study of magnetism, topological phase formation, and response to external fields in strongly correlated quantum systems

— Study of response to external fields and topological phenomena in strongly correlated quantum systems

1. Quantum oscillations in strongly correlated topological Kondo insulators
   Robert Peters, Tsuneya Yoshida, and Norio Kawakami: arXiv:1901.05099
2. Impact of the Rashba Spin Orbit Coupling on f-electron Materials
   Yoshihiro Michishita and Robert Peters: arXiv:1812.10888
3. Interplay between charge, magnetic, and superconducting order in a Kondo lattice with attractive Hubbard interaction
   Benedikt Lechtenberg, Robert Peters, and Norio Kawakami: Phys. Rev. B **98** (2018) 195111.
4. Breakdown of topological Thouless pumping in the strongly interacting regime
   Masaya Nakagawa, Tsuneya Yoshida, Robert Peters, and Norio Kawakami: Phys. Rev. B **98** (2018) 115147.
5. Magnetic states in a three-dimensional topological Kondo insulator
   Robert Peters, Tsuneya Yoshida, and Norio Kawakami: Phys. Rev. B **98** (2018) 075104.
6. Non-Hermitian perspective of the band structure in heavy-fermion systems
   Tsuneya Yoshida, Robert Peters, and Norio Kawakami: Phys. Rev. B **98** (2018) 035141.
7. Topological properties of magnetically ordered heavy-fermion systems in the presence of mirror symmetry
   Kazuhiro Kimura, Tsuneya Yoshida, and Norio Kawakami: J. Phys. Soc. Jpn. **87** (2018) 084705.
8. Reduction of topological Z classification in cold-atom systems
   Tsuneya Yoshida, Ippei Danshita, Robert Peters, and Norio Kawakami: Phys. Rev. Lett. **121** (2018) 025301.
9. Equilibrium and real-time properties of the spin correlation function in the two-impurity Kondo model
   Benedikt Lechtenberg and Frithjof B. Anders: Phys. Rev. B **98** (2018) 035109.
10. Chaotic-integrable transition in the Sachdev-Ye-Kitaev model
    Antonio M. Garcia-Garcia, Bruno Loureiro, Aurelio Romero-Bermudez, and Masaki Tezuka: Phys. Rev. Lett **120** (2018) 241603.

KAWAMURA, Hikaru [B,C,E class; 24000 (B), 0 (C)] (207,208)
— *Novel order in frustrated magnets*
— *Numerical simulations on statistical models of earthquakes*

1. Slow-slip phenomena represented by the one-dimensional Burridge-Knopoff model of earthquakes
   H. Kawamura, M. Yamamoto and Y. Ueda: J. Phys. Soc. Jpn. **87**, (2018) 053001.
2. Randomness-induced quantum spin liquid behavior in the $s = 1/2$ random $J_1 - J_2$ Heisenberg antiferromagnet on the square lattice
   K. Uematsu and H. Kawamura: Phys. Rev. B **98**, (2018) 134427.
3. Nature of the high-speed rupture of the two-dimensional Burridge-Knopoff model of earthquakes
   H. Kawamura, K. Yoshimura, and S. Kakui: Phil. Trans. R. Soc. A **377** (2018) 20170391.
4. Spin ordering induced by lattice distortions in classical Heisenberg antiferromagnets on the breathing pyrochlore lattice
   K. Aoyama and H. Kawamura: Phys. Rev. B **99**, (2019) 1444062.

KAWASHIMA, Naoki [E class; 46000 (B), 6000 (C)] (204,337)
— *Tensornetwork Method and Its Application to Non-Magnetic States*

1. A series of magnon crystals appearing under ultrahigh magnetic fields in a kagome antiferromagnet
   R. Okuma, D. Nakamura, T. Okubo, A. Miyake, A. Matsuo, K. Kindo, M. Tokunaga, N. Kawashima, S. Takeyama and Z. Hiroi: Nature Communications **10**, 1229/1-7 (2019).
2. Calculation of higher-order moments by higher-order tensor renormalization group
   Satoshi Morita, Naoki Kawashima: Computer Physics Communications **236**, 65-71 (2019)
3. Detecting signals of weakly first-order phase transitions in two-dimensional Potts models
   Shumpei Iino, Satoshi Morita, Anders W. Sandvik, and Naoki Kawashima: J. Phys. Soc. Jpn. **88**, 034006/1-8 (2019).
4. Spin-one bilinear-biquadratic model on a star lattice
   Hyun-Yong Lee, and Naoki Kawashima: Phys. Rev. B **97**, 205123/1-7 (2018).
5. Spin Thermal Hall Conductivity of a Kagome Antiferromagnet
   Hayato Doki, Masatoshi Akazawa, Hyun-Yong Lee, Jung Hoon Han, Kaori Sugii, Masaaki Shimozawa, Naoki Kawashima, Migaku Oda, Hiroyuki Yoshida, and Minoru Yamashita: Phys. Rev. Lett. **121**, 097203/1-4 (2018).
6. Fast algorithm for generating random bit strings and multispin coding for directed percolation
   Hiroshi Watanabe, Satoshi Morita, Synge Todo, and Naoki Kawashima: J. Phys. Soc. Jpn. **88**, 024004 (2019).

KITA, Takafumi [C class; 5500 (B), 0 (C)] (242,244)
— *Analysis of many-body effects in Bose-Einstein condensate*
— *Microscopic calculation of the flux-flow Hall effect baed on the augmented quasiclassical equations*

1. Charging in a Superconducting Vortex Due to the Three Force Terms in Augmented Eilenberger Equations
   Hikaru Ueki, Marie Ohuchi, and Takafumi Kita: J. Phys. Soc. Jpn. **87** (2018) 044704.
2. A Variational Approach to Many-Body Problems Incorporating Many-Body Effects at Finite Temperature
   Akimitsu Kirikoshi, Wataru Kohno, and Takafumi Kita: J. Phys. Soc. Jpn., in press.

KITAO, Akio [C class; 5500 (B), 900 (C)] (235)
— *Efficient sampling simulation of the soft modes significantly contribute to protein properties*

1. Dissociation Process of a MDM2/p53 Complex Investigated by Parallel Cascade Selection Molecular Dynamics and the Markov State Model
   D.P. Duy and A. Kitao: J. Phys. Chem. B, **123** (2019) 2469.
2. Refining evERdock: Improved selection of good protein-protein complex models achieved by MD optimization and use of multiple conformations
   A. Shinobu, K. Takemura, N. Matubayasi, and A Kitao: J. Chem. Phys., **149** (2018) 195101.
3. Similarities and Differences between Thymine (6–4) Thymine/Cytosine DNA Lesion Repairs by Photolyases
   H.M. Dokainish and A. Kitao: J. Phys. Chem. B, **122** (2018) 8537.

4. ColDock: Concentrated Ligand Docking with All-Atom Molecular Dynamics Simulation
K. Takemura, C. Sato, and A. Kitao: J. Phys. Chem. B, **122** (2018) 7191.

KOBAYASHI, Katsuyoshi [B class; 400 (B), 50 (C)] (163)
— *Study on electronic properties in new nanoscale surfaces and interfaces*

KOBAYASHI, Nobuhiko [C class; 4500 (B), 800 (C)] (84)
— *First-principles study of quantum transport in nanostructures*

1. Theory of electron transport at the atomistic level
N. Kobayashi, H. Ishii, K. Hirose: Jpn. J. Appl. Phys. 57, 08NA01 (2018).
2. Computational Study on Atomic Structures, Electronic Properties, and Chemical Reactions at Surfaces and Interfaces and in Biomaterials
Y. Takano, N. Kobayashi, Y. Morikawa: J. Phys. Soc. Jpn. 87, 061013 (2018).
3. Quantitative mobility evaluation of organic semiconductors using quantum dynamics based on density functional theory
H. Ishii, J. Inoue, N. Kobayashi, K. Hirose: Phys. Rev. B 98, 235422 (2018).
4. Surface Structure of Organic Semiconductor [n]Phenacene Single Crystals
Y. Wakabayashi, M. Nakamura, K. Sasaki, T. Maeda, Y. Kishi, H. Ishii, N. Kobayashi, S. Yanagisawa, Y. Shimo, Y. Kubozono: J. Am. Chem. Soc. 140, 14046 (2018).
5. Operando Direct Observation of Charge Accumulation and the Correlation with Performance Deterioration in PTB7 Polymer Solar Cells
T. Kubodera, M. Yabusaki, V. Rachmat, Y. Cho, T. Yamanari, Y. Yoshida, N. Kobayashi, K. Marumoto: ACS Appl. Mater. Interfaces 10, 26434 (2018).
6. Theory of Electrical Conduction
N. Kobayashi, H. Ishii, K. Hirose: 3D Local Structure and Functionality Design of Materials eds H. Daimon, Y. C. Sasaki (World Scientific, 2018) p133.

KOGA, Akihisa [C class; 8000 (B), 1450 (C)] (180)
— *Competition between superconductivity and orbital order emerging in strongly correlated electron systems*
— *Stability of magnetic phases in strongly correlated electron systems with various electron filling*

1. Quantum and classical behavior of spin-S Kitaev models in an anisotropic limit
T. Minakawa, J. Nasu, and A. Koga, Phys. Rev. B 99, 104408/1-8 (2019)
2. Staggered ordered phases in the three-orbital Hubbard model
K. Ishigaki, J. Nasu, A. Koga, S. Hoshino, and P. Werner, Phys. Rev. B 99, 085131/1-11 (2019)
3. Symmetry breaking states in the half-filled two-orbital Hubbard model with crystalline electric field
K. Ishigaki, J. Nasu, and A. Koga, J. Phys. Soc. Jpn. 88, 024702/1-5 (2019)
4. Spontaneously orbital-selective superconductivity in a three-orbital Hubbard model
K. Ishigaki, J. Nasu, A. Koga, S. Hoshino, and P. Werner, Phys. Rev. B 98, 235120/1-7 (2018)
5. Incipient and well-developed entropy plateaus in spin-S Kitaev models
J. Oitmaa, A. Koga, and R. R. P. Singh, Phys. Rev. B 98, 214404/1-6 (2018)
6. Successive Majorana Topological Transitions Driven by a Magnetic Field in the Kitaev Model
J. Nasu, Y. Kato, Y. Kamiya, and Y. Motome, Phys. Rev. B 98, 060416/1-6 (2018)
7. Majorana quantization and half-integer thermal quantum Hall effect in a Kitaev spin liquid
Y. Kasahara, T. Ohnishi, Y. Mizukami, O. Tanaka, Sixiao Ma, K. Sugii, N. Kurita, H. Tanaka, J. Nasu, Y. Motome, T. Shibauchi, and Y. Matsuda, Nature 559, 227-231 (2018)
8. Unusual Thermal Hall Effect in a Kitaev Spin Liquid Candidate α-RuCl3
Y. Kasahara, K. Sugii, T. Ohnishi, M. Shimozawa, M. Yamashita, N. Kurita, H. Tanaka, J. Nasu, Y. Motome, T. Shibauchi, and Y. Matsuda, Phys. Rev. Lett. 120, 217205/1-6 (2018)
9. Magnetoelectric Effect in a Spin-State Transition System
M. Naka, E. Mizoguchi, J. Nasu, and S. Ishihara, J. Phys. Soc. Jpn. 87, 063709/1-5 (2018)
10. Ground-state and thermodynamic properties of an S=1 Kitaev model
A. Koga, H. Tomishige, and J. Nasu, J. Phys. Soc. Jpn. 87, 063703 (2018)

KOMATSU, Yu [B class; 600 (B), 90 (C)] (298)
— *Constructing the database of exited states for desigining photosynthetic pigments to absorb the longer wavelength radiation*

KOURA, Akihide [C class; 4000 (B), 0 (C)] (103)
— *Ab initio molecular dynamics study of static structure of glasses*
1. Peculiar atomic dynamics in liquid GeTe with asymmetrical bonding: Observation by inelastic x-ray scattering
   M. Inui, A. Koura, Y. Kajihara, S. Hosokawa, A. Chiba, K. Kimura, F. Shimojo, S. Tsutsui, and A. Q. R. Baron: Phys. Rev. B **97**, (2018) 174203.
2. Static Structure of Liquid GeSe Under Pressure: *Ab Initio* Molecular Dynamics Simulations
   A. Koura and F. Shimojo: Phys. Status Solidi B **255** (2018) 1800103.
3. Electronic structures and impurity cluster features in Mg-Zn-Y alloys with a synchronized long-period stacking ordered phase
   S. Hosokawa, K. Maruyama, K. Kobayashi, J. R. Stellhorn, B. Paulus, A. Koura, F. Shimojo, T. Tsumuraya, M. Yamasaki, Y. Kawamura, S. Yoshioka, and H. Sato: J. Alloys Compd. **762** (2018) 797.

KUNISADA, Yuji [C class; 10500 (B), 0 (C)] (55)
— *Reduction of Rare Metals in Formic Acid Decomposition Catalysts and Oxygen Storage Materials*
1. Sr Substitution Effects on Atomic and Local Electronic Structure of $Ca_2AlMnO_{5+\delta}$
   Y. Kunisada, G. Saito, K. Hayami, T. Nomura, N. Sakaguchi: Surf. Inter. Anal. **51** (2019) 65.
2. Interaction of Localized Surface Plasmons of a Silver Nanosphere Dimer Embedded in a Uniform Medium: STEM-EELS and DDA Simulation
   N. Sakaguchi, S. Matsumoto, Y. Kunisada, M. Ueda: J. Phys. Chem. C **123** (2019) 6735.

KUROKI, Kazuhiko [C class; 11500 (B), 1800 (C)] (179)
— *First principles and model study of electron correlation and superconductivity in multiband systems*
— *Numerical study on unconventional superconductivity in bilayer strongly correlated systems*
1. Effective interaction for vanadium oxyhydrides $Sr_{n+1}V_nO_{2n+1}H_n$ ($n = 1$ and $n \to \infty$): A constrained-RPA study
   M. Ochi, K. Kuroki: Phys. Rev. B. **99** (2019) 155143.

KUSAKABE, Koichi [C class; 3000 (B), 0 (C)] (124)
— *Theoretical analysis of dynamical effects of nanographene*
1. Edge States Caused by Shift of Dirac Points at the Armchair Edge of Distorted nanographene
   K. Kusakabe, K. Nishiguchi, S. Teranishi, Y. Wicaksono: J. Phys. Soc. Jpn. **87** (2018) 084716.
2. Tunable induced magnetic moment and in-planeconductance of graphene in Ni/Graphene/Ni nano spin-valve like structure: a first principles study
   Y. Wicaksono, S. Teranishi, K. Nishiguchi, K. Kusakabe: CARBON **143** (2018) 828.
3. Supercondictivity arising from layer- differen- tiation in multi-layer cuprates with inter-layer effects
   K. Nishiguchi, S. Teranishi, K. Kusakabe, H. Aoki: Phys. Rev. B **98** (2018) 174508.
4. Material-dependent screening of Coulomb interaction in single-layer cuprates
   S. Teranishi, K. Nishiguchi, K. Kusakabe: J. Phys. Soc. Jpn. **87** (2018) 114701.
5. ナノグラファイトの構造と電子状態の関係：トポロジカル物性の予測
   草部浩一: ニューダイヤモンド **35** (2018) 38.

MACHIDA, Manabu [B class; 600 (B), 0 (C)] ()
— *Optical properties of random media*

MAKINO, Takayuki [B,C class; 1000 (B), 420 (C)] (138)
— *Study on electronic structures in Yb2O3 crystals*
— *Study on optical transition and density of states in Yb2O3*
1. Temperature Dependent Localization Dynamics of Excitons in MgZnO Alloyed Semiconductor
   Md. Sherajul Islam, Md. Soyaeb Hasan, E. Kobayashi, T. Makino: Physica B 558, 127 (2019)

MAO, Wei [C class; 4000 (B), 750 (C)] ()
— *First-principles calculation of microscopic behaviors of hydrogen in metal oxides for tritium permeation barrier*

MASAKI-KATO, Akiko [C class; 6000 (B), 950 (C)] ()
— *Study of excitation dynamics of Heisenberg models*

MATSUDA, Yasuhiro [B class; 500 (B), 70 (C)] (304)
— *Estimation of the density of states using Maximum entropy method and Sparse modeling*

MATSUKAWA, Hiroshi [C class; 2000 (B), 550 (C)] ()
— *Physics of Friction*

MATSUMOTO, Munehisa [C class; 11000 (B), 1350 (C)] (233)
— *Bridging space-time scales via coarse grained Green's function and reverse Monte Carlo between microscopic electronic structure and macroscopic observation*
— *Integration of ab initio data of microscopic electronic structure and experimental data of mesoscopic domain structure for ferromagnetic f-d intermetallics*

1. First-principles calculations of the magnetocrystalline anisotropy of the prototype 2:17 cell boundary phase $Y(Co_{1-x-y}Fe_xCu_y)_5$
   Christopher E. Patrick, Munehisa Matsumoto, Julie B. Staunton: Journal of Magnetism and Magnetic Materials 477 (2019) 147.
2. Calculated Curie temperatures for rare-earth permanent magnets: *ab initio* inspection on localized magnetic moments in *d*-electron ferromagnetism
   preprint (arXiv: 1812.04842)
3. Site preference of dopant elements in $Nd_2Fe_{14}B$
   Munehisa Matsumoto: preprint (arXiv: 1812.10945)
4. Navigating the trends in the proximity to magnetic quantum critical point and superconductivity for Ce-based heavy-fermion compounds
   Munehisa Matsumoto: preprint (arXiv: 1812.11502)
5. Optimal uni-axial ferromagnetism in (La,Ce)2Fe14B for permanent magnets
   Munehisa Matsumoto, Masaaki Ito, Noritsugu Sakuma, Masao Yano, Tetsuya Shoji, Hisazumi Akai: preprint (arXiv: 1901.10119)
6. Anisotropic ferromagnetism and structure stability in $4f$-$3d$ intermetallics: *ab initio* structure optimization and magnetic anisotropy for RCo_5 (R=Ce, La, and Y)
   Munehisa Matsumoto: preprint (arXiv: 1901.11498)
7. Electronic Structure Calculations of $CeRh_3B_2$
   Shotaro Doi and Munehisa Matsumoto: preprint (arXiv: 1903.08480)

MATSUNAKA, Daisuke [B class; 600 (B), 0 (C)] (158)
— *First-principles Study of Defects of Magnesium Alloys*

1. EAM ポテンシャルにおける異種原子間相互作用の検討
   小細浩輔, 藤岡芳弥, 吉川創, 松中大介: 計算工学講演論文集, **24** (2019) A-03-04.
2. Molecular Dynamics Simulation on Defect Nucleation from Pre-existing I1 Stacking Fault in Magnesium
   S. Yoshikawa and D. Matsunaka: to be submitted.

MATSUSHITA, Katsuyoshi [C class; 1000 (B), 600 (C)] (276)
— *Numerical Analysis of Instability in Motion of Crowding Cellular Tissue*
— *Numerical study of collective motion transition of crowding cells with anisotropic shape.*

1. Katsuyoshi Matsushita, Emergence of collective propulsion through cell-cell adhesion
   Physical Review E: 97 (2018) 042413
2. Cell Migration driven by Receptor Density Polarity of Cell-Matrix Adhesion
   Katsuyoshi Matsushita, Kazuya Horibe, Naoya Kamamoto and Koichi Fujimoto, Proceedings of

the Symposium on Simulation of Traffic Flow 24, (2018) 5

MAYUMI, Koichi [B class; 600 (B), 80 (C)] (301)
— *Study on Dynamics of Ring and Axial Molecules of Slide-Ring Gel Under Deformation*

1. Sliding Dynamics of Ring on Polymer in Rotaxane: a Coarse-Grained Molecular Dynamics Simulation Study.
   Y. Yasuda, M. Toda, K. Mayumi, H. Yokoyama, H. Morita, and K. Ito: accepted.
2. Molecular Dynamics of Polyrotaxane in Solution Investigated by Quasi-Elastic Neutron Scattering and Molecular Dynamics Simulation: Sliding Motion of Rings on Polymer.
   Y. Yasuda, Y. Hidaka, K. Mayumi, T. Yamada, K. Fujimoto, S. Okazaki, H. Yokoyama, and K. Ito, submitted.

MISAWA, Masaaki [B class; 700 (B), 0 (C)] (150)
— *Molecular dynamics study on pressure-induced transformation of silicates*

MISAWA, Takahiro [E class; 14500 (B), 2500 (C)] (15)
— *Superconductivity and quantum spin liquid in multi-orbital systems with inverted Hund's rule coupling*

1. Ab initio effective Hamiltonians for cuprate superconductors
   Motoaki Hirayama, Youhei Yamaji, Takahiro Misawa, and Masatoshi Imada: Phys. Rev. B **98**, 134501 (2018).
2. mVMC - Open-source software for many-variable variational Monte Carlo method
   Takahiro Misawa, Satoshi Morita, Kazuyoshi Yoshimi, Mitsuaki Kawamura, Yuichi Motoyama, Kota Ido, Takahiro Ohgore, Masatoshi Imada, and Takeo Kato :Comput. Phys. Commun. **235**, 447 (2019).

MIYASHITA, Seiji [C class; 6000 (B), 950 (C)] (223)
— *Manipulation of quantum state by external fields*

1. Optical bistability in a low-photon-density regime
   Tatsuhiko Shirai, Synge Todo, Hans de Raedt, and Seiji Miyashita:Phys. Rev. A **98**, 043802 (2018).
2. Mechanism for subgap optical conductivity in honeycomb Kitaev materials
   A. Bolens, H. Katsura, M. Ogata, and S. Miyashita:Phys. Rev. B**97**, 161108 (R), (1-5) (2018)
3. Exploration of the effects of dipole-dipole interactions in $Nd_2Fe_{14}B$ thin films based on a stochastic cutoff method with a novel efficient algorithm,
   T. Hinokihara, M. Nishino, Y. Toga, and S. Miyashita:Phys. Rev. B**97**, 104427(1-8) (2018)
4. Anisotropy of exchange stiffness based on atomic-scale magnetic properties in the rare-earth permanent magnet $Nd_2Fe_{14}B$
   Yuta Toga, Masamichi Nishino, Seiji Miyashita, Takashi Miyake, and Akimasa Sakuma: Phys. Rev. B**98**, 054418 (2018).

MIZUGUCHI, Tomoko [C class; 2500 (B), 0 (C)] (265)
— *Effect of interface on the dynamics of water confined in mesoporous silica*

1. Hydrogen bond analysis of confined water in mesoporous silica using the reactive force field
   T. Mizuguchi, K. Hagita, S. Fujiwara and T. Yamada: submitted to Mol. Sim.

MIZUKAMI, Wataru [C class; 2000 (B), 0 (C)] (125)
— *Exploration of surface reactions on model real catalyst*

MOMIDA, Hiroyoshi [C class; 3000 (B), 500 (C)] (113)
— *Theoretical design of energy harvesting and storage device materials by first-principles calculations*

1. First-Principles Study on Cathode Properties of Li_2MTiO_4 (M = V, Cr, Mn, Fe, Co, and Ni) with Oxygen Deficiencies for Li-Ion Batteries
   M. Hamaguchi, H. Momida, and T. Oguchi, J. Phys. Soc. Jpn. **87**, 044805 (2018).
2. Elucidation of Discharge Mechanism and Evaluation of Na-Ion Battery Performance of Tin Sulfide (SnS) Electrode by using First-Principles Calculation

H. Kotaka, H. Momida, A. Kitajou, S. Okada, and T. Oguchi, J. Comput. Chem. Jpn. **18**, 78 (2019).

3. First-Principles Study of Na-Ion Battery Performance and Reaction Mechanism of Tin Sulfide as Negative Electrode
   H. Kotaka, H. Momida, A. Kitajou, S. Okada, and T. Oguchi, Chem. Rec. (2019) in press.

MORI, Takashi [C class; 3000 (B), 0 (C)] (261)
— *Semiclassical dynamics of quantum spin systems*

1. Prethermalization in the transverse-field Ising chain with long-range interactions
   T. Mori: J. Phys. A **52**, 054001 (2019).

MORIKAWA, Yoshitada [C class; 2500 (B), 900 (C)] (114)
— *First-principles Thermodynamics and Statistical Mechanics Simulations of Catalytic Reactions at Solid Surfaces*

1. A New Pentacene Polymorph Induced by Interaction with a Bi(0001) Substrate
   T. Shirasawa, S. Yanagisawa, S. Hatada, W. Voegeli, Y. Morikawa, and T. Takahashi: J. Phys. Chem. C **122** (2018) 6240.
2. Platinum-catalyzed hydrolysis etching of SiC in water: A density functional theory study
   P. V. Bui, D. Toh, A. Isohashi, S. Matsuyama, K. Inagaki, Y. Sano, K. Yamauchi, and Y. Morikawa: Jpn. J. Appl. Phys. **57** (2018) 055703.
3. Computational Study on Atomic Structures, Electronic Properties, and Chemical Reactions at Surfaces and Interfaces and in Biomaterials
   Y. Takano, N. Kobayashi, and Y. Morikawa: J. Phys. Soc. Jpn. **87** (2018) 061013.
4. Hydrogen-bond Induced Nitric Oxide Dissociation on Cu(110)
   T. N. Pham, M. Sugiyama, F. Muttaqien, S. E. M. Putra, K. Inagaki, D. N. Son, Y. Hamamoto, I. Hamada, and Y. Morikawa: J. Phys. Chem. C **122** (2018) 11814.
5. Enhancement of CO_2 adsorption on oxygen-functionalized epitaxial graphene surface under near-ambient conditions
   S. Yamamoto, K. Takeuchi, Y. Hamamoto, R. Liu, Y. Shiozawa, T. Koitaya, T. Someya, K. Tashima , H. Fukidome, K. Mukai, S. Yoshimoto, M. Suemitsu, Y. Morikawa, J. Yoshinobu, and I. Matsuda: Phys. Chem. Chem. Phys. **20** (2018)19532.
6. Diffusion mechanism of Na ionpolaron complex in potential cathode materials $NaVOPO_4$ and $VOPO_4$ for rechargeable sodium-ion batteries
   H. D. Luong, T. D. Pham, Y. Morikawa, Y. Shibutani, and V. A. Dinh: Phys. Chem. Chem. Phys., **20** (2018) 23625.
7. Effects of Surface Termination and Layer Thickness on Electronic Structures of $LaNiO_3$ Thin Films
   H. D. Nguyen, B. T. Cong, and Y. Morikawa: J. Phys. Soc. Jpn. **87** (2018) 114704.
8. First-principles study of polar, nonpolar, and semipolar GaN surfaces during oxide vapor phase epitaxy growth
   T. Kawamura*, A. Kitamoto, M. Imade, M. Yoshimura, Y. Mori, Y. Morikawa, Y. Kangawa, K. Kakimoto, and T. Akiyama: Jpn. J. Appl. Phys. **57** (2018) 115504.
9. Platinum Single-atom Adsorption on Graphene: A Density Functional Theory Study
   S. A. Wella, Y. Hamamoto, Suprijadi, Y. Morikawa, and I. Hamada: Nanoscale Adv. **1** (2019) 1165.
10. Experimental and Computational Studies on Ruthenium(II) Bis-diimine Complexes of N,N'-Chelate Ligand: The Origin of the Change in the Absorption Spectra upon Oxidation and Reduction
    S. S. Tan, S. Yanagisawa, K. Inagaki, M. B. Kassim and Y. Morikawa: Phys. Chem. Chem. Phys. **21** (2019) 7973.
11. Van der Waals Density Functional Study of Formic Acid Adsorption and Decomposition on Cu(111)
    S. E. M. Putra, F. Muttaqien, Y. Hamamoto, K. Inagaki, I. Hamada, and Y. Morikawa: J. Chem. Phys. **150** (2019) 154707.

MORIMOTO, Kenichi [C class; 2000 (B), 0 (C)] ()
— *RANS-LES Hybrid Analysis of Turbulent Heat Transfer*

MORITA, Satoshi [B class; 700 (B), 90 (C)] (290)
— *Quantum many-body problem solver with tensor network methods*

1. Calculation of higher-order moments by higher-order tensor renormalization group
   S. Morita and N. Kawashima: Comput. Phys. Commun. **236**, 6571 (2019).
2. Detecting signals of weakly first-order phase transitions in two-dimensional Potts models
   S. Iino, S. Morita, N. Kawashima, and A. W. Sandvik: J. Phys. Soc. Jpn. **88**, 034006 (2019).
3. Fast Algorithm for Generating Random Bit Strings and Multispin Coding for Directed Percolation
   H. Watanabe, S. Morita, S. Todo, and N. Kawashima: J. Phys. Soc. Jpn. **80**, 024004 (2019).

MOTOME, Yukitoshi [C,D class; 16000 (B), 1950 (C)] (173)
— *Dynamics of Majorana particles in Kitaev spin liquids in a magnetic field*
— *Numerical study on novel quantum phenomena in spin-orbit coupled materials*
— *Numerical study on quantum magnetism in spin-orbit coupled materials*

1. Unusual Thermal Hall Effect in a Kitaev Spin Liquid Candidate α-$RuCl_3$
   Y. Kasahara, K. Sugii, T. Ohnishi, M. Shimozawa, M. Yamashita, N. Kurita, H. Tanaka, J. Nasu, Y. Motome, T. Shibauchi, and Y. Matsuda: Phys. Rev. Lett. **120** (2018) 217205.
2. Nonreciprocal spin Seebeck effect in antiferromagnets
   R. Takashima, Y. Shiomi, and Y. Motome: Phys. Rev. B **98** (2018) 020401(R).
3. Majorana quantization and half-integer thermal quantum Hall effect in a Kitaev spin liquid
   Y. Kasahara, T. Ohnishi, Y. Mizukami, O. Tanaka, Sixiao Ma, K. Sugii, N. Kurita, H. Tanaka, J. Nasu, Y. Motome, T. Shibauchi, and Y. Matsuda: Nature **559** (2018) 227.
4. Successive Majorana topological transitions driven by a magnetic field in the Kitaev model
   J. Nasu, Y. Kato, Y. Kamiya, and Y. Motome: Phys. Rev. B **98** (2018) 060416(R).
5. Néel and Bloch-Type Magnetic Vortices in Rashba Metals
   S. Hayami and Y. Motome: Phys. Rev. Lett. **121** (2018) 137202.
6. Magnetic structural unit with convex geometry: A building block hosting an exchange-striction-driven magnetoelectric coupling
   K. Kimura, Y. Kato, K. Yamauchi, A. Miyake, M. Tokunaga, A. Matsuo, K. Kindo, M. Akaki, M. Hagiwara, S. Kimura, M. Toyoda, Y. Motome, and T. Kimura: Phys. Rev. Materials **2** (2018) 104415.
7. Multiple-Q magnetic orders in Rashba-Dresselhaus metals
   K. N. Okada, Y. Kato, and Y. Motome: Phys. Rev. B **98** (2018) 224406.
8. Band crossings in honeycomb-layered transition metal compounds
   Y. Sugita and Y. Motome: Phys. Rev. B **99** (2019) 041101(R).
9. Magnetoelectric behavior from cluster multipoles in square cupolas: Study of $Sr(TiO)Cu_4(PO_4)_4$ in comparison with Ba and Pb isostructurals
   Y. Kato, K. Kimura, A. Miyake, M. Tokunaga, A. Matsuo, K. Kindo, M. Akaki, M. Hagiwara, S. Kimura, T. Kimura, and Y. Motome: Phys. Rev. B **99** (2019) 024415.
10. Effect of magnetic anisotropy on skyrmions with a high topological number in itinerant magnets
    S. Hayami and Y. Motome: Phys. Rev. B **99** (2019) 094420.
11. Antiferromagnetic Kitaev Interaction in f-Electron Based Honeycomb Magnets
    S.-H. Jang, R. Sano, Y. Kato, and Y. Motome: preprint (arXiv:1807.01443), submitted to Phys. Rev. B.
12. Magnetoelectric effect in band insulator-ferromagnet heterostructures
    K. N. Okada, Y. Kato, and, Y. Motome: preprint (arXiv:1902.04204), accepted for the publication in Phys. Rev. B.
13. Spin-current diode with a monoaxial chiral magnet
    S. Okumura, H. Ishizuka, Y. Kato, J. Ohe, and Y. Motome: preprint (arXiv:1903.12358), submitted to Appl. Phys. Lett.

MOTOYAMA, Yuichi [B class; 800 (B), 100 (C)] (199)
— *Drawing phase diagram from many-variable variational wave functions with machine learning*

MURASHIMA, Takahiro [E class; 20000 (B), 3000 (C)] (209)
— *Numerical analysis of non-equilibrium dynamics of polymeric liquid*

1. Elongational Viscosity of Weakly Entangled Polymer Melt via Coarse-Grained Molecular Dynamics Simulation
   T. Murashima, K. Hagita, T. Kawakatsu: J. Soc. Rheol. Jpn. **46** (2018) 207.
2. Coupling Finite Element Method with Large Scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) for Hierarchical Multiscale Simulations
   T. Murashima, S. Urata, S. Li: arXiv:1902.09171, submitted to EPJB.

NADA, Hiroki [B,C class; 4000 (B), 90 (C)] (256,257)
— *Analysis of Formation Mechanism of Calcium Phosphate Crystal by Large-Scale Molecular Dynamics Simulation Combined with Metadynamics Method*
— *Large-Scale Molecular Dynamics Simulation Study on the Crystallization Mechanism of Water Including Air Molecules*

1. A New Methodology for Evaluating the Structural Similarity Between Different Phases Using a Dimensionality Reduction Technique
   H. Nada: ACS Omega, **3** (2018) 5789.
2. Computer Simulations: Essential Tools for Crystal Growth Studies
   H. Nada: Crystals, **8** (2018) 314.
3. Shock Growth of Ice Crystals Near Equilibrium Melting Pressure Under Dynamic Compression
   Y.-J. Kim, Y.-H. Lee, S. Lee, H. Nada and G. W. Lee: Proc. Natl. Acad. Sci. U.S.A., in press.
4. Anisotropy in Stable Conformations of Hydroxylate Ions Between the 001 and 110 Planes of TiO_2 Rutile Crystals for Glycolate, Lactate, and 2-Hydroxybutyrate Ions Studied by Metadynamics Method
   H. Nada, M. Kobayashi and M. Kakihana: submitted to ACS Omega.

NAKAHARA, Akio [B class; 700 (B), 90 (C)] ()
— *Numerical simulation for memory effect in paste of flow and vibration*

NAKAMURA, Kazuma [C class; 4500 (B), 0 (C)] (96,335)
— *Ab initio derivation of effective low-energy model for excitonic insulator Ta2NiSe5*
— *Development of ab initio many-body perturbation calculation software RESPACK*

1. Hydrostatic pressure effects on superconducting transition of nanostructured niobium highly strained by high-pressure torsion
   M. Mito, Y. Kitamura, T. Tajiri, K. Nakamura, R. Shiraishi, K. Ogata, H. Deguchi, T. Yamaguchi, N. Takeshita, T. Nishizaki, K. Edalati, Z. Horita: J. Appl. Phys. **125**, (2019) 125901.

NAKANO, Hiroki [C class; 4500 (B), 1100 (C)] (240)
— *Numerical study on low-energy states of quantum spin systems*

1. Impact of Dzyaloshinskii-Moriya Interactions and Tilts of g Tensors on the Magnetization of a Spherical Kagome Cluster in $\{W_{72}V_{30}\}$
   Y. Fukumoto, Y. Yokoyama, and H. Nakano: J. Phys. Soc. Jpn. **87** (2018) 124710(1-6)
2. Third Boundary of the Shastry-Sutherland Model by Numerical Diagonalization
   H. Nakano and T. Sakai: J. Phys. Soc. Jpn. **87** (2018) 123702(1-5)
3. Precise Estimation of the $S = 2$ Haldane Gap by Numerical Diagonalization
   H. Nakano and T. Sakai: J. Phys. Soc. Jpn. **87** (2018) 105002(1-2)
4. Numerical-Diagonalization Study of Magnetization Process of Frustrated Spin-1/2 Heisenberg Antiferromagnets in Two Dimensions: – Triangular- and Kagome-Lattice Antiferromagnets–
   H. Nakano and T. Sakai: J. Phys. Soc. Jpn. **87** (2018) 063706(1-5)
5. Metamagnetic jump in the spin-1/2 antiferromagnetic Heisenberg model on the square kagome lattice
   Y. Hasegawa, H. Nakano, and T. Sakai: Phys. Rev. B **98** (2018) 014404(1-9)
6. Ground state with nonzero spontaneous magnetization of the two-dimensional spin-1/2 Heisenberg antiferromagnet with frustration

T. Sakai and H. Nakano: AIP Adv. **8** (2018) 101408(1-5)

7. Gapless spin excitations in the S=1/2 Kagome- and triangular-lattice Heisenberg antiferromagnets
   T. Sakai and H. Nakano: Physica B **536** (2018) 85-88
8. Spontaneous Magnetization of the Spin-1/2 Heisenberg Antiferromagnet on the Triangular Lattice with a Distortion
   A. Shimada, T. Sakai, H. Nakano, and K. Yoshimura: J. Phys.: Conf. Series **969** (2018) 012126(1-6)
9. Quantum Spin Fluid Behaviors of the Kagome- and Triangular-Lattice Antiferromagnets
   T. Sakai and H. Nakano: J. Phys.: Conf. Series **969** (2018) 012127(1-6)

NAKAYAMA, Takashi [C class; 5500 (B), 950 (C)] (73)

— First-principles study of ionization and diffusion of metal atoms at metal/solid interfaces in electric fields: toward semiconductor and organic substrates

1. Physics of Fermi-Level "Unpinning" at Metal/Ge Interfaces; First-Principles View
   T. Nakayama, T. Nishimoto: ECS Transactions **86** (2018) 291.
2. Structural and Charging Stability of Metal Nanodot Memory in SiO2; First-Principles Study
   T. Nakayama, S. Yamazaki, Y. Shiraishi: ECS Transactions **86** (2018) 69.
3. Metal-atom penetration and diffusion in organic solids: difference between sigma- and pai- orbital molecular systems
   S. Watanabe, T. Nakayama: Jpn. J. Appl. Phys. (2019) in press.

NISHIDATE, Kazume [C class; 1500 (B), 0 (C)] (135)

— Density functional calculations of the catalytic site of fuel cell and photocatalyst

1. Oxygen reduction reaction of FeN_4 center embedded in graphene and carbon nanotube: Density functional calculations
   S. Aoyama, J. Kaiwa, P. Chantngarm, S. Tanibayashi, H. Saito, M. Hasegawa, and K. Nishidate: AIP Advances **8** (2018) 115113.

NISHIGUCHI, Kazutaka [B class; 500 (B), 0 (C)] (306)

— Theoretical study for superconductivity in multilayer cuprates with two-particle self-consistent approach

1. Superconductivity arising from layer differentiation in multilayer cuprates
   K. Nishiguchi, S. Teranishi, K. Kusakabe, and H. Aoki: Phys. Rev. B **98** (2018) 174508.

NOGUCHI, Hiroshi [C class; 13000 (B), 1900 (C)] (210)

— structure formation of biomembranes

1. Angular-momentum conservation in discretization of the Navier-Stokes equation for viscous fluids
   H. Noguchi: Phys. Rev. E **99**, 023307 (2019).
2. Limiting shapes of confined lipid vesicles
   B. Kavčič, A. Sakashita, H. Noguchi, and P. Ziherl: Soft Matter **15**, 602 (2019).

NOGUCHI, Yoshifumi [C class; 6000 (B), 950 (C)] (68)

— XPS simulation using self-consistent GW method

1. Optical properties of six isomers of three dimensionally delocalized π-conjugated carbon nanocage
   Y. Noguchi, D. Hirose, and O. Sugino: Eur. Phys. J. B **91** (2018) 125.a

NOMURA, Yusuke [C class; 10500 (B), 1700 (C)] (185)

— Development of machine-learning solvers for Hamiltonians with electron-phonon interactions

— Implementation and application of multi-orbital TRILEX -a new method to bridge weak-coupling and strong coupling methods-

1. Stripe and superconducting order competing in the Hubbard model on a square lattice studied by a combined variational Monte Carlo and tensor network method
   Andrew S. Darmawan, Yusuke Nomura, Youhei Yamaji, and Masatoshi Imada: Phys. Rev. B **98** (2018) 205132.
2. Constructing exact representations of quantum many-body systems with deep neural networks

Giuseppe Carleo, Yusuke Nomura, and Masatoshi Imada: Nat. Commun. **9** (2018) 5322.

NUGRAHA, Ahmad Ridwan Tresna [B class; 200 (B), 30 (C)] (164)
— *Coherent phonon spectroscopy of atomic layer materials*

OBATA, Masao [C class; 3000 (B), 300 (C)] (116)
— *Analysis on atomic and magnetic structure in magnetic molecular complex, crystal and interface and investigation of electron correlation effect*
— *Analysis on atomic structure in magnetic molecular complex, crystal and interface using spin dependent van der Waals density functional and investigation of electron correlation effect*

1. Implementation of Magnetic Dipole Interaction in the Planewave-Basis Approach for Slab Systems
   T. Oda and M. Obata: J. Phys. Soc. Jpn. **87** (2018) 064803.
2. A Comprehensive Study of Sign Change in Electric Field Control Perpendicular Magnetic Anisotropy Energy at Fe/MgO Interface: First Principles Calculation
   I. Pardede, T. Kanagawa, N. Ikhsan, I. Murata, D. Yoshikawa, M. Obata, and T. Oda: IEEE Transactions on Magnetics **55**, (2018) 1700104.
3. Investigation of magnetic dipole-dipole interaction using magnetic density on solid oxygen based on first-principles approach
   M. Obata, M. Christivana, and T. Oda: AIP Advances **8** (2018) 101419.
4. Shape Magnetic Anisotropy From Spin Density in Nanoscal Slab Systems
   T. Oda, I. Pardede, T. Kanagawa, N. Ikhsan, D. Yoshikawa, and M. Obata: IEEE Transactions on Magnetics **55**, (2018) 1300104.
5. Noncollinear magnetic structure with spin-dependent van der Waals density functional approach: β-phase solid oxygen
   M. Christivana, M. Obata, and T. Oda: submitted to J. Phys. Soc. Jpn.

ODA, Masato [C class; 2500 (B), 600 (C)] (119)
— *Modulation of phonon modes originate from impurities in GaN*

1. Investigation of the electronphonon interactions around Ga vacancies in GaN and their role in the first stage of defect reactions
   M. Oda: Jpn. J. Appl. Phys., in press

ODA, Tatsuki [E class; 28500 (B), 4650 (C)] (46,48)
— *Analyses on atomic, magnetic, and electronic structures in high-performance spintronics materials*
— *Analyses on magnetic and electronic structures in high-performance spintronics materials*

1. Implementation of magnetic dipole interaction in the planewave-basis approach for slab systems
   Tatsuki Oda and Masao Obata: Journal of the Physical Society of Japan, 87, 064803 (2018)
2. A comprehensive Study of Sign Change in Electric Field Control Perpendicular Magnetic Anisotropy Energy at Fe/MgO Interface: First Principles Calculation
   Indra Pardede, Tomosato Kanagawa, Nurul Ikhsan, Itsuki Murata, Daiki Yoshikawa, Masao Obata, and Tatsuki Oda: IEEE Transactions on Magnetics, 55, 1700104 (2018)
3. Ab Initio study of martensitic transition in Ni2MnGa
   T. Koubský, P. Sedlák, H. Seiner, Jaroslava Fojtíková, Masao Obata, Tatsuki Oda, and Ladislav Kalvoda: ACTA PHYSICA POLONICA A, 134, 804 (2018)
4. Shape Magnetic Anisotropy from Spin Density in Nanoscale Slab Systems
   Tatsuki Oda, Indra Pardede, Tomosato Kanagawa, Nurul Ikhsan, Daiki Yoshikawa, and Masao Obata: IEEE Transactions on Magnetics, 55, 1300104 (2018)
5. Perpendicular and in-plane magnetic anisotropies in Cr-buffered Fe(x)/MgO interface from first-principles approach
   Nurul Ikhsan, Tomosato Kanagawa, Indra Pardede, Daiki Yoshikawa, and Tatsuki Oda: The Science Reports of Kanazawa University, 62, 23 (2018)
6. Fermi level smearing effect in the perpendicular interface Fe/MgO magnetic anisotropy
   Nurul Ikhsan, Indra Pardede, Tomosato Kanagawa, Daiki Yoshikawa, and Tatsuki Oda: The Science Reports of Kanazawa University, 62, 37 (2018)
7. Investigation of magnetic dipole-dipole interaction using magnetic density on solid oxygen based

on first-principles approach
Masao Obata, Mega Christivana, and Tatsuki Oda: AIP Advances, 8, 101419 (2018)

8. Noncollinear magnetic structure with spin-dependent van der Waals density functional approach: β-phase solid oxygen
Mega Christivana, Masao Obata, and Tatsuki Oda: submitted for publication, (2018)
9. Large nonvolatile control of magnetic anisotropy in CoPt/ZnO magnetic tunnel junctions
Muftah Al-Mahdawi, Mohamed Belmoubarik, Masao Obata, Daiki Yoshikawa, Hideyuki Sato, Tomohiro Nozaki, Tatsuki Oda, Masashi Sahashi: submitted for publication, (2018)

OHBA, Tomonori [B class; 700 (B), 0 (C)] (293)
— *Organic Electrolyte Solution in Nanospaces*

1. Anomalous changes of intermolecular distance in aqueous electrolytes in narrow pores of carbon nanotubes
S. M. Khan, S. Faraezi, Y. Oya, K. Hata, T. Ohba: Adsorption, in press.
2. Phase Transition of $S = 1/2$ Heisenberg Antiferomagnet
A. Karatrantos, S. Khan, T. Ohba, Q. Cai: Phys. Chem. Chem. Phys. **20** (2018) 6307.

OHGOE, Takahiro [C class; 10500 (B), 1700 (C)] (239)
— *Development of the diagrammatic Monte Carlo method and its application to cold Fermi gases*
— *Highly accurate numerical analysis of Tan's contact of two-component cold Fermi gases*

1. Diagrammatic Monte Carlo algorithm for the resonant Fermi gas
K. Van Houcke, F. Werner, T. Ohgoe, N.V. Prokof'ev and B. V. Svistunov: Phys. Rev. B **99** (2019) 035140.
2. Contact and Momentum distribution of the Unitary Fermi Gas
R. Rossi, T. Ohgoe, E. Kozik, N. Prokof'ev, B. Svistunov, K. Van Houcke, and F. Werner: Phys. Rev. Lett. **121** (2018) 130406.
3. Resummation of diagrammatic series with zero convergence radius for strongly correlated fermions
R. Rossi, T. Ohgoe, K. Van Houcke, and F. Werner: Phys. Rev. Lett. **121** (2018) 130405.

OHMURA, Satoshi [C class; 3000 (B), 0 (C)] (123)
— *Effects of light elements on transport properties of liquid Fe alloy under ultrahigh pressure condition : ab initio molecular-dynamics simulations*

1. Structural change in liquid sulphur from chain polymeric liquid to atomic simple liquid under high pressure
S Ohmura and F Shimojo: Journal of Physics: Condensed Matter **31** (2019) 215101.
2. Selective reduction mechanism of graphene oxide driven by photon mode versus thermal mode
Hada Masaki, Miyata Kiyoshi, Ohmura Satoshi, Arashida Yusuke, Ichiyanagi Kohei, Katayama Ikufumi, Suzuki Takayuki, Chen Wang, Mizote Shota, Sawa Takayoshi, Yokoya Takayoshi, Seki Toshio, Matsuo Jiro, Tokunaga Tomoharu, Itoh Chihiro, Tsuruta Kenji, Fukaya Ryo, Nozawa Shunsuke, Adachi Shin-ichi, Takeda Jun, Onda Ken, Koshihara Shin-ya, Hayashi Yasuhiko Nishina Yuta: ACS Nano under review

OHNISHI, Masato [C class; 3500 (B), 750 (C)] (98)
— *Analysis of Thermoelectric Properties of Clathrate Compounds with Ab Initio Calculations*

1. Perspective: Towards ultimate impedance of phonon transport by nanostructure interface
Masato Ohnishi, Junichiro Shiomi: APL Materials, 7, 013102 (2019).

OHSAWA, Kazuhito [C class; 1000 (B), 0 (C)] (144)
— *Study of interaction between radiation damage and interstitial atom*

OHTO, Tatsuhiko [C,D class; 9000 (B), 0 (C)] (59,60,61)
— *Ab initio molecular dynamics simulation of doped-graphene/water interfaces*
— *First-principles molecular dynamics simulation of the interface between water and a supramolecular self-assembled monolayer*
— *Interaction between osmolytes in water revealed by ab initio molecular dynamics simulation*

1. Chemical dopants on edge of holey graphene accelerate electrochemical hydrogen evolution reaction
   Akichika Kumatani, Chiho Miura, Hirotaka Kuramochi, Tatsuhiko Ohto, Mitsuru Wakisaka, Yuki Nagata, Hiroki Ida, Yasufumi Takahashi, Kailong Hu, Samuel Jeong, Jun-ichi Fujita, Tomokazu Matsue, Yoshikazu Ito: Adv. Sci. in press.
2. Boosting Electrochemical Water Splitting via Ternary NiMoCo Hybrid Nanowire Arrays
   Kailong Hu, Mingxing Wu, Satoshi Hinokuma, Tatsuhiko Ohto, Mitsuru Wakisaka, Jun-ichi Fujita, and Yoshikazu Ito: J. Mater. Chem. A 7, 2156 (2019)
3. Structure and Dynamics of Water at the Water-Air Interface Using First Principles Molecular Dynamics Simulations within Generalized Gradient Approximation
   Tatsuhiko Ohto, Mayank Dodia, Sho Imoto, and Yuki Nagata: J. Chem. Theory Comput. 15, 595 (2019)
4. Orientational Distribution of Free O-H Groups of Interfacial Water Is Exponential
   Shumei Sun, Fujie Tang, Sho Imoto, Daniel R. Moberg, Tatsuhiko Ohto, Francesco Paesani, Mischa Bonn, Ellen H. G. Backus, and Yuki Nagata: Phys. Rev. Lett. 121, 246101 (2018)
5. Single-molecule rectifiers based on voltage-dependent deformation of molecular orbitals in carbazole oligomers
   Ryo Yamada, Ken Albrecht, Tatsuhiko Ohto, Keigo Minode, Kimihisa Yamamoto, and Hirokazu Tada: Nanoscale 10, 19818 (2018)
6. Large Hydrogen Bond Mismatch between TMAO and Urea Promotes Their Hydrophobic Association
   Wen Jun Xie, Seoncheol Cha, Tatsuhiko Ohto, Wataru Mizukami, Yuezhi Mao, Manfred Wagner, Mischa Bonn, Johannes Hunger, and Yuki Nagata: Chem 4, 2615 (2018)
7. Graphene Layer Encapsulation of Non-Noble Metal Nanoparticles as Acid-Stable Hydrogen Evolution Catalysts
   Kailong Hu, Tatsuhiko Ohto, Linghan Chen, Jiuhui Han, Mitsuru Wakisaka, Yuki Nagata, Jun-ichi Fujita, and Yoshikazu Ito: ACS Energy Letters 3, 1539 (2018)
8. Structure and Dynamics of Water at Water-Graphene and Water-Hexagonal Boron Nitride Sheet Interfaces Revealed by Ab Initio Sum-Frequency Generation Spectroscopy
   Tatsuhiko Ohto, Hirokazu Tada, and Yuki Nagata: Phys. Chem. Chem. Phys. 20, 12979 (2018)
9. Aggregation-Induced Emission Enhancement from Disilane-Bridged Donor–Acceptor–Donor Luminogens Based on the Triarylamine Functionality
   Tsukasa Usuki, Masaki Shimada, Yoshinori Yamanoi, Tatsuhiko Ohto, Hirokazu Tada, Hidetaka Kasai, Eiji Nishibori, Hiroshi Nishihara: ACS Appl. Mater. Interfaces, 10, 12164 (2018)
10. Cooperation between holey graphene and NiMo alloy for hydrogen evolution in an acidic electrolyte
    Yoshikazu Ito, Tatsuhiko Ohto, Daisuke Hojo, Mitsuru Wakisaka, Yuki Nagata, Linghan Chen, Kailong Hu, Masahiko Izumi, Jun-ichi Fujita, and Tadafumi Adschiri ACS Catal. 8, 3579 (2018)

OHTSUKI, Tomi [C class; 5500 (B), 900 (C)] (232)
— *Scaling theories of random topological and non topological systems*

1. Unconventional Scaling Theory in Disorder-Driven Quantum Phase Transition
   X. Luo, T. Ohtsuki, R. Shindou: Physical Review B **98**, 020201 (2018)
2. Critical Exponent of the Anderson Transition Using Massively Parallel Supercomputing
   K. Slevin, T. Ohtsuki: Journal of the Physical Society of Japan **87**, 094703 (2018)
3. Topological Matter in the Absence of Translational Invariance
   Advanced Topological Insulators, 109-157, Wiley online (2019)

OKADA, Susumu [B class; 600 (B), 80 (C)] ()
— *Physical properties of nanoscale carbon materials under an external electric field*

OKAMOTO, Yuko [E class; 3000 (B), 0 (C)] (259)
— *Study on complex systems by generalized-ensemble algorithms*

OKITSU, Kouhei [C class; 1500 (B), 0 (C)] (277)
— *Study on 'cubic algorithm' for solving n-beam Takagi-Taupin equation*

1. Experimentally obtained and computer-simulated X-ray asymmetric eight-beam pinhole topographs for a silicon crystal
   K. Okitsu, Y. Imai, Y. Yoda and Y. Ueji: Acta Cryst. **A75** (2019) In Press in Advansed Section.
2. Experimentally obtained and computer-simulated X-ray non-coplanar 18-beam pinhole topographs for a silicon crystal
   K. Okitsu, Y. Imai and Y. Yoda: Acta Cryst. **A75** (2019) In Press in Advansed Section.

OKUBO, Tatsuya [C class; 1500 (B), 0 (C)] ()
— *Theoretical and experimental investigation on phase selectivity in zeolite syntheses*

OKUBO, Tsuyoshi [C class; 5500 (B), 900 (C)] (230)
— *Novel phases in honeycomb lattice Kitaev materials*

1. Field-enhanced quantum fluctuation in an $S = \frac{1}{2}$ frustrated square lattice
   H. Yamaguchi, Y. Sasaki, T. Okubo, M. Yoshida, T. Kida, M. Hagiwara, Y. Kono, S. Kittaka, T. Sakakibara, M. Takigawa, Y. Iwasaki and Y. Hosokoshi: Phys. Rev. B **98** (2018) 094402.
2. A series of magnon crystals appearing under ultrahigh magnetic fields in a kagom antiferromagnet
   R. Okuma, D. Nakamura, T. Okubo, A. Miyake, A. Matsuo, K. Kindo, M. Tokunaga, N. Kawashima, S. Takeyama and Z. Hiroi: Nat. Commun. **10** (2019) 1229.
3. Gapless Kitaev Spin Liquid to Classical String Gas through Tensor Networks
   H.-Y. Lee, R. Kaneko, T. Okubo and N. Kawashima: arXiv:1901.05786.
4. Multiple–q states of the J_1–J_2 classical honeycomb-lattice Heisenberg antiferromagnet under magnetic fields
   T. Shimokawa, T. Okubo and H. Kawamura: arXiv:1902.01582.

OKUMURA, Hisashi [C class; 6500 (B), 0 (C)] (224)
— *Oligomerization process of full-length amyloid-beta peptides studied by molecular dynamics simulations*

1. Effects of a hydrophilic/hydrophobic interface on amyloid-β- peptides studied by molecular dynamics simulations and NMR experiments
   S. G. Itoh, M. Yagi-Utsumi, K. Kato, and H. Okumura: J. Phys. Chem. B **123** (2019) 160.
2. Cavity closure of 2-hydroxypropyl-β- cyclodextrin: Replica exchange molecular dynamics simulations
   K. Kerdpol, J. Kicuntod, P. Wolschann, S. Mori, C. Rungnim, M. Kunaseth, H. Okumura, N. Kungwan, and T. Rungrotmongkol: Polymers **11** (2019) 145.
3. Conformational properties of an artificial GM1 glycan cluster based on a metal-ligand complex
   Y. Tachi, Y. Okamoto, and H. Okumura: J. Chem. Phys. **149** (2018) 135101.

ONISHI, Hiroaki [C class; 2000 (B), 0 (C)] (270)
— *Magnetic excitation and spin transport in frustrated quantum spin chain*

1. Dynamical quadrupole structure factor of ferromagnetic frustrated chain
   H. Onishi, Physica B 536, 346-349 (2018).
2. Magnetic excitations and transport properties in frustrated ferromagnetic chain
   H. Onishi, J. Magn. Magn. Mater. 479, 88-90 (2019).

ONO, Tomoya [C class; 9000 (B), 1350 (C)] (56)
— *Development of first-principles electronic-structure and transport calculation method based on real-space finite-difference approach*

1. Complex band structure calculations based on the overbridging boundary matching method without using Green's functions
   S. Tsukamoto, T. Ono, S. Iwase, and S. Blügel: Phys. Rev. B **98** (2018) 195422.
2. Contour integral method for obtaining the self-energy matrices of electrodes in electron transport calculations
   S. Iwase, Y. Futamura, A. Imakura, T. Sakurai, S. Tsukamoto, and T. Ono: Phys. Rev. B, **97** (2018) 195449.

3. First-principles study on leakage current caused by oxygen vacancies at $HfO_2/SiO_2/Si$ interface
   K. Takagi and T. Ono: Jpn. J. Appl. Phys. **57** (2018) 066501.
4. DFT calculation for oxidation reaction of SiC(0001)
   T. Ono: Materials Science Forum, accepted.

ONO, Yoshiaki [C class; 4000 (B), 750 (C)] (189)
— *First-principles calculation and dynamical mean-field theory for superconductivity in multi-band systems*

1. FFLO Superconductivity Mediated by Excitonic Fluctuation in Semimetallic Ta_2NiSe_5
   Takemi Yamada, Kaoru Domon, Yoshiaki Ono: J. Phys. Soc. Jpn., in press

OSHIKAWA, Masaki [B class; 800 (B), 0 (C)] ()
— *Numerical study of many-body polarization and quantum dynamics*

OSHIYAMA, Atsushi [E class; 34500 (B), 5250 (C)] (44)
— *Mechanisms of Semiconductor Interface Formation and its Electronic Properties based on Quantum Theory*

1. Structural stability and energy levels of carbon-related defects in amorphous SiO_2 and its interface with SiC
   Y.-i. Matsushita and A. Oshiyama: Jpn. J. Appl. Phys. **57** (2018) 125701
2. Microscopic mechanism of carbon annihilation upon SiC oxidation due to phosphorous treatment: Density functional calculations combined with ion mass spectrometry
   T. Kobayashi, Y.-i. Matsushita, T. Okuda, T. Kimoto and A. Oshiyama: Appl. Phys. Exp. **11** (2018) 121301
3. Reaction Pathway of Surface-Catalyzed Ammonia Decomposition and Nitrogen Incorporation in Epitaxial Growth of Gallium Nitride
   K. M. Bui, J.-I. Iwata, Y. Kangawa, K. Shiraishi, Y. Shigeta, and A. Oshiyama: J. Phys. Chem. C **122** (2018)
4. First-Principle Study of Ammonia Decomposition and Nitrogen Incorporation on the GaN Surface in Metal Organic Vapor Phase Epitaxy
   K. M. Bui, J.-I. Iwata, Y. Kangawa, K. Shiraishi, Y. Shigeta, and A. Oshiyama: J. Cryst. Growth **507** (2019)
5. Structural determination of phosphosilicate glass based on first-principles molecular dynamics calculation
   T. Kobayashi, Y.-i. Matsushita, T. Kimoto and A. Oshiyama: Jpn. J. Appl. Phys. **58** (2019) 011001

OTOMO, Junichiro [B,D class; 1000 (B), 570 (C)] (130)
— *Analysis of ion conduction in materials of proton-conducting solid electrolyte*
— *Theoretical analysis of catalytic surface reaction with proton conductors*

OZEKI, Yukiyasu [C class; 8500 (B), 0 (C)] (221)
— *Study on topological phase transitions by dynamical scaling analysis*
— *Study on topological phase transitions by dynamical scaling analysis II*

1. Dynamical scaling analysis of phase transition and critical properties for the RP^2 model in two dimensions
   Y. Ozeki, A. Matsuda and Y. Echinaka: Phys. Rev E **99** (2019) 012116

RAEBIGER, Hannes [B class; 700 (B), 0 (C)] ()
— *Theory of self-organized nano-structures for electronic devices*

SAITO, Mineo [C class; 8500 (B), 0 (C)] (64)
— *First-principles calculation for muon and positron experiments of wide gap semiconductors*

1. Anisotropic thermoelectric effect on phosphorene and bismuthene: first-principles calculations based on nonequilibrium Green's function theory

Yuto Tanaka, Mineo Saito and Fumiyuki Ishii: J. J. Appl. Phys. **57** (2018) 125201.

2. Electronic band structures of group-V two-dimensional materials
   Nuning Anugrah Putri Namari and Mineo Saito: J. J. Appl. Phys., accepted for publication.

SAITO, Nen [B class; 600 (B), 90 (C)] (297)
— *phase field simulation for amoeboid cells*

SAKAGUCHI, Norihito [C class; 4000 (B), 0 (C)] (102)
— *Reduction of Rare Metals in Fuel Cell Catalysts and Hydrogen Permeable Membrane*

1. Enhanced hydrogen permeability of hafnium nitride nanocrystalline membranes by interfacial hydridic conduction
   青木芳尚，倉千晴，國貞雄治，朱春宇，幅崎浩樹: クリーンエネルギー **27** (2018) 44.
2. Adsorption and Diffusion Properties of a Single Iron Atom on Light-Element-Doped Graphene
   S. Hasegawa, Y. Kunisada, N. Sakaguchi: e-J. Surf. Sci. Nanotech. **16** (2018) 193.
3. Combustion synthesis of AlN doped with carbon and oxygen
   G. Saito, Y. Kunisada, T. Watanabe, X. Yi, T. Nomura, N. Sakaguchi, T. Akiyama: J. Am. Ceram. Soc. **102** (2019) 524.
4. Hydrogen isotope absorption in unary oxides and nitrides with anion vacancies and substitution
   T. Watanabe, Y. Kunisada, N. Sakaguchi: ChemPhysChem in press.
5. グラフェン上での金属原子吸着状態の理論的研究
   長谷川瞬，國貞雄治，坂口紀史: 表面と真空 印刷中
6. Exploration of Long-Life Pt/Heteroatom-Doped Graphene Catalysts in Hydrogen Atmosphere
   S. Hasegawa, Y. Kunisada, N. Sakaguchi: ACS Omega **4** (2019) 6573.

SAKAI, Toru [C class; 8500 (B), 1500 (C)] (218,219)
— *Numerical Diagonalization Study on the Quantum Spin Liquid in Frustrated Spin Systems*
— *Numerical Study on Quantum Phase Transitions of the Spin Tubes*

1. Spin-1/2 Triangular-Lattice Heisenberg Antiferromagnet with $\sqrt{3}\times\sqrt{3}$-Type Distortion -Behavior around the Boundaries of the Intermediate Phse-
   A. Shimada, H. Nakano, T. Saka and K. Yoshimura: J. Phys. Soc. Jpn. 87 (2018) 034706.
2. The Spin-1/2 Heisenberg Antiferromagnet on a Triangular-Lattice with $\sqrt{3}\times\sqrt{3}$-Type Distortion -Magnetization Process and Magnetic Susceptibility-
   A. Shimada, H. Nakano, T. Saka and K. Yoshimurai: J. Jpn. Soc. Powder Powder Metallurgy 65 (2018) 3.
3. Quantum Spin Fluid Behaviors of the Kagome- and Triangular-Lattice Antiferromagnets
   T. Sakai and H. Nakano: J. Phys.: Conf. Ser. 969 (2018) 012127/1-6
4. Spontaneous Magnetization of the Spin-1/2 Heisenberg Antiferromagnet on the Triangular Lattice with a Distortion
   A. Shimada, T. Sakai, H. Nakano and K. Yoshimurai: J. Phys.: Conf. Ser. 969 (2018) 012126/1-6
5. Gapless Spin Excitations in the $S = 1/2$ Kagome- and Triangular-Lattice Heisenberg Antiferromagnets
   T. Sakai and H. Nakano: Physica B 536 (2018) 85-88
6. Numerical Diagonalization Study of Magnetization Process of Frustrated Spin-1/2 Heisenberg Antiferromagnets in Two Dimensions -Triangular- and Kagome-Lattice Antiferromagnets-
   H. Nakano and T. Sakai: J. Phys. Soc. Jpn. 87 (2018) 063706/1-5
7. Precise Estimation of the $S = 2$ Haldane Gap by Numerical Diagonalization
   H. Nakano and T. Sakai: J. Phys. Soc. Jpn. 87 (2018) 105002/1-2
8. Ground-State Phase Diagram of an Anisotropic $S = 1/2$ Ladder with Different Interactions
   T. Tonegawa, T. Hikihara, K. Okamoto, S. C. Furuya and T. Sakai: J. Phys. Soc. Jpn. 87 (2018) 104002/1-11
9. Third Boundary of the Shastry-Sutherland Model by Numerical Diagonalization
   H. Nakano and T. Sakai: J. Phys. Soc. Jpn. 87 (2018), 123702/1-5
10. Ground state with nonzero spontaneous magnetization of the two-dimensional spin-1/2 Heisenberg antiferromagnet with frustration
    T. Sakai and H. Nakano: AIP ADVANCES 8 (2018) 101408/1-5

11. Metamagnetic jump in the spin-1/2 antiferromagnetic Heisenberg model on the square kagome lattice
    Y. Hasegawa, H. Nakano and T. Sakai: Phys. Rev. B 98 (2018) 014404/1-9
12. Analysis of Rashba Effect on Au(111) Model Surface
    M. Fujiwara, N. Shima, K. Makoshi and T. Sakai: J. Phys. Soc. Jpn. 88 (2019), 034604/1-5
13. From kagome strip to kagome lattice: Realizations of frustrated $S = 1/2$ antiferromagnets in Ti(III) fluorides
    H. O. Jeschke, H. Nakano and T. Sakai: Phys. Rev. B 99 (2019) 140410(R)/1-6

SAKAKIBARA, Hirofumi [B class; 800 (B), 100 (C)] (147)
— *Development of the determination technique of model parameters based on the accurate ab-initio quantum simulation*

SAKURAGI, Shunsuke [C class; 1000 (B), 0 (C)] (143)
— *Development and control of surface and interface spin texture by band engineering using quantum-well state*

1. Change in magnetization of ferromagnetic Pd(001) ultrathin films induced by the strain effect of $BaTiO_3$
   Yusuke Ban, Katsuyoshi Komatsu, Shunsuke Sakuragi, Tomoyasu Taniyama, Hiroyuki Kageshima, and Tetsuya Sato: Appl. Phys. Lett. **112** (2018) 142409.
2. Spontaneous distortion via the appearance of ferromagnetism in Pd ultrathin films: Observation of an inverse mechanism for the Stoner criterion
   Shunsuke Sakuragi, Hiroo Tajiri, Hiroyuki Kageshima, and Tetsuya Sato: Phys. Rev. B **97** (2018) 214421.
3. Switching of magnetism via modifying phase shift of quantum-well states by tailoring the interface electronic structure
   Shunsuke Sakuragi, Hiroyuki Kageshima, and Tetsuya Sato: submitted to Phys. Rev. B

SASAKI, Takehiko [C class; 1500 (B), 0 (C)] (133)
— *Reaction processes of polyalcohols in high temperature water by First Principles Calculations*

1. Understanding Competition of Polyalcohol Dehydration Reactions in Hot Water
   Y. L. Chang, T. Sasaki, J. Ribas Ariño, M. Machida, M. Shiga: J. Phys. Chem. B **123** (2019) 1662.

SATO, Tetsuya [C class; 3000 (B), 0 (C)] (122)
— *Magnetic properties of Fe/Pd(001) bilayer affected by quantum-well states in Pd layer*

1. Spontaneous distortion via the appearance of ferromagnetism in Pd ultrathin films: Observation of an inverse mechanism for the Stoner criterion
   SAKURAGI Syunsuke: Phys. Rev. B **97**, 214421 (2018).

SAYYAD, Sharareh [B,E class; 8600 (B), 1930 (C)] ()
— *Nonequilibrium investigation of high temperature superconductors*
— *Numerical study of d-wave superconductors in equilibrium*

SEKINE, Yasushi [C class; 4000 (B), 0 (C)] (101)
— *Elucidation of the surface of supported metal catalyst in an electric field*

1. The important role of N2H formation energy for low-temperature ammonia syntheis in an electric field
   K. Murakami, Y. Tanaka, R. Sakai, K. Toko, K. Ito, A. Ishikawa, T. Higo, T. Yabe, S. Ogo, M. Ikeda, H. Tsuneki, H. Nakai, Y. Sekine : Catal. Today, in press.

SHIGETA, Yasuteru [C class; 6000 (B), 950 (C)] (67)
— *Analyses on self-organization processes using dissimilarity sampling*

1. Programmed Dynamical Ordering in Self-organization Processes of Nano-cube: A Molecular Dynamics Study

R. Harada, T. Mashiko, M. Tachikawa, S. Hiraoka, Y. Shigeta: Phys. Chem. Chem. Phys. **20** (2018) 9115.

2. Coulomb and CH-π interactions in (6-4) photolyaseDNA complex dominate DNA binding and repair abilities
   Y. Terai, R. Sato, T. Yumiba, R. Harada, K. Shimizu, T. Toga, T. Ishikawa-Fujiwara, T. Todo, S. Iwai, Y. Shigeta, J. Yamamoto: Nucl. Acid. Res., **46** (2018) 6761.
3. How low-resolution data can predict conformational changes of a protein: a molecular dynamics study
   R. Harada,Y. Shigeta: Phys. Chem. Chem. Phys. **20** (2018) 17790.
4. On-the-Fly Specifications of Reaction Coordinates in Parallel Cascade Selection Molecular Dynamics Accelerate Conformational Transitions of Proteins
   R. Harada, TY. Shigeta: J. Chem. Theor. Comput. **14** (2018) 3332.

SHIMADA, Toshihiro [B class; 700 (B), 0 (C)] (152)
— Formation mechanism and electronic structures of novel two dimensional materials and nanotubes - BCN and MX2 systems

1. Single crystal growth, structural analysis and electronic band structure of anitrogen-containing polyacene Benzo[i]benzo[6',7']quinoxalino[2',3':9,10]phenanthro[4,5-abc]phenazine
   Nobuhiko Sakai, Takahiro Tamura, Takashi Yanase, Taro Nagahama, Toshihiro Shimada: Jpn. J. Appl. Phys.**58** (2019) SBBG08.
2. Search for new nitrogen-doped carbon materials by compressing molecular crystals
   Ichiro Yamane, Takashi Yanase, Taro Nagahama,Toshihiro Shimada: Jpn. J. Appl. Phys.**58** (2019) SBBG13.

SHIMAMURA, Kohei [C class; 2500 (B), 600 (C)] (118)
— Ab initio molecular dynamics simulation of sustained chemical reaction processes in deep-sea hydrothermal vents

1. *Ab Initio* Molecular Dynamics Study of Prebiotic Production Processes of Organic Compounds at Meteorite Impacts on Ocean
   K. Shimamura, F. Shimojo, A. Nakano, and S. Tanaka: J. Comp. Chem. **40** (2019) 349.

SHIMOJO, Fuyuki [C class; 5000 (B), 0 (C)] (92)
— First-Principles Molecular-Dynamics Study of Structural and Electronic Properties of Covalent Liquids and Glass under Pressure

1. Electronic Structure of Titania Nanosheets with Vacancies Based on Nonadiabatic Quantum Molecular Dynamics Simulations
   Y. Uchida, M. Hara, A. Funatsu, and F. Shimojo: Phys. Status Solidi B **255**, 1700689 (2018).
2. Electronic structures and impurity cluster features in Mg-Zn-Y alloys with a synchronized long-period stacking ordered phase
   S. Hosokawa, K. Maruyama, K. Kobayashi, J. R. Stellhorn, B. Paulus, A. Koura, F. Shimojo, T. Tsumuraya, M. Yamasaki, Y. Kawamura, S. Yoshioka, and H. Sato: J. Alloys Compd. **762**, 797 (2018).
3. Photo-induced lattice contraction in layered materials
   H. Kumazoe, A. Krishnamoorthy, L. Bassman, R. K. Kalia, A. Nakano, F. Shimojo, and P. Vashishta: J. Phys.: Condens. Matter **30**, 32LT02 (2018).
4. Static structure of liquid GeSe under pressure: *ab initio* molecular dynamics simulations
   A. Koura and F. Shimojo: Phys. Status Solidi B **255**, 1800103 (2018).

SHIMOKAWA, Tokuro [C class; 5000 (B), 900 (C)] (237)
— Multiple-Q states of the frustrated Heisenberg model on the honeycomb lattice

1. Ripple state in the frustrated honeycomb-lattice antiferromagnet
   T. Shimokawa and H. Kawamura: submitted to Phys. Rev. Lett.
2. Multiple-q states of the J1-J2 classical honeycomb-lattice Heisenberg antiferromagnet under magnetic fields
   T. Shimokawa, T. Okubo and H. Kawamura: submitted to Phys. Rev. B

SHINAOKA, Hiroshi [C class; 1500 (B), 800 (C)] (193)
— *Dynamical mean-field calculations of strongly correlated transition metal compounds*

SHINODA, Wataru [E class; 13000 (B), 1750 (C)] (35)
— *Molecular basis analysis of Soft Materials using All-Atom and Coarse-Grained Molecular Dynamics Simulations*

1. SPICA Force Field for Lipid Membranes: Domain Formation Induced by Cholesterol.
   Sangjae Seo and Wataru Shinoda: Journal of Chemical Theory and Computation, 15, 762-774 (2019).
2. Free energy analysis of membrane pore formation process in the presence of multiple melittin peptides
   Yusuke Miyazaki, Susumu Okazaki, Wataru Shinoda: BBA-Biomembranes, DOI:10.1016/j.bbamem.2019.03.002
3. Exploring the effect of pendent side chain length on the structural and mechanical properties of hydrated perfluorosulfonic acid polymer membranes by molecular dynamics simulation
   An-Tsung Kuo, Kotono Takeuchi, Atsushi Tanaka, Shingo Urata, Susumu Okazaki, Wataru Shinoda: Polymer, 146, 53-62 (2018).
4. Molecular mechanism of material deformation and failure in butadiene rubber: Insight from all-atom molecular dynamics simulation using a bond breaking potential model
   Rajdeep S. Payal, Kazushi Fujimoto, Changwoon Jang, Wataru Shinoda, Yuki Takei, Hiroshi Shima, Katsuhiko Tsunoda, Susumu Okazaki: Polymer, 170, 113-119 (2019).

SHINOHARA, Yasushi [C,D class; 5000 (B), 650 (C)] (108)
— *First-principles calculations for nonlinear light absorption of insulators*
— *Relaxation effect on high-order harmonic generation from crystalline solids*

1. Polarization-Resolved Study of High Harmonics from Bulk Semiconductors
   K. Kaneshima, Y. Shinohara, K. Takeuchi, N. Ishii, K. Imasaka, T. Kaji, S. Ashihara, K.L. Ishikawa, and J. Itatani: Phys. Rev. Lett. 120 (2018) 243903.
2. High-order harmonic generation from hybrid organicinorganic perovskites thin films
   Hideki Hirori, Peiyu Xia, Yasushi Shinohara, Tomohito Otobe, Yasuyuki Sanari, Hirokazu Tahara, Nobuhisa Ishi, Jiro Itatani, Kenichi L. Ishikawa, Tomoko Aharen, Masashi Ozaki, Atsushi Wakamiya, Yoshihiko Kanemitsu: APL Materials 7, 041107 (2019)

SHIOMI, Junichiro [B,C class; 12600 (B), 1000 (C)] (211,213,214)
— *Control of phonon and electron transport properties using mechanical strain*
— *Screening for Thermal Functional Materials using Materials Informatics*
— *Understanding Mechanical and Thermal Properties of Sustainable Materials through Molecular Simulations*

1. Ultranarrow-Band Wavelength-Selective Thermal Emission with Aperiodic Multilayered Metamaterials Designed by Bayesian Optimization
   A. Sakurai, K. Yada, T. Simomura, S. Ju, M. Kashiwagi, H. Okada, T. Nagao, K. Tsuda, and J. Shiomi: ACS Central Science 5, 319, (2019).
2. Materials Informatics for Heat Transfer: Recent Progresses and Perspectives
   S. Ju, J. Shiomi: Nanoscale and Microscale Thermophysical Engineering 23, 157 (2019).
3. Parametric Model to Analyze the Components of the Thermal Conductivity of a Cellulose-Nanofibril Aerogel
   M. Obori, D. Suh, S. Yamasaki, T. Kodama, T. Saito, A. Isogai, J. Shiomi: Phys. Rev. Appl. 11 (2019) 024044.
4. Corrrection to Thermal Boundary Conductance Across Heteroepitaxial ZnO/GaN Interfaces: Assessment of the Phonon Gas Model
   John Gaskins, George Kotsonis, Ashutosh Giri, Shenghong Ju, Andrew Rohskopf, Yekan Wang, Tingyu Bai, Edward Sachet, Christopher Shelton, Zeyu Liu, Zhe Cheng, Brian Foley, Samuel Graham, Tengfei Luo, Asegun Henry, Mark S. Goorsky, Junichiro Shiomi, Jon-Paul Maria, and Patrick E. Hopkins: Nano Lett., 19, 14081408 (2019).
5. High-working-pressure Sputtering of ZnO for Stable and Efficient Perovskite Solar Cells

Abhishek Thote, Il Jeon, Hao-Sheng Lin, Sergei Manzhos, Takafumi Nakagawa, Donguk Suh, Junho Hwang, Makoto Kashiwagi, Junichiro Shiomi, Shigeo Maruyama, Daiguji Hirofumi, Yutaka Matsuo: ACS Applied Electronic Materials, 1, 389396 (2019).

6. Quantifying phonon particle and wave transport in nanostructures–The unexpectedly strong particle effect in silicon nanophononic metamaterial with cross junction
   Dengke Ma, Anuj Arora, Shichen Deng, Junichiro Shiomi, Nuo Yang: Materials Today Physics, 8, 56-61 (2019).
7. Tuning phonon transport spectrum for better thermoelectric materials
   Takuma Hori, Junichiro Shiomi: Science and Technology of Advanced Materials, 20, 10-25 (2018).
8. Akhiezer mechanism limits coherent heat conduction in phononic crystals
   Yuxuan Liao, Takuma Shiga, Makoto Kashiwagi, and Junichiro Shiomi: Physical Review B 98, 134307 (2018).
9. Thermal boundary conductance across heteroepitaxial ZnO/GaN interfaces: Failures of the phonon gas model
   John Gaskins, George Kotsonis, Ashutosh Giri, Shenghong Ju, Andrew Rohskopf, Yekan Wang, Tingyu Bai, Edward Sachet, Christopher Shelton, Zeyu Liu, Zhe Cheng, Brian Foley, Samuel Graham, Tengfei Luo, Asegun Henry, Mark S. Goorsky, Junichiro Shiomi, Jon-Paul Maria, and Patrick E. Hopkins: Nano letters, 18, 7469-7477 (2018).
10. Modulating temperature dependence of thermal conductivity by nanostructuring
    Takuma Shiga, Junichiro Shiomi: Japanese Journal of Applied Physics, 57, 120312 (2018).
11. Thermal phonon engineering by tailored nanostructures
    Masahiro Nomura, Junichiro Shiomi, Takuma Shiga, and Roman Anufriev: Japanese Journal of Applied Physics 57, 080101 (2018).
12. Revisiting PbTe to identify how thermal conductivity is really limited
    Shenghong Ju, Takuma Shiga, Lei Feng and Junichiro Shiomi: Phys. Rev. B 97, 184305 (2018).
13. Modelling heat conduction in nanoporous silicon with geometry distributions
    Makoto Kashiwagi, Yuta Sudo, Takuma Shiga, and Junichiro Shiomi: Physical Review Applied, 10, 044018 (2018).

SHIRAI, Tatsuhiko [B class; 700 (B), 0 (C)] (292)

— *Application of Eigenstate Thermalization Hypothesis to Non-equilibrium steady states*

1. Optical bistability in a low-photon-density regime
   T. Shirai, S. Todo, H. de Raedt and S. Miyashita: Pays. Rev. A **98** (2018) 043802.
2. Thermalization in Open Many-Body Systems Based on Eigenstate Thermalization Hypothesis
   T. Shirai and T. Mori: submitted to Phys. Rev. Lett.

SHIRAISHI, Kenji [C class; 6000 (B), 950 (C)] ()

— *Multiphysics Simulation of MOVPE Growth of Nitride Semiconductor Based on Unification of First Principles Calculations and Fluid Dynamics*

SHUDO, Ken-ichi [B class; 600 (B), 0 (C)] (157)

— *Chemical doping of nano-structured PbS*

1. Electronic states of 3D aromatic molecules on Au(111) surfaces: adsorption of carboranethiol
   Takuto Aoki, Yuta Nakahama, Tadao Ikeda, Masako Shindo, Masanobu Uchiyama, and Ken-ichi Shudo: Journal of Materials Science, *in press* (2019).
2. Chemical synthesis and band gap control of Ga2O3:Co nanocrystals
   Kohki Mukai , Akira Tsuno, Ken-ichi Shudo, and Hiroyuki Otani: Japanese Journal of Applied Physics **58**, SBBK05 (2019).
3. Core electron topologies in chemical compounds: case study of carbon vs. silicon
   Daisuke Yoshida, Hannes Raebiger, Ken-ichi Shudo, and Koichi Ohno: Angewandte Chemie Int. Ed. **57**, 7012–7018 (2018).

SUGINO, Osamu [E class; 13000 (B), 2350 (C)] (50)

— *Functional property of electrodes*

1. Direct coupling of first-principles calculations with replica exchange Monte Carlo sampling of ion

disorder in solids
Shusuke Kasamatsu and Osamu Sugino, J. Phys. Cond. Mat., 31. 085901 (2019).
2. Hydrogen adsorption on Pt (111) revisited from random phase approximation
Lei Yan, Yang Sun, Yoshiyuki Yamamoto, Shusuke Kasamatsu, Ikutaro Hamada, and Osamu Sugino, J. Chem. Phys. 149, 164702 (2018).
3. First-principles investigation of polarization and ion conduction mechanisms in hydroxyapatite
Shusuke Kasamatsu and Osamu Sugino, Phys. Chem. Chem. Phys. 20 8744 (2018).

SUZUKI, Takafumi [C class; 8500 (B), 1600 (C)] (216)
— *Dynamical properties of honeycomb-lattice Kitaev-Heisenberg models in magnetic fields*
— *Ramman spectra in the effective models for honeycomb-lattice magnet $RuCl_3$*
1. Effective model with strong Kitaev interactions for α-$RuCl_3$
Takafumi Suzuki and Sei-ichiro Suga: Phys. Rev. B **97** (2018) 134424.
2. Thermal properties of spin-S Kitaev-Heisenberg model on a honeycomb lattice
Takafumi Suzuki and Youhei Yamaji: Physica B **536** (2018) 637-639.
3. Field dependence of THz spectra of effective models for α-$RuCl_3$
Takafumi Suzuki and Sei-ichiro Suga: AIP Advances **8** (2018) 101414.
4. Quantized $\Delta S = 2$ Excitation Spectra by Confinement in an $S = 1$ Spin Chain
Takafumi Suzuki and Sei-ichiro Suga: Accepted in J. Phys. Soc. Jpn.

SUZUKI, Tatsuo [C class; 2000 (B), 550 (C)] ()
— *Theoretical search for high-efficient monolayer water-splitting photocatalysts II*

SUZUKI, Yuji [C class; 8500 (B), 0 (C)] (62)
— *Development of High-performance Polymer Electret*
1. 量子化学計算を用いた高性能アモルファスフッ素ポリマー・エレクトレットの開発
S. Kim, K.Suzuki, and Y. Suzuki: 日本機械学会熱工学コンファレンス 2018, 富山, 2018 年 10 月 20 日-10 月 21 日, D126.
2. Development of A High-performance Amorphous Fluorinated Polymer Electret Based on Quantum Chemical Analysis
18th Int. Conf. on Micro and Nanotechnology for Power Generation and Energy Conversion Applications (PowerMEMS 2018), Daytona Beach, T4B-01, (2018)
3. 量子化学計算を用いた高電子親和力官能基を持つ アモルファスフッ素ポリマーエレクトレットの開発
応用物理学会春季学術講演会，東京，2019 年 3 月 9 日-12 日, 11p-W242-2

TAKAE, Kyohei [B class; 800 (B), 0 (C)] (289)
— *Dynamics of structure formation in charged colloids*
1. Hydrodynamic simulations of charge-regulation effects in colloidal suspensions
K. Takae and H. Tanaka: Soft Matter **14** (2018) 4711.
2. Self-organization into ferro- and antiferroelectric crystals via the interplay between particle shape and dipolar interaction
K. Takae and H. Tanaka: Proc. Natl. Acad. Sci. **115** (2018) 9917.

TAKETSUGU, Tetsuya [C class; 3500 (B), 700 (C)] (99)
— *Ab initio study on the structure and functions of nanomaterials*
1. Low-lying Excited States of hqxcH and Zn-hqxc Complex: Toward Understanding Intramolecular Proton Transfer Emission
M. Ebina, Y. Kondo, T. Iwasa, T. Taketsugu: Inorg. Chem., **58**, (2019) 4686-4698.
2. Photoluminescence Properties of [Core+exo]-Type Au6 Clusters: Insights into the Effect of Ligand Environments on the Excitation Dynamics
Y. Shichibu, M. Zhang, T. Iwasa, Y. Ono, T. Taketsugu, S. Omagari, T. Nakanishi, Y. Hasegawa, K. Konishi: J. Phys. Chem. C, **123**, (2019) 6934-6939.
3. Ammonia-rich combustion and ammonia combustive decomposition properties of various supported catalysts

S. Hinokuma, K. Araki, T. Iwasa, S. Kiritoshi, Y. Kawabata, T. Taketsugu, and M. Machida: Catal. Commun., **123**, (2019) 64-68.

4. Combined Automated Reaction Pathway Searches and Sparse Modeling Analysis for Catalytic Properties of Lowest Energy Twins of Cu_13
   T. Iwasa, T. Sato, M. Takagi, M. Gao, A. Lyalin, M. Kobayashi, K. Shimizu, S. Maeda, T. Taketsugu: J. Phys. Chem. A, **123**, (2019) 210-217.
5. 金・銀・銅クラスターの安定構造，異性化反応経路，および NO 解離反応経路の探索とその電子物性
   近藤有輔，高原里奈，毛利広野，高木牧人，前田理，岩佐豪, 武次徹也: J. Comput. Chem. Jpn., **18**, (2019) 64-69.
6. First principles calculations toward understanding SERS of 2,2′ -bipyridyl adsorbed on Au, Ag and Au-Ag alloy
   M. Takenaka, Y. Hashimoto, T. Iwasa, T. Taketsugu, G. Seniutinas, A. Balčytis, S. Juodkazise, Y. Nishijima: J. Comput. Chem., **40**, (2019) 925-932.
7. Supported binary CuOx − Pt catalysts with high activity and thermal stability for the combustion of NH3 as a carbon-free energy source
   S. Kiritoshi, T. Iwasa, K. Araki, Y. Kawabata, T. Taketsugu, S. Hinokuma, and M. Machida: RSC Advances, **8**, (2018) 41491-41498.
8. Spiral Eu(III) Coordination Polymers with Circularly Polarized Luminescence
   Y. Hasegawa, Y. Miura, Y. Kitagawa, S. Wada, T. Nakanishi, K. Fushimi, T.Seki, H. Ito, T. Iwasa, T. Taketsugu, M. Gon, K. Tanaka, Y. Chujo, S. Hattori, M. Karasawa, and K. Ishii: Chem. Commun., **54**, (2018) 10695-10697.
9. Insights into Geometries, Stabilities, Electronic Structures, Reactivity Descriptors, and Magnetic Properties of Bimetallic NimCun-m (m = 1, 2; n = 3-13) Clusters: Comparison with Pure Copper Clusters
   R. K. Singh, T. Iwasa, and T. Taketsugu: J. Comput. Chem., **39**,(2018) 1878-1889 .

TAMURA, Ryo [C class; 1500 (B), 400 (C)] (272)

— Development of effective model estimation method by machine learning for multiple input measured data

1. Functional nanoparticles-coated nanomechanical sensor arrays for machine learning-based quantitative odor analysis
   K. Shiba, R. Tamura, T. Sugiyama, Y. Kameyama, K. Koda, E. Sakon, K. Minami, H. T. Ngo, G. Imamura, K. Tsuda, and G. Yoshikawa: ACS Sensors **3** (2018) 1592.
2. Hunting for organic molecules with artificial intelligence: Molecules optimized for desired excitation energies
   M. Sumita, X. Yang, S. Ishihara, R. Tamura, and K. Tsuda: ACS Central Science **4** (2018) 1126.
3. Machine learning forces trained by Gaussian process in liquid states: Transferability to temperature and pressure
   R. Tamura, J. Lin, and T. Miyazaki: Journal of the Physical Society of Japan **88** (2019) 044601.
4. Efficient construction method for phase diagrams using uncertainty sampling
   K. Terayama, R. Tamura, Y. Nose, H. Hiramatsu, H. Hosono, Y. Okuno, and K. Tsuda: Physical Review Materials **3** (2019) 033802.
5. Quantum Phase Transition in Fully-Connected Quantum Wajnflasz–Pick Model
   Y. Seki, S. Tanaka and S. Kawabata: J. Phys. Soc. Jpn. **88** (2019) 054006.
6. Application of Ising Machines and a Software Development for Ising Machines
   K. Tanahashi, S. Takayanagi, T. Motohashi and S. Tanaka: J. Phys. Soc. Jpn., in press.
7. A Fully-Connected Ising Model Embedding Method and Its Evaluation for CMOS Annealing Machines
   D. Oku, K. Terada, M. Hayashi, M. Yamaoka, S. Tanaka and N. Togawa: IEICE Transactions in press.
8. Li-ion conductive Li3PO4-Li3BO3-Li2SO4 mixture: Prevision through density functional molecular dynamics and machine learning
   M. Sumita, R. Tamura, K. Homma, C. Kaneta, and K. Tsuda: Bulletin of the Chemical Society of Japan in press.
9. Expanding the horizon of automated metamaterials discovery via quantum annealing

K. Kitai, J. Guo, S. Ju, S. Tanaka, K. Tsuda, J. Shiomi and R. Tamura: submitted.

TANAKA, Hajime [B class; 1700 (B), 0 (C)] (274)
— *Hydrodynamic effects on crystal nucleation in a hard-sphere colloidal system*
— *Schmidt number dependence on dynamics in colloidal suspensions*

1. Numerical prediction of colloidal phase separation by direct computation of Navier-Stokes equation
   Michio Tateno and Hajime Tanaka: npj Computational Materials **5** (2019) 40
2. Physical foundation of the fluid particle dynamics method for colloid dynamics simulation
   Akira Furukawa, Michio Tateno and Hajime Tanaka: Soft Matter **14** (2018) 3738

TANAKA, Shu [C class; 1000 (B), 200 (C)] (286)
— *Study on quantum annealing from a viewpoint of statistical mechanics*

1. Quantum Phase Transition in Fully-Connected Quantum Wajnflasz–Pick Model
   Y. Seki, S. Tanaka and S. Kawabata: J. Phys. Soc. Jpn. **88** (2019) 054006.
2. Application of Ising Machines and a Software Development for Ising Machines
   K. Tanahashi, S. Takayanagi, T. Motohashi and S. Tanaka: J. Phys. Soc. Jpn., in press.
3. A Fully-Connected Ising Model Embedding Method and Its Evaluation for CMOS Annealing Machines
   D. Oku, K. Terada, M. Hayashi, M. Yamaoka, S. Tanaka and N. Togawa: IEICE Transactions in press.
4. Expanding the horizon of automated metamaterials discovery via quantum annealing
   K. Kitai, J. Guo, S. Ju, S. Tanaka, K. Tsuda, J. Shiomi and R. Tamura: submitted.
5. Functional nanoparticles-coated nanomechanical sensor arrays for machine learning-based quantitative odor analysis
   K. Shiba, R. Tamura, T. Sugiyama, Y. Kameyama, K. Koda, E. Sakon, K. Minami, H. T. Ngo, G. Imamura, K. Tsuda, and G. Yoshikawa: ACS Sensors **3** (2018) 1592.
6. Hunting for organic molecules with artificial intelligence: Molecules optimized for desired excitation energies
   M. Sumita, X. Yang, S. Ishihara, R. Tamura, and K. Tsuda: ACS Central Science **4** (2018) 1126.
7. Machine learning forces trained by Gaussian process in liquid states: Transferability to temperature and pressure
   R. Tamura, J. Lin, and T. Miyazaki: Journal of the Physical Society of Japan **88** (2019) 044601.
8. Efficient construction method for phase diagrams using uncertainty sampling
   K. Terayama, R. Tamura, Y. Nose, H. Hiramatsu, H. Hosono, Y. Okuno, and K. Tsuda: Physical Review Materials **3** (2019) 033802.
9. Li-ion conductive Li_3PO_4-Li_3BO_3-Li_2SO_4 mixture: Prevision through density functional molecular dynamics and machine learning
   M. Sumita, R. Tamura, K. Homma, C. Kaneta, and K. Tsuda: Bulletin of the Chemical Society of Japan in press.

TATENO, Masaru [C class; 4000 (B), 0 (C)] ()
— *Molecular dynamics free energy calculations of functional mechanisms of biological macromolecular complex systems*

TATETSU, Yasutomi [C class; 4000 (B), 800 (C)] (95)
— *First-principles calculations of a search for subphases and large-scale calculations for the grain boundaries of Nd-Fe-B magnets*

1. First-principles study on substitution effects in $Nd_2(Fe, X)_{14}B$
   Y. Tatetsu, S. Tsuneyuki, and Y. Gohda: Materialia, 4, 388-394 (2018).
2. Dynamic interface formation in magnetic thin film heterostructures
   S. Nakashima, T. Miyamachi, Y. Tatetsu, Y. Takahashi, Y. Takagi, Y. Gohda, T. Yokoyama, and F. Komori: Advanced Functional Materials, 29, 1804594 (2018).
3. Role of typical elements in $Nd_2Fe_{14}X$ (X = B, C, N, O, F)
   Yasutomi Tatetsu, Yosuke Harashima, Takashi Miyake, and Yoshihiro Gohda: Physical Review Materials 2, 0744100-1 − 0744100-9 (9) (2018).

TATEYAMA, Yoshitaka [C class; 4500 (B), 950 (C)] (82)
— *DFT sampling studies on interfacial properties of batteries and catalysts*

1. A General Representation Scheme for Crystalline Solids based on Voronoi-Tessellation Real Feature Values and Atomic Property Data
   R. Jalem, M. Nakayama, Y. Noda, T. Le, I. Takeuchi, Y. Tateyama, H. Yamazaki: Sci. Tech. Adv. Mater. **19** (2018) 231-242.
2. First-Principles Microkinetic Analysis of NO + CO Reactions on Rh(111) Surface toward Understanding NOx Reduction Pathways
   A. Ishikawa, Y. Tateyama: J. Phys. Chem. C **122** (2018) 17378-17388.
3. Liquid electrolyte informatics using an exhaustive search with linear regression
   K. Sodeyama, Y. Igarashi, T. Nakayama, Y. Tateyama, M. Okada: Phys. Chem. Chem. Phys. **20** (2018) 22585-22591.
4. Dynamical Solvent Effects on the Charge and Reactivity of Ceria-Supported Pt Nanoclusters
   L. Szabova, M. F. Camellone, F. N. Ribeiro, V. Matolin, Y. Tateyama, S. Fabris: J. Phys. Chem. C **122** (2018) 27507-27515.
5. Structures, Electronic States, and Reactions at Interfaces between LiNi0.5Mn1.5O4 Cathode and Ethylene Carbonate Electrolyte: A First-Principles Study
   Y. Okuno, K. Ushirogata, K. Sodeyama, G. Shukri, Y. Tateyama: J. Phys. Chem. C **123** (2019) 2267-2277.
6. Oxygen Redox Promoted by Na Excess and Covalency in Hexagonal and Monoclinic Na2-xRuO3 Polymorphs
   M. H. N. Assadi, M. Okubo, A. Yamada, Y. Tateyama: J. Electrochem. Soc. **166** (2019) A5343-A5348.

TERAO, Takamichi [B class; 1100 (B), 150 (C)] (283)
— *Molecular simulation of colloidal suspensions*

1. Generalised local bond order parameter analysis: application to colloidal particles with dendritic polymer brushes
   R. Mizuno, K. Okumura, J. Oguri, and T. Terao: Mol. Simul. **45** (2019) 743. .

TERASAWA, Asako [B,C class; 4200 (B), 650 (C)] (93)
— *First principles calculations and development of graph analysis method for magnetic alloys and amorphous grain boundary phases in permanent magnets*
— *First principles calculations and mathematical analyses of amorphous magnetic alloys and amorphous grain boundary phases in permanent magnets*

1. Hidden order in amorphous structures: Extraction of nearest neighbor networks of amorphous NdFe alloys with Gabriel graph analyses
   A. Terasawa and Y. Gohda, J. Chem. Phys., **149**, 154502, (2018).

TODO, Synge [C class; 5500 (B), 900 (C)] (229)
— *Topological Order and Quantum Dynamics in Quantum Many-body Systems*

1. Crystal structure prediction supported by incomplete experimental data
   N. Tsujimoto, D. Adachi, R. Akashi, S. Todo, S. Tsuneyuki, Phys. Rev. Materials 2, 053801 (7pp) (2018)
2. Optical bistability in a low-photon-density regime
   T. Shirai, S. Todo, H. de Raedt, S. Miyashita, Phys. Rev. A 98, 043802 (13pp) (2018)
3. ZN Berry phase and symmetry protected topological phases of SU(N) antiferromagnetic Heisenberg chain
   Y. Motoyama, S. Todo, , Phys. Rev. B 98, 195127 (6pp) (2018)
4. Localized mode and nonergodicity of a harmonic oscillator chain
   F. Ishikawa, S. Todo, Phys. Rev. E 98, 062140 (8pp) (2018)
5. Parallel loop cluster quantum Monte Carlo simulation of quantum magnets based on global union-find graph algorithm
   S. Todo, H. Matsuo, H. Shitara, Comp. Phys. Comm. 239, 84-93 (2019)

6. Fast algorithm for generating random bit strings and multispin coding for directed percolation
   H. Watanabe, S. Morita, S. Todo, N. Kawashima, J. Phys. Soc. Jpn. 88, 024004 (8pp) (2019)
7. Search for Common Minima in Joint Optimization of Multiple Cost Functions
   D. Adachi, N. Tsujimoto, R. Akashi, S. Todo, S. Tsuneyuki, to appear in Comp. Phys. Comm.

TOHYAMA, Takami [C class; 4500 (B), 850 (C)] (246)
— *Dynamical DMRG study of spin dynamics in frustrated quantum spin systems*

1. Magnetic phase diagram of a frustrated spin ladder
   T. Sugimoto, M. Mori, T. Tohyama, and S. Maekawa: Phys. Rev. B **97**, (2018) 144424.
2. Dynamical density matrix renormalization group study of spin and charge excitations in the four-leg t-t'-J ladder
   T. Tohyama, M. Mori, and S. Sota: Phys. Rev. B **97**, (2018) 235137.
3. Ground state phase diagram of the Kitaev-Heisenberg model on a honeycomb-triangular lattice
   M. Kishimoto, K. Morita, Y. Matsubayashi, S. Sota, S. Yunoki, and T. Tohyama: Phys. Rev. B **98**, (2018) 054411.
4. Ground-state phase diagram of the Kitaev-Heisenberg model on a kagome lattice
   K. Morita, M. Kishimoto, and T. Tohyama: Phys. Rev. B **98**, (2018) 134437.
5. Syntheses and first-principles calculations of the pseudobrookite compound $AlTi_2O_5$
   T. Tohyama, R. Ogura, K. Yoshinaga, S. Naito, N. Miyakawa, and E. Kaneshita: J. Phys. Chem. Solids **127**, (2019) 035121.
6. Magnetization plateau and supersolid phases in the spin-1/2 antiferromagnetic Heisenberg model on a tetragonally distorted fcc lattice
   K. Morita and T. Tohyama: Phys. Rev. B **99**, (2019) 144417.

TOKIWA, Hiroaki [C class; 3500 (B), 0 (C)] (112)
— *Theoretical Study of Industrial Enzyme and Drug Target Protein using the Forth Revolution*

1. Development of analysis toolkit to visualize interaction energies generated by fragment molecular orbital calculations
   Takaki Tokiwa, Shogo Nakano, Yuta Yamamoto, Takeshi Ishikawa, Sohei Ito, Vladimir Sladek, Kaori Fukuzawa, Yuji Mochizuki, Hiroaki Tokiwa, Fuminori Misaizu, and Yasuteru Shigeta: J. Chem. Info. Model (DOI:10.1021/acs.jcim.8b00649) 59(1), 25-30 (2018)
2. Protein residue networks from energetic and geometric data: Are they identical?
   Vladimir Sladek, Hiroaki Tokiwa, Hitoshi Shimano, Yasuteru Shigeta: J. Chem. Theor. Comp. (DOI: 10.1021/acs.jctc.8b00733) 14(12), 6623-6631 (2018)
3. Dual conformation of the ligand induces the partial agonistic activity of retinoid X receptor α (RXR α)
   Yurina Miyashita, Nobutaka Numoto, Sundaram Arulmozhiraja, Shogo Nakano, Naoya Matsuo, Kanade Shimizu, Osamu Shibahara, Michiko Fujiwara, Hiroki Kakuta, Sohei Ito, Teikichi Ikura, Nobutoshi Ito, Hiroaki Tokiwa: FEBS Lett. (DOI: 10.1002/1873-3468.13301) 593(2), 242-250 (2018)
4. Benchmark analysis of native and artificial NAD^+-dependent enzymes generated by a sequence based design method with or without phylogenetic data
   Shogo Nakano, Tomoharu Motoyama, Yurina Miyashita, Yuki Ishizuka, Naoya Matsuo, Hiroaki Tokiwa, Suguru Shinoda, Yasuhisa Asano, and Sohei Ito: Biochem. (DOI: 10.1021/acs.biochem.8b00339) 57(26), 3722-3732 (2018)
5. Molecular association model of PPARα and its new specific and efficient ligand, pemafibrate: Structural basis for SPPARMα
   Yuta Yamamoto, Kenta Takei, Sundaram Arulmozhiraja, Vladimir Sladek, Naoya Matsuo, Songiee Han, Takashi Matsuzaka, Motohiro Sekiya, Takaki Tokiwa, Mitsuo Shoji, Yasuteru Shigeta, Yoshimi Nakagawa, Hiroaki Tokiwa,Hitoshi Shiman: Biochem. Biophys. Res. Comm. (DOI: 10.1016/j.bbrc.2018.03.135) 499(2), 239-245 (2018)
6. Total Synthesis of Termicalcicolanone A via Organocatalysis and Regioselective Claisen Rearrangement
   Saki Ito, Taiki Kitamura, Sundaram Arulmozhiraja, Kei Manabe, Hiroaki Tokiwa, and Yumiko Suzuki: Org. Lett.(DOI: 10.1021/acs.orglett.9b00731) 21(8), 2777-2781 (2019)

7. 25S-Adamantyl-23-yne-26,27-dinor-1α,25-dihydroxyvitamin D_3: Synthesis, Tissue Selective Biological Activities, and X-ray Crystal Structural Analysis of Its Vitamin D Receptor Complex
   Rocio Otero, Michiyasu Ishizawa, Nobutaka Numoto, Teikichi Ikura, Nobutoshi Ito, Hiroaki Tokiwa, Antonio Mourin, Makoto Makishima, and Sachiko Yamada: J. Med. Chem. (DOI: 10.1021/acs.jmedchem.8b00427) 61(15), 6658-6673 (2018).
8. 3-(Triflyloxy)benzynes Enable the Regiocontrolled Cycloaddition of Cyclic Ureas to Synthesize 1,4-Benzodiazepine Derivatives
   Hideki Kaneko, Takashi Ikawa, Yuta Yamamoto, Sundaram Arulmozhiraja, Hiroaki Tokiwa, Shuji Akai: Syn. Lett. (DOI: 10.1055/s-0036-1591924) 29(07), 943-948 (2018).

TONEGAWA, Takashi [B class; 1200 (B), 0 (C)] (284)
— *Numerical Study of the One-Dimensional Quantum Spin Systems with Spatial Structures*

1. Ground-State Phase Diagram of an Anisotropic $S = 1/2$ Ladder with Different Leg Interactions
   T. Tonegawa, T. Hikihara, K. Okamoto, S. C. Furuya, and T. Sakai: J. Phys. Soc. Jpn. **87**, 104002 (2018)

TOYAO, Takashi [B class; 500 (B), 70 (C)] (159)
— *Calculation of catalyst electronic structures for catalyst informatics*

TOYODA, Masayuki [B class; 700 (B), 0 (C)] (151)
— *Theoretical Study on Magnetoelectric Effects of Localized Spin Systems in Quadrupole Alignemnt*

1. A-cation control of magnetoelectric quadrupole order in $A(\mathrm{TiO})\mathrm{Cu}_4(\mathrm{PO}_4)_4$ (A = Ba, Sr, and Pb)
   K. Kimura, M. Toyoda, P. Babkevich, K. Yamauchi, M. Sera, V. Nassif, H. M. Rønnow, and T. Kimura: Physical Review B, 97, 134418 (2018)

TSUMURAYA, Takao [C class; 500 (B), 0 (C)] (161)
— *First-principles study on the formation mechanism of long-period stacking ordered structure in Fe based shape memory alloys and Mg alloys*

TSUNETSUGU, Hirokazu [B class; 600 (B), 0 (C)] (303)
— *Numerical study of vortices in ferromagnetic superconductor*

TSUNEYUKI, Shinji [C class; 7000 (B), 1000 (C)] (65)
— *Development and application of first-principles simulation methods: from structure prediction to superconductivity*

1. First-principles study on substitution effects in $\mathrm{Nd}_2(\mathrm{Fe, X})_{14}\mathrm{B}$
   Y. Tatetsu, S. Tsuneyuki and Y. Gohda: Materialia **4** (2018) 388.
2. First-principles study of phonon anharmonicity and negative thermal expansion in ScF_3
   Y. Oba, T. Tadano, R. Akashi and S. Tsuneyuki: Phys. Rev. Materials **3** (2019) 033601.
3. Ab initio prediction of structural phase-transition temperature of SrTiO_3 from finite-temperature phonon calculation
   T. Tadano and S. Tsuneyuki: J. Ceram. Soc. Jpn., in press.
4. Crystal structure prediction supported by incomplete experimental data
   N. Tsujimoto, D. Adachi, R. Akashi, S. Todo and S. Tsuneyuki: Phys. Rev. Materials **2** (2018) 053801.
5. Neural-network Kohn-Sham exchangecorrelation potential and its out-of-training transferability
   R. Nagai, R. Akashi, S. Sasaki and S. Tsuneyuki: J. Chem. Phys. **148** (2018) 241737.
6. Ferromagnetism above 1000 K in highly cation-ordered double-perovskite insulator $\mathrm{Sr}_3\mathrm{OsO}_6$
   Y.K. Wakabayashi, Y. Krockenberger, N. Tsujimoto, T. Boykin, S. Tsuneyuki, Y. Taniyasu and H. Yamamoto: Nat. Commun. **10** (2019) 535.
7. Search for common minima in joint optimization of multiple cost functions
   D. Adachi, N. Tsujimoto, R. Akashi, S. Todo and S. Tsuneyuki: Comp. Phys. Commun., in press.

TSURUTA, Kenji [C class; 1500 (B), 0 (C)] (132)
— *Ab-initio Metaheuristics for Functional Design of Nanocarbon*

1. Metaheuristic Ab-initio Optimum Search for Doping Effects in Nanocarbons
   Kenji Tsuruta, Keiichi Mitani, Md. Abdullah Al Asad, Yuta Nishina, Kazuma Gotoh, and Atsushi Ishikawa: Materials Science Forum

UCHIDA, Takashi [B class; 300 (B), 80 (C)] (310)
— *Theory of multiple spin density waves and magnetic skyrmions in frustrated itinerant magnets*

UDAGAWA, Masafumi [C,D class; 11500 (B), 450 (C)] (215)
— *Dynamics of fractional excitations in quantum spin liquid*
— *Gauge charge picture of spin liquids: Structure formation and magnetic correlation*

1. Vison-Majorana complex zero-energy resonance in Kitaev's spin liquid
   Masafumi Udagawa: Physical Review B **98**, 220404(R)-1-5
2. Spectrum of itinerant fractional excitations in quantum spin ice
   Masafumi Udagawa, Roderich Moessner: Phys. Rev. Lett. **122** (2019) 117201
3. Magnetic clustering, half-moons, and shadow pinch points as signals of a proximate Coulomb phase in frustrated Heisenberg magnets
   Tomonari Mizoguchi, Ludovic D. C. Jaubert, Roderich Moessner, Masafumi Udagawa: Phys. Rev. B **98** (2018) 144446

WAKABAYASHI, Daisuke [B class; 700 (B), 0 (C)] (291)
— *Compression behavior and inhomogeneous structure of silica glass in its intermediate state in structural transformations*

WATANABE, Hiroshi [B class; 800 (B), 100 (C)] (288)
— *Data compression for molecular dynamics simulation on the basis of multiresolution analysis*

1. Fast algorithm for generating random bit strings and multispin coding for directed percolation
   H. Watanabe, S. Morita, S. Todo, and N. Kawashima, J. Phys. Soc. Jpn. **88**, 024004 (2019)

WATANABE, Hiroshi [B class; 600 (B), 0 (C)] (201)
— *Novel phenomena induced by intradimer charge degree of freedom in molecular conductors*

1. Mechanism of superconductivity and electron-hole doping asymmetry in κ-type molecular conductors
   H. Watanabe, H. Seo, and S. Yunoki: submitted, arXiv: 1811.09035.

WATANABE, Kazuyuki [C class; 10000 (B), 1750 (C)] (53)
— *First-Principles Study of Excited Electron, Positron and Atom Dynamics and Optical Responses of Nanostructures*

1. Electron scattering in time-dependent density functional theory
   L. Lacombe, Y. Suzuki, K. Watanabe, and N. T. Maitra, The European Physical Journal B **91**, 96 (2018).
2. Secondary-electron emission from multi-layer graphene: time-dependent first-principles study
   Y. Ueda, Y. Suzuki, and K. Watanabe, Appl. Phys. Express **11**, 105101 (2018).
3. Time-Dependent Multicomponent Density Functional Theory for Coupled Electron-Positron Dynamics
   Y. Suzuki, S. Hagiwara and K. Watanabe, Phys. Rev. Lett. **121**, 133001 (2018).
4. Thermal effects on laser-assisted field evaporation from a Si surface: A real-time first-principles study
   K. Uchida, Y. Suzuki, and K. Watanabe, submitted.

WATANABE, Satoshi [C class; 12000 (B), 1850 (C)] (51)
— *Theoretical Analyses on Various Properties Concerning Nanodevices*

1. CO-tip manipulation using repulsive interactions
   N. K. M. Nazriq, E. Minamitani, and T. K. Yamada: Nanotechnology **29** (2018) 495701.

2. Inelastic electron tunneling spectroscopy by STM of phonons at solid surfaces and interfaces
   E. Minamitani, N. Takagi, R. Arafune, T. Frederiksen, T. Komeda, H. Ueba, and S. Watanabe: Prog. Surf. Sci. **93** (2018) 131.
3. Phonon Angular Momentum Induced by the Temperature Gradient
   M. Hamada, E. Minamitani, M. Hirayama, S. Murakami: Phys. Rev. Lett. 121 (2018) 175301.
4. 固体表面を舞台とした電子フォノン相互作用の研究
   南谷英美: 固体物理 **53** (2018) 609.
5. 電子相関とスピン軌道相互作用が生み出す吸着分子の新奇な磁性
   南谷英美, 高木紀明: 日本物理学会誌 **73** (2018) 690.
6. ニューラルネットワークを用いたアモルファス物質中の原子拡散の研究
   安藤康伸, 李文文 and 渡邉 聡: 固体物理 **53** (2018) 389.
7. A Comparative Study on the Diffusion Behaviors of Metal and Oxygen Ions in Metal-Oxide Based Resistance Switches via Ab Initio Molecular Dynamics Simulations
   B. Xiao, X.-F. Yu, and S. Watanabe: ACS Appl. Electronic Mater., in press.
8. Moisture Effect on the Diffusion Behaviors of Cu ions in $Cu/Ta_2O_5/Pt$ and $Cu/SiO_2/Pt$ Resistance Switches: A First-Principle Study
   B. Xiao and S. Watanabe: submitted to Sci. Technol. Adv. Mater.
9. Mechanically tunable spontaneous vertical charge redistribution in few-layer WTe_2
   Z. Ni, E. Minamitani, K. Kawahara, R. Arafune, C.-L. Lin, N. Takagi, and S. Watanabe: submitted to ACS Nano
10. First-principles study of Li-ion distribution at γ-Li_3PO_4/metal interfaces
    K. Shimizu, W. Liu, W. Li, S. Kasamatsu, Y. Ando, E. Minamitani, and S. Watanabe: submitted to Phys. Rev. Mater.

YAMADA, Atsuo [C class; 5500 (B), 900 (C)] (75)
— *First-principles investigations of battery materials*

1. Redox-Driven Spin Transition ina Layered Battery Cathode Material
   E. Watanabe, W. Zhao, A. Sugahara, B.Mortemard de Boisse, L. Lander, D. Asakura, Y.Okamoto, T. Mizokawa, M. Okubo and A.Yamada: Chem. Mater. **31** (2019) 2358.
2. Combined Theoretical and Experimental Studies of Sodium Battery Materials
   E. Watanabe, S. Chung, S. Nishimura, Y.Yamada, M. Okubo and A. Yamada: Chem. Rec. **19** (2019)1.

YAMADA, Atsushi [C class; 2500 (B), 600 (C)] (191)
— *Superconductivity and magnetic properties of the Hubbard model*

YAMAGUCHI, Shu [C class; 5000 (B), 0 (C)] (90)
— *Bronsted Acidity on Oxide Surface Induced by Neutralization of Lewis Acid Sites by Molecules*

YAMAJI, Youhei [E class; 12000 (B), 2250 (C)] (175)
— *Numerical studies on fractional excitations in strongly correlated electron systems*

1. Path to stable quantum spin liquids in spin-orbit coupled correlated materials
   Andrei Catuneanu, Youhei Yamaji, Gideon Wachtel, Yong Baek Kim, and Hae-Young Kee: npj Quantum Materials **3** (2018) 23.
2. Ab initio effective Hamiltonians for cuprate superconductors
   Motoaki Hirayama, Youhei Yamaji, Takahiro Misawa, and Masatoshi Imada: Phys. Rev. B **98** (2018) 134501.
3. Classical and quantum spin dynamics of the honeycomb Γ model
   Anjana M. Samarakoon, Gideon Wachtel, Youhei Yamaji, D. A. Tennant, Cristian D. Batista, and Yong Baek Kim: Phys. Rev. B **98** (2018) 045121.
4. Stripe and superconducting order competing in the Hubbard model on a square lattice studied by a combined variational Monte Carlo and tensor network method
   Andrew S. Darmawan, Yusuke Nomura, Youhei Yamaji, and Masatoshi Imada: Phys. Rev. B **98** (2018) 205132.

YAMAMOTO, Norifumi [B class; 800 (B), 100 (C)] (146)
— *Theoretical Study on the Aggregation-Induced Emission*

YAMASHITA, Koichi [C class; 6000 (B), 0 (C)] (77)
— *Large scale ab initio calculations on the fundamental processes of solar energy convergence devices and on designing principles for new materials*

1. Investigations on the charge transfer mechanism at donor/acceptor interfaces in quest of descriptors of organic solar cell performance
   A. Muraoka, M. Fujii, K. Mishima, H. Matsunaga, H. Benten, H. Ohkita, S. Ito and K. Yamashita: Phys. Chem. Chem. Phys. **20** (2018) 1219312199.
2. Halogen in materials design: Revealing the nature of hydrogen bonding and other non-covalent interactions in the polymorphic transformations of methylammonium lead tribromide perovskite
   A. Varadwaj, P. R. Varadwaj, H. M. Marques and K. Yamashita: Mater. Today Chem. **9** (2018) 116.
3. *cis*-1 Isomers of tethered bismethano[70]fullerene as electron acceptors in organic photovoltaics
   T. Umeyama, S. Takahara, S. Shibata, K. Igarashi, T. Higashino, K. Mishima, K. Yamashita and H. Imahori: RSC Adv. **8** (2018) 1831618326.
4. Influence of the aggregate state on band structure and optical properties of C60 computed with different methods
   A. Pal, S. Arabnejad, K. Yamashita and S. Manzhos: J. Chem. Phys. **148** (2018) 204301.
5. Palladium‐ Catalyzed Intramolecular CH Arylation versus 1,5-Palladium Migration: A Theoretical Investigation
   N. Misawa, T. Tsuda, R. Shintani, K. Yamashita and K. Nozaki: Chem. Asian J. **13** (2018) 25662572.
6. Revealing the Cooperative Chemistry of the Organic Cation in the Methylammonium Lead Triiodide Perovskite Semiconductor System
   A. Varadwaj, P. R. Varadwaj and K. Yamashita: ChemistrySelect **3** (2018) 72697282.
7. Two-dimensional optical excitations in the mixed-valence $Cs_2Au_2I_6$ fully inorganic double perovskite
   G. Giorgi, K. Yamashita and M. Palummo: J. Mater. Chem. C **6** (2018) 1019710201.
8. Anion-Substitution-Induced Non-Rigid Variation of Band Structure in $SrNbO_{3-x}N_x$ $(0 \leq x \leq 1)$ Epitaxial Thin Films
   D. Oka, Y. Hirose, M. Kaneko, S. Nakao, T. Fukumura, K. Yamashita and T. Hasegawa: ACS Appl. Mater. Interfaces **10** (2018) 3500835015.
9. Can Combined Electrostatic and Polarization Effects Alone Explain the F$\cdots$F Negative-Negative Bonding in Simple Fluoro-Substituted Benzene Derivatives? A First-Principles Perspective
   P. R. Varadwaj, A. Varadwaj, H. M. Marques and K. Yamashita: Computation **6** (2018) 51.
10. Nature of the Electronic and Optical Excitations of RuddlesdenPopper Hybrid OrganicInorganic Perovskites: The Role of the Many-Body Interactions
    G. Giorgi, K. Yamashita and M. Palummo: J. Phys. Chem. Lett. **9** (2018) 58915896.
11. Halogen in materials design: Chloroammonium lead triiodide perovskite ($ClNH_3PbI_3$) a dynamical bandgap semiconductor in 3D for photovoltaics
    P. R. Varadwaj, A. Varadwaj, H. M. Marques and K. Yamashita: J. Comput. Chem. **39** (2018) 19021912.
12. Probing the nature of the Co(III) ion in corrins: The reactions of aquacyano-5-seco-cobyrinic acid heptamethyl ester with anionic ligands
    M. Nowakowska, S. M. Chemaly, A. L. Rousseau, P. P. Govender, P. R. Varadwaj, A. Varadwaj, K. Yamashita and H. M. Marques: Inorg. Chim. Acta **484** (2018) 402413.
13. Epitaxy of $(GaN)_{1-x}(ZnO)_x$ Solid-Solution Thin Films with Widely Tunable Chemical Composition and Strong Visible Absorption
    C. Yang, Y. Hirose, T. Wakasugi, N. Kashiwa, H. Kawai, K. Yamashita and T. Hasegawa: Phys. Rev. Applied **10** (2018) 44001.
14. A Theoretical study on the charge and discharge states of Na- ion battery cathode material, $Na_{1+x}FePO_4F$
    C. Shinagawa, Y. Morikawa, S. Nishimura, H. Ushiyama, A. Yamada and K. Yamashita: J.

Comput. Chem **40** (2019) 237246.
15. Molecular QTAIM Topology Is Sensitive to Relativistic Corrections
J. S. M. Anderson, J. I. Rodriguez, P. W. Ayers, D. E. Trujillo-Gonzalez, A. W. Goetz, J. Autschbach, F. L. Castillo-Alvarado and K. Yamashita: Chem. Eur. J. **25** (2019) 25382544.
16. Significance of hydrogen bonding and other noncovalent interactions in determining octahedral tilting in the $CH_3NH_3PbI_3$ hybrid organic-inorganic halide perovskite solar cell semiconductor
P. Varadwaj, A. Varadwaj, H. M. Marques and K. Yamashita: Sci. Rep. **9** (2019) 50.
17. Regression model for stabilization energies associated with anion ordering in perovskite-type oxynitrides
M. Kaneko, M. Fujii, T. Hisatomi, K. Yamashita, K. Domen: J. Energy Chem. **36** (2019) 714.
18. Effect of Nuclear Motion on Charge Transport in Fullerenes: A Combined Density Functional Tight BindingDensity Functional Theory Investigation
S. Arabnejad, A. Pal, K. Yamashita and S. Manzhos: Front. Energy Res. **7** (2019) 3.
19. Li and Na Interaction with Ti_2C-MXene: A First-Principles Calculation
S. Kurahashi, S. Arabnejad, H. Ushiyama and K. Yamashita: J. Comput. Chem. Jpn. **18** (2019) 8494.
20. First-principles study on visible light absorption of defected $SrNbO_3$
M. Kaneko, K. Mishima and K. Yamashita: J. Photochem. Photobiol. A: Chem. **375** (2019) 175180.

YAMASHITA, Tomoki [C class; 3000 (B), 850 (C)] (106)
— *Developments of new materials using materials informatics*

1. Fine-grained optimization method for crystal structure prediction
K.Terayama, T. Yamashita, T. Oguchi, and K. Tsuda, npj Comput. Mater. **4**, 32 (2018).

YAMAUCHI, Kunihiko [C class; 6000 (B), 0 (C)] (76)
— *First-Principles DFT Calculations for Topological Matter*

1. Ultrathin Bismuth Film on 1T-TaS_2: Structural Transition and Charge- Density-Wave Proximity Effect
Keiko Yamada, Seigo Souma, Kunihiko Yamauchi, Natsumi Shimamura, Katsuaki Sugawara, Chi Xuan Trang, Tamio Oguchi, Keiji Ueno, Takashi Takahashi, and Takafumi Sato: Nano Lett. **18** (2018) 3235.
2. *A*-cation control of magnetoelectric quadrupole order in $A(TiO)Cu_4(PO_4)_4$ (A =Ba, Sr, and Pb)
K. Kimura, M. Toyoda, P. Babkevich, K. Yamauchi, M. Sera, V. Nassif, H. M. Rønnow, and T. Kimura: Phys. Rev. B **97** (2018) 2268.
3. Ultrathin Bismuth Film on High-Temperature Cuprate Superconductor $Bi_2Sr_2CaCu_2O_{8+\delta}$ as a Candidate of a Topological Superconductor
Natsumi Shimamura, Katsuaki Sugawara, Sukrit Sucharitakul, Seigo Souma, Katsuya Iwaya, Kosuke Nakayama, Chi Xuan Trang, Kunihiko Yamauchi, Tamio Oguchi, Kazutaka Kudo, Takashi Noji, Yoji Koike, Takashi Takahashi, Tetsuo Hanaguri, and Takafumi Sato: ACS Nano **12** (2018) 10977.
4. Magnetic structural unit with convex geometry: A building block hosting an exchange-striction-driven magnetoelectric coupling
Kenta Kimura, Yasuyuki Kato, Kunihiko Yamauchi, Atsushi Miyake, Masashi Tokunaga, Akira Matsuo, Koichi Kindo, Mitsuru Akaki, Masayuki Hagiwara, Shojiro Kimura, Masayuki Toyoda, Yukitoshi Motome, and Tsuyoshi Kimura: Phys. Rev. Mater. **2** (2018) 10415.

YANAGISAWA, Susumu [C class; 3000 (B), 0 (C)] (120)
— *First-principles band structure calculation of organic crystals at finite-temperature*
— *Search for adsorption geometry of an organic molecular layer on a metal surface with the first-principles molecular dynamics*

1. Impact of the molecular quadrupole moment on ionization energy and electron affinity of organic thin films: Experimental determination of electrostatic potential and electronic polarization energies
K. Yamada, S. Yanagisawa, T. Koganezawa, K. Mase, N. Sato, and H. Yoshida: Phys. Rev. B

97 (2018) 245206.
2. Surface Structure of Organic Semiconductor [n]Phenacene Single Crystals
Y. Wakabayashi, M. Nakamura, K. Sasaki, T. Maeda, Y. Kishi, H. Ishii, N. Kobayashi, S. Yanagisawa, Y. Shimo, and Y. Kubozono: J. Am. Chem. Soc. **140** (2018) 14046.
3. Nano-scale first-principles electronic structure simulations of materials relevant to organic electronics
S. Yanagisawa and I. Hamada: A Chapter in Theoretical Chemistry for Advanced Nanomaterials - Functional Analysis by Computation and Experiment edited by Taku Onishi (Springer Nature, 2019)

YANAGISAWA, Takashi [B class; 800 (B), 130 (C)] (198)
— *Optimization variational Monte Carlo study of strongly correlated electron systems*
— *Study of strongly correlated electron systems based on optimization Monte Carlo method and first-principles calculations*

1. Possibility of flat-band ferromagnetism in hole doped pyrochlore oxide $Sn_2Nb_2O_7$ and $Sn_2Ta_2O_7$
I. Hase, T. Yanagisawa, Y. Aiura, K. Kawashima: Physical Review Letters 120 (2018) 196401.
2. Antiferromagnetism, Superconductivity and phase diagram in the two-dimensional Hubbard model
T. Yanagisawa: J. Phys. Soc. Jpn. 88 (2019) 054702.a
3. Optimized wave function by kinetic renormalization effect in strongly correlated region of the three-band Hubbard model
T. Yanagisawa, M. Miyazaki, I. Hase and K. Yamaji: J. Phys. Conf.Ser. 1054 (2018) 012017.a
4. Electronic structure of novel binary superconductor $SrGe_2$
I. Hase, T. Yanagisawa, A. Iyo, H. Eisaki, Y. Yoshida and K. Kawashima: J. Phys. Conf. Series 1054 (2018) 012004.
5. The Competition between CDW and the superconducting state in valence skip compounds
I. Hase, T. Yanagisawa and K. Kawashima: Communications in Computational Physics 23 (2018) 773.
6. Crossover induced electron pairing and superconductivity by kinetic renormalization in correlated electron systems
T. Yanagisawa, M. Miyazaki, K. Yamaji: Condensed Matter 3 (2018) 26.a
7. Massless and quantized modes of kinks in the phase space of superconductors
T. Yanagisawa: Phys. Lett. A382 (2018) 3483.
8. Renormalization group analysis of the hyperbolic sine-Gordon model
T. Yanagisawa: Prog. Theor. Exp. Phys. 2019 (2019) 023A01.
9. Antiferromagnetism, Superconductivity and phase diagram in the three-band model of hig temperature superconductors
T. Yanagisawa: J. Phys. Conf. Ser. (2019) in press.a
10. Green's functions of Nambu-Goldstone and Higgs modes in superconductors
T. Yanagisawa: J. Supercond. Novel Magne. 2018 (2018) 4983 on line.

YASUDA, Chitoshi [C class; 2500 (B), 300 (C)] (263)
— *Randomness Effects on Spin-Peierls System*

1. Antiferromagnetic Long-Range Order for $S = 1/2$ Two-Dimensional Site-Diluted Heisenberg Model Coupled to Lattice Degree of Freedom
S. Miyara and C. Yasuda: J. Phys. Soc. Jpn. **87** (2018) 104702.
2. Ground-state properties of spin-1/2 Heisenberg antiferromagnets with frustration on the diamond-like-decorated square and triangular lattices
Y. Hirose, S. Miura, C. Yasuda, and Y. Fukumoto: AIP Advances **8** (2018) 101427.

YASUOKA, Kenji [C class; 9500 (B), 0 (C)] (58)
— *Study on the Temperature Induced Stability of Defects on Rutile TiO2(110) Surfaces*
— *The Effect of Defect Density on O_2 Absorption Reactions on Rutile TiO_2(110) Surfaces*

YOKO, Akira [B class; 500 (B), 0 (C)] (160)
— *Structural study on surface reconstruction and solvent effects of nanoparticles*

1. Impact of Surface Energy on the Formation of Composite Metal Oxide Nanoparticles
   A. Yoko, N. Umezawa, T. Ohno, and Y. Oshima: J. Phys. Chem. C **122**, 24350-24358 (2018).

YOSHIDA, Tsuneya [C class; 7000 (B), 0 (C)] (181)
— *Anomalous phenomena induced for correlated topological systems*
— *Non-Hermitian properties induced by strong correlations*

1. Symmetry-protected exceptional rings in two-dimensional correlated systems with chiral symmetry
   Tsuneya Yoshida, Robert Peters, Norio Kawakami, and Yasuhiro Hatsugai: Phys. Rev. B 99, (2019) 121101(R)
2. Breakdown of topological Thouless pumping in the strongly interacting regime
   Masaya Nakagawa, Tsuneya Yoshida, Robert Peters, and Norio Kawakami: Phys. Rev. B 98, (2018) 115147
3. Magnetic states in a three-dimensional topological Kondo insulator
   Robert Peters, Tsuneya Yoshida, and Norio Kawakami: Phys. Rev. B 98, (2018) 075104
4. Non-Hermitian perspective of the band structure in heavy-fermion systems
   Tsuneya Yoshida, Robert Peters, and Norio Kawakami: Phys. Rev. B 98, (2018) 035141
5. Topological Properties of Magnetically Ordered Heavy-Fermion Systems in the Presence of Mirror Symmetry
   Kazuhiro Kimura Tsuneya Yoshida, and Norio Kawakami: J. Phys. Soc. Jpn. 87, (2018) 084705
6. Reduction of Topological Z Classification in Cold-Atom Systems
   Tsuneya Yoshida, Ippei Danshita, Robert Peters, and Norio Kawakami: Phys. Rev. Lett. 121, (2018) 025301

YOSHIDOME, Takashi [C class; 2000 (B), 700 (C)] (264)
— *Quantitative computation of the dissociation rate of a protein-ligand complex using a manifold-learning technique*

1. An Automatic Classification of Molecular Dynamics Simulation Data into States, and Its Application to the Construction of a Markov State Model
   R. Ito and T. Yoshidome: J. Phys. Soc. Jpn. **87** (2018) 114802.

YOSHINO, Hajime [C class; 2000 (B), 0 (C)] (269)
— *Spinglass transitions in frustrated vector spin models*

□ SCCMS Projects

FUJITA, Takatoshi [3000 (B), 0 (C)] (323)
— *Development of an excited-state theory based on many-body Green's functions and fragment molecular orbital method*

1. Development of the fragment-based COHSEX method for large and complex molecular systems
   T. Fujita, Y. Noguchi, Phys. Rev. B **98** (2018) 205140.
2. Thousand-atom ab initio calculations of excited states at organic/organic interfaces: toward first-principles investigations of charge photogeneration
   T. Fujita, A. M, Khorshed, T. Hoshi, Phys. Chem. Chem. Phys. **20** (2018) 26443.

FUKUSHIMA, Tetsuya [5000 (B), 500 (C)] (324)
— *First-principles materials design by multi-scale simulation*

1. Anomalous Hall conductivity and electronic structures of Si-substituted Mn2CoAl epitaxial films
   K. Arima, F. Kuroda, S. Yamada, T. Fukushima, T. Oguchi, and K. Hamaya: Phys. Rev. B **97** (2018) 054427.
2. First-principles prediction of the control of magnetic properties in Fe-doped GaSb and InSb
   H. Shinya, T. Fukushima, A. Masago, K. Sato, and H. Katayama-Yoshida: J. Appl. Phys. **124** (2018) 103962.
3. Magnetism of Eu-doped GaN modulations by spinodal nanodecomposition
   A. Masago, H. Shinya, T. Fukushima, K. Sato, and H. Katayama-Yoshida: Phys. Rev. B **98** (2018) 214426.
4. Magnetic and transport properties of equiatomic quaternary Heusler CoFeVSi epitaxial films
   S. Yamada, S. Kobayashi, F. Kuroda, K. Kudo, S. Abo, T. Fukushima, T. Oguchi, and K. Hamaya: Phys. Rev. Materials **2** (2018) 124403.

GOHDA, Yoshihiro [5000 (B), 500 (C)] (328)
— *First-principles calculations of interface magnetic properties at magnetic materials*

1. First-principles study of magnetoelectric coupling at Fe/$BiFeO_3$(001)interfaces
   K. Fujita and Y. Gohda: Phys. Rev. Appl. **11**, 024006 (2019).
2. First-principles prediction of one-dimensional giant Rashba splittings in Bi adsorbed In atomic chains
   T. Tanaka and Y. Gohda: Phys. Rev. B **98**, 241409(R) (2018).
3. First-principles study on substitution effects in Nd_2(Fe, X)$_{14}$B
   Y. Tatetsu, S. Tsuneyuki, and Y. Gohda: Mater. **4**, 388 (2018).
4. Hidden order in amorphous structures: extraction of nearest neighbor networks of amorphous Nd-Fe alloys with Gabriel graph analyses
   A. Terasawa and Y. Gohda:J. Chem. Phys. **149**, 154502 (2018).
5. Role of typical elements in $Nd_2Fe_{14}X$ (X=B, C, N, O, F)
   Y. Tatetsu, Y. Harashima, T. Miyake, and Y. Gohda: Phys. Rev. Mater. **2**, 074410 (2018).

HOSHI, Takeo [5000 (B), 500 (C)] (80)
— *Large-scale device-material research by massively parallel electronic structure calculation and data-driven science*

1. Solution of the k-th eigenvalue problem in large-scale electronic structure calculations
   Dongjin Lee, Takeo Hoshi, Tomohiro Sogabe, Yuto Miyatake, Shao-Liang Zhang, submitted; Preprint (arXiv.1710.05134)

IITAKA, Toshiaki [20000 (B), 100 (C)] (330,332)
— *Computational study of hydrous minerals using the path integral molecular dynamics method II*
— *Structure study of silicate melts using linear scaling ab initio molecular dynamics*

IMADA, Masatoshi [20000 (B), 2000 (C)] (168,171)

— *Emergent Phenomena from Combined Strong Electron Correlation and Electron-Phonon Coupling*

— *Applications of highly accurate lattice model solvers with tensor network and machine learning for mechanisms of superconductivity*

1. Competition among various charge-inhomogeneous states and d-wave superconducting state in Hubbard models on square lattices
   Kota Ido, Takahiro Ohgoe, and Masatoshi Imada: Phys. Rev. B **97** (2018) 045138.
2. Quantum spin liquid signatures in Kitaev-like frustrated magnets
   Matthias Gohlke, Gideon Wachtel, Youhei Yamaji, Frank Pollmann, and Yong Baek Kim: Phys. Rev. B **97**, (2018) 075126.
3. Ab initio effective Hamiltonians for cuprate superconductors
   Motoaki Hirayama, Youhei Yamaji, Takahiro Misawa, and Masatoshi Imada: Phys. Rev. B. **98** (2018) 134501.
4. Direct connection between Mott insulators and d-wave high-temperature superconductors revealed by continuous evolution of self-energy poles
   Shiro Sakai, Marcello Civelli, and Masatoshi Imada : Phys. Rev. B.**98** (2018) 195109
5. Stripe and superconducting order competing in the Hubbard model on a square lattice studied by a combined variational Monte Carlo and tensor network method
   Andrew S. Darmawan, Yusuke Nomura, Youhei Yamaji, and Masatoshi Imada: Phys. Rev. B 98,**98** (2018) 205132.
6. Resummation of diagrammatic series with zero convergence radius for strongly correlated fermions
   Riccardo Rossi, Takahiro Ohgoe, Kris Van Houcke, and Felix Werner: Phys. Rev. Lett. **121** (2018) 130405.
7. Contact and Momentum distribution of the Unitary Fermi Gas
   Riccardo Rossi, Takahiro Ohgoe, Kris Van Houcke, and Felix Werner: Phys. Rev. Lett. **121** (2018) 130406.
8. mVMC-Open-source software for many-variable variational Monte Carlo method
   Takahiro Misawa, Satoshi Morita, Kazuyoshi Yoshimi, Mitsuaki Kawamura, Yuichi Motoyama, Kota Ido, Takahiro Ohgoe, Masatoshi Imada, Takeo Kato: Compt. Phys. Commun.,**235** (2019) 447.
9. Excitons and Dark Fermions as Origins of Mott Gap, Pseudogap and Superconductivity in Cuprate Superconductors — General Idea and Basic Concept Based on Gap Physics
   Takafumi J. Suzuki, Masatoshi Imada: J. Phys. Soc. Jpn. **88** (2019) 024701.

KAWAKATSU, Toshihiro [10000 (B), 1000 (C)] (329)

— *Multiscale simulations on complex multiphase flows*

1. Supercomputer System at ISSP
   T.Murashima, K. Hagita and T.Kawakatsu: J. Soc. Rheol. Jpn. **46** (2018) 207-220.

KAWASHIMA, Naoki [20000 (B), 2000 (C)] (320)

— *Application of Tensor Network Methods to Condensed Matter Physics*

— *Tensor Network Method and Its Application to Condensed Matter Physics*

1. A series of magnon crystals appearing under ultrahigh magnetic fields in a kagome antiferromagnet
   R. Okuma, D. Nakamura, T. Okubo, A. Miyake, A. Matsuo, K. Kindo, M. Tokunaga, N. Kawashima, S. Takeyama and Z. Hiroi: Nature Communications **10**, 1229/1-7 (2019).
2. Calculation of higher-order moments by higher-order tensor renormalization group
   Satoshi Morita, Naoki Kawashima: Computer Physics Communications **236**, 65-71 (2019)
3. Detecting signals of weakly first-order phase transitions in two-dimensional Potts models
   Shumpei Iino, Satoshi Morita, Anders W. Sandvik, and Naoki Kawashima: J. Phys. Soc. Jpn. **88**, 034006/1-8 (2019).
4. Spin-one bilinear-biquadratic model on a star lattice
   Hyun-Yong Lee, and Naoki Kawashima: Phys. Rev. B **97**, 205123/1-7 (2018).
5. Spin Thermal Hall Conductivity of a Kagome Antiferromagnet
   Hayato Doki, Masatoshi Akazawa, Hyun-Yong Lee, Jung Hoon Han, Kaori Sugii, Masaaki Shimozawa, Naoki Kawashima, Migaku Oda, Hiroyuki Yoshida, and Minoru Yamashita: Phys. Rev.

Lett. **121**, 097203/1-4 (2018).

6. Fast algorithm for generating random bit strings and multispin coding for directed percolation
Hiroshi Watanabe, Satoshi Morita, Synge Todo, and Naoki Kawashima: J. Phys. Soc. Jpn. **88**, 024004 (2019).

KOHYAMA, Masanori [20000 (B), 2000 (C)] (312,313)

— *First-Principles Phase Field Mapping*

1. Accurate quasiparticle calculation of x-ray photoelectron spectra of solids
T. Aoki and K. Ohno: J. Phys.: Condensed Mat. **30** (2018) 21LT01.
2. GW($\Gamma\Theta$) method without the Bethe-Salpeter equation for photoabsorption energies of spin-polarized systems
T. Isobe, R. Kuwahara, and K. Ohno: Phys. Rev. A **97**, (2018) 060502(R).
3. A first-principles phase field method for quantitatively predicting multi-composition phase separation without thermodynamic empirical parameter
Swastibrata Bhattacharyya, Ryoji Sahara, and K. Ohno: in submission to Nature Communications.

MISAWA, Takahiro [10000 (B), 1000 (C)] (15)

— *Spin Hall magnetization switching in topological Dirac semimetal*

— *Study of correlated quantum many-body systems using RESPACK*

1. Ab initio effective Hamiltonians for cuprate superconductors
Motoaki Hirayama, Youhei Yamaji, Takahiro Misawa, and Masatoshi Imada: Phys. Rev. B **98**, 134501 (2018).
2. mVMC - Open-source software for many-variable variational Monte Carlo method
Takahiro Misawa, Satoshi Morita, Kazuyoshi Yoshimi, Mitsuaki Kawamura, Yuichi Motoyama, Kota Ido, Takahiro Ohgore, Masatoshi Imada, and Takeo Kato :Comput. Phys. Commun. **235**, 447 (2019).

MIYAKE, Takashi [2500 (B), 0 (C)] (326)

— *Development of permanent magnet materials*

1. First-principles study of spin-wave dispersion in $Sm(Fe_{1-x}Co_x)_{12}$
Taro Fukazawa, Hisazumi Akai, Yosuke Harashima and Takashi Miyake: J. Mag. Mag. Mater. **469** (2019) 296.
2. Effect of R-site substitution and pressure on stability of RFe_{12}: A first-principles study
Yosuke Harashima, Taro Fukazawa, Hiori Kino, and Takashi Miyake: J. Appl. Phys. **124** (2018) 163902.
3. Anisotropy of exchange stiffness based on atomic-scale magnetic properties in rare-earth permanent magnet $Nd_2Fe_{14}B$
Yuta Toga, Masamichi Nishino, Seiji Miyashita, Takashi Miyake and Akimasa Sakuma: Phys. Rev. B **98** (2018) 054418.
4. Important descriptors and descriptor groups of Curie temperatures of rare-earth transition-metal binary alloys
Hieu-Chi Dam, Viet Cuong Nguyen, Tien Lam Pham, Anh Tuan Nguyen, Kiyoyuki Terakura, Takashi Miyake, and Hiori Kino: J. Phys. Soc. Jpn. **87** (2018) 113801.
5. Leaning structure-property relationship in crystalline materials: A study of lanthanide-transition metal alloys
Tien-Lam Pham, Duong-Nguyen Nguyen, Van Doan Nguyen, Hiori Kino, Takashi Miyake, and Hieu Chi Dam: J. Chem. Phys. **148** (2018) 204106.

MORITA, Akihiro [5000 (B), 0 (C)] ()

— *Molecular simulation of ion transport and desolvation at electrode interface*

NOGUCHI, Hiroshi [10000 (B), 1000 (C)] (205)

— *Molecular Dynamics Simulation of Complex Fluids*

1. Polymer effects on Karman vortex: Molecular dynamics study

Y. Asano, H. Watanabe, and H. Noguchi: J. Chem. Phys. **148**,(2018) 144901.

OGATA, Shuji [5000 (B), 0 (C)] (321)
— *Simulation of organic-inorganic interfaces*

1. Unveiling the Chemical Reactions Involved in Moisture-Induced Weakening of Adhesion between Aluminum and Epoxy Resin
   S. Ogata and M. Uranagase: J. Phys. Chem. C (2018) 122 17748-17755.
2. E cient scheme for calculating work of adhesion between a liquid and polymer-grafted substrate
   M. Uranagase, S. Ogata, K. Tanaka, H. Mori, and S. Tajima: J. Chem. Phys. **148** (2018) 064703/1-9.

OGUCHI, Tamio [5000 (B), 0 (C)] (326)
— *Electron Theory on Sodium Secondary-Battery Materials*

1. First-Principles Study on Cathode Properties of Li_2MTiO_4 (M = V, Cr, Mn, Fe, Co, and Ni) with Oxygen Deficiencies for Li-ion Batteries
   M. Hamaguchi, H. Momida, and T. Oguchi, J. Phys. Soc. Jpn. **87**, 044805 (2018).
2. Elucidation of discharge mechanism and evaluation of Na-ion battery performance of tin sulfide (SnS) electrode by using first-principles calculation
   H. Kotaka, H. Momida, A. Kitajou, S. Okada, and T. Oguchi, J. Comput. Chem. Jpn. **18**, 78 (2019).
3. First-Principles Study of Na-Ion Battery Performance and Reaction Mechanism of Tin Sulfide as Negative Electrode
   H. Kotaka, H. Momida, A. Kitajou, S. Okada, and T. Oguchi, Chem. Rec. **19**, 811 (2019).

OKAZAKI, Susumu [10000 (B), 1000 (C)] (322)
— *Conversion and storage of energy - Fuel cells and secondary batteries: Research and development of fundamental technologies of battery simulators*

1. Exploring the Effect of Pendent Side Chain Length on the Structural and Mechanical Properties of Hydrated Perfluorosulfonic Acid Polymer Membranes by Molecular Dynamics Simulation
   A. Kuo, K. Takeuchi, A. Tanaka, S. Urata, S. Okazaki, and W. Shinoda: Polymer,146, 53-62 (2018)
2. Molecular Mechanism of Material Deformation and Failure in Butadiene Rubber: Insight from All-Atom Molecular Dynamics Simulation Using a Bond Breaking Potential Model
   R. S. Payal, K. Fujimoto, C. Jang, W. Shinoda, Y. Takei, H. Shima, K. Tsunoda, and S. Okazaki: Polymer, 170, 113-119 (2019)
3. Difference in molecular mechanisms governing changes in membrane properties of phospholipid bilayers induced by addition of nonionic and zwitterionic surfactants
   Y. Andoh, S. Kitou, S. Okazaki: J. Mol. Liquids, 271, 933-941(2018)

OSHIYAMA, Atsushi [10000 (B), 1000 (C)] (44)
— *Exploration of new-functionality and high-performance semiconductor devices*

1. Structural stability and energy levels of carbon-related defects in amorphous SiO_2 and its interface with SiC
   Y.-i. Matsushita and A. Oshiyama: Jpn. J. Appl. Phys. **57** (2018) 125701
2. Microscopic mechanism of carbon annihilation upon SiC oxidation due to phosphorous treatment: Density functional calculations combined with ion mass spectrometry
   T. Kobayashi, Y.-i. Matsushita, T. Okuda, T. Kimoto and A. Oshiyama: Appl. Phys. Exp. **11** (2018) 121301
3. Reaction Pathway of Surface-Catalyzed Ammonia Decomposition and Nitrogen Incorporation in Epitaxial Growth of Gallium Nitride
   K. M. Bui, J.-I. Iwata, Y. Kangawa, K. Shiraishi, Y. Shigeta, and A. Oshiyama: J. Phys. Chem. C **122** (2018)
4. First-Principle Study of Ammonia Decomposition and Nitrogen Incorporation on the GaN Surface in Metal Organic Vapor Phase Epitaxy
   K. M. Bui, J.-I. Iwata, Y. Kangawa, K. Shiraishi, Y. Shigeta, and A. Oshiyama: J. Cryst. Growth

507 (2019)
5. Structural determination of phosphosilicate glass based on first-principles molecular dynamics calculation
T. Kobayashi, Y.-i. Matsushita, T. Kimoto and A. Oshiyama: Jpn. J. Appl. Phys. **58** (2019) 011001

SAITO, Susumu [5000 (B), 500 (C)] ()
— *Materials design using B, C, and N for next-generation device*

SHIBA, Hayato [10000 (B), 1000 (C)] (316)
— *Molecular dynamics simulation of the hierarchical dynamics and functional dynamics of electrolyte liquids*
— *Numerical simulations of universal features of slow glassy dynamics from molecular liquids to electrolytes*

1. Molecular dynamics study of mesophase transitions upon annealing of imidazolium-based ionic liquids with long-alkyl chains
H. Peng, M. Kubo, and H. Shiba: Phys. Chem. Chem. Phys. 9796-9805 (2018).

SUGINO, Osamu [10000 (B), 1000 (C)] (314)
— *Priority project 5 – energy conversion (chemical energy)*

1. Direct coupling of first-principles calculations with replica exchange Monte Carlo sampling of ion disorder in solids
Shusuke Kasamatsu and Osamu Sugino, J. Phys. Cond. Mat., 31. 085901 (2019).
2. Hydrogen adsorption on Pt (111) revisited from random phase approximation
Lei Yan, Yang Sun, Yoshiyuki Yamamoto, Shusuke Kasamatsu, Ikutaro Hamada, and Osamu Sugino, J. Chem. Phys. 149, 164702 (2018).
3. First-principles investigation of polarization and ion conduction mechanisms in hydroxyapatite
Shusuke Kasamatsu and Osamu Sugino, Phys. Chem. Chem. Phys. 20 8744 (2018).

TAKETSUGU, Tetsuya [10000 (B), 1000 (C)] (99)
— *Ab initio study on abundant nano-catalysts free from precious metals*
— *Ab initio study toward abundant element nanocatalysts with less precious metals*

1. Low-lying Excited States of hqxcH and Zn-hqxc Complex: Toward Understanding Intramolecular Proton Transfer Emission
M. Ebina, Y. Kondo, T. Iwasa, T. Taketsugu: Inorg. Chem., **58**, (2019) 4686-4698.
2. Photoluminescence Properties of [Core+exo]-Type Au6 Clusters: Insights into the Effect of Ligand Environments on the Excitation Dynamics
Y. Shichibu, M. Zhang, T. Iwasa, Y. Ono, T. Taketsugu, S. Omagari, T. Nakanishi, Y. Hasegawa, K. Konishi: J. Phys. Chem. C, **123**, (2019) 6934-6939.
3. Ammonia-rich combustion and ammonia combustive decomposition properties of various supported catalysts
S. Hinokuma, K. Araki, T. Iwasa, S. Kiritoshi, Y. Kawabata, T. Taketsugu, and M. Machida: Catal. Commun., **123**, (2019) 64-68.
4. Combined Automated Reaction Pathway Searches and Sparse Modeling Analysis for Catalytic Properties of Lowest Energy Twins of Cu_13
T. Iwasa, T. Sato, M. Takagi, M. Gao, A. Lyalin, M. Kobayashi, K. Shimizu, S. Maeda, T. Taketsugu: J. Phys. Chem. A, **123**, (2019) 210-217.
5. 金・銀・銅クラスターの安定構造，異性化反応経路，および NO 解離反応経路の探索とその電子物性
近藤有輔，高原里奈，毛利広野，高木牧人，前田理，岩佐豪, 武次徹也: J. Comput. Chem. Jpn., **18**, (2019) 64-69.
6. First principles calculations toward understanding SERS of 2,2′ -bipyridyl adsorbed on Au, Ag and Au-Ag alloy
M. Takenaka, Y. Hashimoto, T. Iwasa, T. Taketsugu, G. Seniutinas, A. Balčytis, S. Juodkazise, Y. Nishijima: J. Comput. Chem., **40**, (2019) 925-932.
7. Supported binary CuOx − Pt catalysts with high activity and thermal stability for the combustion

of NH3 as a carbon-free energy source
S. Kiritoshi, T. Iwasa, K. Araki, Y. Kawabata, T. Taketsugu, S. Hinokuma, and M. Machida: RSC Advances, **8**, (2018) 41491-41498.

8. Spiral Eu(III) Coordination Polymers with Circularly Polarized Luminescence
Y. Hasegawa, Y. Miura, Y. Kitagawa, S. Wada, T. Nakanishi, K. Fushimi, T.Seki, H. Ito, T. Iwasa, T. Taketsugu, M. Gon, K. Tanaka, Y. Chujo, S. Hattori, M. Karasawa, and K. Ishii: Chem. Commun., **54**, (2018) 10695-10697.
9. Insights into Geometries, Stabilities, Electronic Structures, Reactivity Descriptors, and Magnetic Properties of Bimetallic NimCun-m (m = 1, 2; n = 3-13) Clusters: Comparison with Pure Copper Clusters
R. K. Singh, T. Iwasa, and T. Taketsugu: J. Comput. Chem., **39**,(2018) 1878-1889 .

TOHYAMA, Takami [5000 (B), 0 (C)] (246)
— *Cooperation Research with Big Experimental Facilities*

1. Magnetic phase diagram of a frustrated spin ladder
T. Sugimoto, M. Mori, T. Tohyama, and S. Maekawa: Phys. Rev. B **97**, (2018) 144424.
2. Dynamical density matrix renormalization group study of spin and charge excitations in the four-leg t-t'-J ladder
T. Tohyama, M. Mori, and S. Sota: Phys. Rev. B **97**, (2018) 235137.
3. Ground state phase diagram of the Kitaev-Heisenberg model on a honeycomb-triangular lattice
M. Kishimoto, K. Morita, Y. Matsubayashi, S. Sota, S. Yunoki, and T. Tohyama: Phys. Rev. B **98**, (2018) 054411.
4. Ground-state phase diagram of the Kitaev-Heisenberg model on a kagome lattice
K. Morita, M. Kishimoto, and T. Tohyama: Phys. Rev. B **98**, (2018) 134437.
5. Syntheses and first-principles calculations of the pseudobrookite compound $AlTi_2O_5$
T. Tohyama, R. Ogura, K. Yoshinaga, S. Naito, N. Miyakawa, and E. Kaneshita: J. Phys. Chem. Solids **127**, (2019) 035121.
6. Magnetization plateau and supersolid phases in the spin-1/2 antiferromagnetic Heisenberg model on a tetragonally distorted fcc lattice
K. Morita and T. Tohyama: Phys. Rev. B **99**, (2019) 144417.

YABANA, Kazuhiro [15000 (B), 1500 (C)] (319)
— *Dynamics in nano-interface excited by high-intensity pulsed light*
— *Unified Photonic-Electronic Devices*

1. 電子動力学シミュレーションコードのメニーコアプロセッサと GPU における性能比較
廣川祐太, 朴泰祐, 植本光治, 佐藤駿丞, 矢花一浩, 情報処理学会研究報告 2018-HPC-163, 1-11
2. SALMON: Scalable Ab-initio LightMatter simulator for Optics and Nanoscience
M. Noda, S.A. Sato, Y. Hirokawa, M. Uemoto, T. Takeuchi, S. Yamada, A. Yamada, Y Shinohara, M. Yamaguchi, K. Iida, I. Floss, T. Otobe, K.-M. Lee, K. Ishimura, T. Boku, G.F. Bertsch, K. Nobusada, K. Yabana, Comp. Phys. Comm. 235, 356 (2019)

YAMADA, Atsuo [5000 (B), 500 (C)] (75)
— *Theoretical design of electrode materials with oxygen redox activity*

1. Redox-Driven Spin Transition ina Layered Battery Cathode Material
E. Watanabe, W. Zhao, A. Sugahara, B.Mortemard de Boisse, L. Lander, D. Asakura, Y.Okamoto, T. Mizokawa, M. Okubo and A.Yamada: Chem. Mater. **31** (2019) 2358.
2. Combined Theoretical and Experimental Studies of Sodium Battery Materials
E. Watanabe, S. Chung, S. Nishimura, Y.Yamada, M. Okubo and A. Yamada: Chem. Rec. **19** (2019)1.

YOSHIMI, Kazuyoshi [10000 (B), 1000 (C)] (317)
— *Study of many-body correlation effects on spin relaxation rate in quantum dots*
— *Study of spatial anisotropy potential effects on spin relaxation rate in quantum dots*

□ Doctor Theses

1. **HIROKAWA, Yuta**
   Co-design of the ab-initio electron dynamics simulation in advanced high performance computer systems (in Japanese)
   University of Tsukuba, 2018-09

2. **IMOTO, Fumihiro**
   Development of Orbital-Free Density Functional Theory with Machine Learning and its Applications
   the University of Tokyo, 2019-03

3. **INOMOTO, Fumihiro**
   Development of Orbital-Free Density Functional Theory with Machine Learning and its Applications
   the University of Tokyo, 2019-03

4. **KAWASAKI, Airi**
   Geminal theory for strongly correlated few-body systems
   the University of Tokyo, 2019-03

5. **KIM, Seonwoo**
   Development of A High-performance Fluorinated Polymer Electret based on Quantum Chemical Analysisa
   the University of Tokyo, 2019-03

6. **KUMAZOE, Hiroyuki**
   Non-adiabatic ab initio molecular dynamics study of structural and dynamic properties of two-dimensional transition metal dichalcogenides
   Kumamoto University, 2019-03

7. **MIYARA, Shouta**
   Study of Dilution Effects in the Two-Dimensional Antiferromagnetic Heisenberg Model Coupled to the Lattice Degree of Freedom
   University of the Ryukyus, 2019-03

8. **NURUL, Ikhsan**
   Development of first principles approach on the magnetic anisotropy in Fe/MgO interfaces
   Kanazawa University, 2018-09

9. **ONO, Atsushi**
   Theory of Photoinduced Ultrafast Spin Dynamics
   Tohoku University, 2019-03

10. **PRAYITNO, Teguh Budi**
    First-principles Study on Spin Spiral using Linear Combination of Pseudo Atomic Orbitals
    Kanazawa University, 2018-09

11. **SATO, Ryuhei**
    The Research on the Basicity and Proton Conductivity on Hydrated Zrironia
    the University of Tokyo, 2018-09

12. **SUGITA, Yusuke**
Theoretical study of spin-orbit coupled systems with honeycomb-layered structures
the University of Tokyo, 2019-03

13. **TAMURA, Takahiro**
Development and Exploration of New Materials Related with Carbon and Boron Nitride
Hokkaido University, 2018-09

14. **TANAKA, Yuta**
Effect of the electronic entropy on structural change and ablation of metals by an ultrashort laser pulse
the University of Tokyo, 2019-03

15. **TATENO, Michio**
Phase ordering dynamics of colloidal suspensions
the University of Tokyo, 2019-03

16. **TSUJIMOTO, Naoto**
Data assimilation for crystal structure prediction: Construction and implementation of the algorithm and its application
the University of Tokyo, 2019-03

17. **UEDA, Yoshihiro**
Secondary electron emission from nanographene studied by time-dependent density functional theory
The Tokyo University of Science, 2019-03

18. **YAMAMURA, Ryosuke**
Microscopic Theory of Γ_3 Quadrupole Ordering in Pr Compounds on the Basis of a j-j Coupling Scheme
Tokyo Metropolitan University, 2019-03

19. **YOSHITAKE, Junki**
Spin dynamics at finite temperatures in the Kitaev model
the University of Tokyo, 2019-03

□ Master Theses

1. **AKAI, Satoshi**
   First-principles calculation of doping properties in Pb-perovskite halide semiconductors
   Chiba University, 2019-03

2. **CHANG, Yong Lik**
   Elucidation of Reaction Mechanism of Polyalcohol Dehydration in High Temperature Water with Metadynamics
   the University of Tokyo, 2019-03

3. **CHRISTIVANA, Mega**
   First-Principles Calculation on Crystal Structure and Magnetism in β-phase Solid Oxygen
   Kanazawa University, 2018-09

4. **FUJIMOTO, Jun**
   First-principles Study on the Isotope Effect in Hydrocarbons Adsorbed on Noble Metal Surfaces
   Osaka University, 2019-03

5. **FPUTRA, Septia Eka Marsha**
   Theoretical Study of Formic Acid (HCOOH)) on the Cu(111) Surface: Single Molecule and Polymeric Structures
   Osaka University, 2018-09

6. **HASEGAWA, Miki**
   Analysis on the Catalytic Effect of Pt for Etching of Ga at Stepped and Kinked GaN(0001) Surfaces
   Osaka University, 2019-03

7. **HIZUME, Yuma**
   Theoretical study on the effect of spin-fluctuation in superconductivity in iron under high pressure
   the University of Tokyo, 2019-03

8. **IWAHASHI, Daichi**
   Analysis of Cu ion migration in amorphous Ta_2O_5 using neural network potentials
   the University of Tokyo, 2019-03

9. **KANEHIRA, Shinichi**
   Development of descriptor for crystal structure prediction using deep learning
   Osaka University, 2019-03

10. **KANG, Gun-Woo**
    Construction of neural network potentials to analyze ion migration in non-stoichiometric amorphous TaO_x
    the University of Tokyo, 2019-03

11. **KIMURA, Kazuhiro**
    Topological magnetic phases protected by crystalline symmetry in heavy fermion systems
    Kyoto University, 2019-03

12. **KIRIKOSHI, Akimitsu**
    Construction of a Variational Approach for Incorporating Many-Body Effects Self-Consistently in Bose–Einstein Condensed Phase at Finite Temperature
    Hokkaido University, 2019-03

13. **KITAGUCHI, Tomohiro**
First-principles analysis on magnetic properties of systems consisting of transition metal dichalcogenides and adsorbed magnetic metal atoms
the University of Tokyo, 2019-03

14. **KURODA, Yuki**
Hybridization Effects of Molecular Orbitals on Valence Band of Organic Semiconductors
University of Tsukuba, 2019-03

15. **MICHISHITA, Yoshihiro**
The impacts of Rashba spin-orbit coupling, non-hermiticity and periodic laser driving on f-electron materials
Kyoto University, 2019-03

16. **MOCHIHARA, Kosuke**
Magnetic properties of Fe/Pd(001) bilayer affected by quantum-well states formed in Pd layer
Keio University, 2019-03

17. **MORIYA, Tomotaka**
Construction of high-dimensional neural network potentials to analyze Li ion migration in Li_3PO_4 under applied electric fields
the University of Tokyo, 2019-03

18. **MURATA, Itsuki**
Implementation and extension of the band-unfolding method in supercell electronic structure calculation
Kanazawa University, 2019-03

19. **NAGASAWA, Riki**
Defect formation at metal/semiconductor interfaces in electric field: first-principles study
Chiba University, 2019-03

20. **NAITO, Tomoya**
Density functional theory with finite-light-speed correction
the University of Tokyo, 2019-03

21. **NAKAMURA, Kengo**
Research of Kondo effect in two-orbital Anderson model using numerical renormalization group method
Tokyo Metropolitan University, 2019-03

22. **NAKANISHI, Ken M.**
Quantum-classical hybrid algorithm for estimating excited energies of quantum many-body systems
the University of Tokyo, 2019-03

23. **NAKAYAMA, Takafumi**
Evaluation of Optical Activity of Chiral Perylene Derivative (Chiral-PTCDI) Using Classical Molecular Dynamics and Machine Learning Techniques
Osaka University, 2019-03

24. **NISHIMOTO, Toshiki**
Origin of Fermi-level depinning at metal/Ge interfaces: first-principles study
Chiba University, 2019-03

25. **OGURA, Masayoshi**
Development of neural network potentials for calculations of thermal conductivity
the University of Tokyo, 2019-03

26. **ONO, Takanori**
Coarse grained molecular dynamics study of PEGylated lipid effect on physical properties of lipid membranes
Nagoya University, 2019-03

27. **SUGITA, Megumi**
First-principles study of noble metal surfaces and noble metal/oxides interfaces
Kanazawa University, 2019-03

28. **SUZUKI, Motoi**
Event-chain path-integral Monte Carlo and its application to novel quantum phase of Bosons
the University of Tokyo, 2019-03

29. **TAKEDA, Kazuki**
Evaluation of the Structural Stability and Magnetism of Co-doped Anatase TiO_2
Osaka University, 2019-03

30. **TAKEUCHI, Kotono**
Molecular dynamics study on hydrogen permeability for polymer electrolyte membranes
Nagoya University, 2019-03

31. **TAMURA, Miyu**
Multi-dimensional free energy analysis on membrane permeation of ionizable drug
Nagoya University, 2019-03

32. **TANAKA, Yuto**
Anisotropic thermoelectric effect on phosphorene and bismuthene: first-principles calculations based on nonequilibrium Green's function theory
Kanazawa University, 2019-03

33. **WATANABE, Shunta**
First-principles calculation of metal-atom penetration into organic molecular solids
Chiba University, 2019-03

34. **WAZA, Kazunori**
Femtosecond Time-Resolved Spectroscopy in YO Epitaxial Films
University of Fukui, 2019-03

35. **YAJIMA, Yuji**
Study of Dynamical Properties of Silicon Oxide based on First-principles Molecular Dynamics
Shimane University, 2019-03

36. **YAMAGUCHI, Satoshi**
First-principles calculations and experimental consideration of ferromagnetism in Pt(100) ultra thin films
Keio University, 2019-03

37. **YOSHIDA, Hidetaka**
Description of the interaction between magnetic molecules using the DFT+U method
the University of Tokyo, 2019-03