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
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□ ISSP Joint Research Projects

AKAGI, Kazuto [C class; 5000 (B), 0 (C)] (104)
— *Elucidation of diffusion process of ionic species in organic solvent*

AKAGI, Yutaka [B class; 900 (B), 100 (C)] ()
— *Novel Topological Excitation in Magnet*

AKAI, Hisazumi [B class; 1800 (B), 100 (C)] (146, 147)
— *Data accumulation of magnetic properties of rare earth mixed crystal*
— *Data accumulation of magnetic properties of rare earth mixed crystal magnetic materials*
1. Calculating Curie temperatures for rare-earth permanent magnets: Ab initio inspection of localized magnetic moments in d-electron ferromagnetism
   M.Matsumoto and H.Akai : Phys. Rev. B **101**, 1444402 (2020).
2. Curie temperature of Sm_2Fe_{17} and $Nd_2Fe_{14}B$: a first-principles study
   T. Fukazawa, H.Akai, Y. Harashima, and T. Miyake : IEEE Trans. Magn. **55**,2101305 (2019).
3. Ab initio Study of High-field NMR Shift of ^{59}Co in the Ferromagnetic Heusler Alloy Co_2TiGa
   H.Nishihara, H.Akai, K.Sato, T.Kanomata, M.Geshi, T.Sakon, and T.Wada : J. Phys. Soc. Jpn. **88**, 034712 (2019).
4. First-principles study of spin-wave dispersion in $Sm(Fe_{1-x}Co_x)_{12}$
   T. Fukazawa, H.Akai, Y. Harashima, and T. Miyake : J. Magn. Magn. Mater. **469**, 296 (2019).

AKASHI, Ryosuke [C class; 5000 (B), 850 (C)] (89)
— *Ab initio study on the metallization and superconductivity in metallic superhydrides*
1. Superconductivity of LaH_{10} and LaH_{16} polyhydrides
   I. A. Kruglov, D. V. Semenok, H. Song, R. Szczęániak, I. A. Wrona, R. Akashi, M. M. D. Esfahani, D. Duan, T. Cui, A. G. Kvashnin, and A. R. Oganov: Phys. Rev. B **101** (2020) 024508.
2. Archetypical ”push the band critical point” mechanism for peaking of the density of states in three-dimensional crystals: Theory and case study of cubic H_3S
   Phys. Rev. B **101** (2020) 075126.

AOYAMA, Kazushi [B class; 1500 (B), 190 (C)] (301)
— *Effects of a magnetic field on spin-lattice-coupled orders in breathing pyrochlore antiferromagnets*
— *Transport properties of the antiferromagnetic classical XXZ model in two dimensions*
1. Effects of magnetic anisotropy on spin and thermal transport in classical antiferromagnets on the square lattice
   K. Aoyama and H. Kawamura: Phys. Rev. B **100** (2019) 144416.
2. Spin Current as a Probe of the $\mathbf{Z}_2$-Vortex Topological Transition in the Classical Heisenberg Antiferromagnet on the Triangular Lattice

K. Aoyama and H. Kawamura: Phys. Rev. Lett. **124** (2020) 047202.

ARAI, Munehito [C class; 9000 (B), 0 (C)] (252)
— *Computational rational design of novel proteins for industrial and pharmaceutical applications*
— *Protein design toward the development of anti-allergy drugs*

ARAI, Toyoko [C class; 2000 (B), 600 (C)] (135)
— *DFT calculation of atomic displacement captured by energy dissipation channel of noncontact atomic force microscope*

ARIMA, Kenta [B class; 700 (B), 90 (C)] (178)
— *Simulation of STM images of graphene sheet after chemical reduction*

ASANO, Yuta [E class; 30000 (B), 4600 (C)] (241)
— *Karman-Vortex Cavitation in a Complex Fluid*
— *Molecular Dynamics Simulation of Cavitating Flow in a Complex Fluid*

1. Effects of cavitation on Kármán vortex behind circular-cylinder arrays: A molecular dynamics study
   Y. Aasno, H. Watanabe, and H. Noguchi: J. Chem. Phys. **152** (2020) 034501.
2. 分子動力学計算による複雑流体中のカルマン渦の解析
   浅野 優太, 渡辺 宙志, 野口 博司: 分子シミュレーション研究会会誌“アンサンブル”**22**, 157 (2020).

DEKURA, Haruhiko [B class; 800 (B), 0 (C)] (173)
— *First-principles calculation of the higher-order phonon-phonon scattering strength*

EGAMI, Yoshiyuki [C class; 2500 (B), 800 (C)] (119)
— *First-principles study on controlling of electronic structures and electron-transport properties of 2-D materials*
— *First-principles study on controlling of electronic structures and electron-transport properties of atomic layered materials*

1. Efficient calculation of the self-energy matrices for electron-transport simulations
   Y. Egami, S. Tsukamoto and T. Ono: Phys. Rev. B. **100** (2019) 075413.
2. Efficient calculation of the Green's function in scattering region for electron-transport simulations
   Y. Egami, S. Tsukamoto and T. Ono: submitted to Phys. Rev. Lett.

FUCHIZAKI, Kazuhiro [C class; 4500 (B), 200 (C)] (283)
— *Kinetics of phase transition and polyamorphism*

1. Predicting the Melting Curve of MgO: An Essential Update
   K. Fuchizaki: J. Phys. Soc. Jpn. **88** (2019) 065003.

FUJII, Keisuke [B class; 400 (B), 0 (C)] (351)
— *Quantum simulation for quantum many body systems using noisy-intermediate-scale quantum computers*

FUJIMOTO, Yoshitaka [C class; 1500 (B), 0 (C)] (155)
— *First-principles investigation of electronic properties of carbon nanotubes and graphene*

1. 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. **58**, SIIB03 (2019).
2. Electronic structures and scanning tunneling microscopy images of heterostructures consisting of graphene and carbon-doped hexagonal boron nitride layers
   T. Haga, Y. Fujimoto, and S. Saito: Phys. Rev. B **100**, 125403 (2019).
3. Atomic structures and scanning tunneling microscopy of nitrogen-doped carbon nanotubes
   Y. Fujimoto and S. Saito: IOP Conf. Ser.: Mater. Sci. Eng. **744**, 012032 (2020).
4. First-Principles Materials Design for Graphene-based Sensor Devices

Y. Fujimoto: Sustainable Materials for Next Generation Energy Devices (Elsevier 2020),Accepted.

FUJISHIRO, Hiroki [C class; 1500 (B), 0 (C)] (153)
— *Strained Band-Structure Engineering for Antimonide-Based Terahertz Transistors*

FUKUDA, Jun-ichi [B class; 1500 (B), 0 (C)] (312)
— *Calculation of ordered structures and their optical properties of soft materials*

FUKUDA, Masahiro [B class; 800 (B), 100 (C)] (169)
— *Local physical quantities analysis based on the quantum field theory in material surface*

FUKUDA, Tuneo [B class; 700 (B), 0 (C)] (181)
— *First Principles Calculation of 2-Dimensional Silicides Formed on Nickel Surfaces*

1. Formation of two-dimensional silicide on the Ni(100) surface
   T. Fukuda, I. Kishida and K. Umezawa: Jpn. J. Appl. Phys., in press.

FUKUI, Ken-ichi [C class; 1500 (B), 0 (C)] (311)
— *Analysis on Structuring and Dynamics of Ionic Liquid Forming Electric Double Layer as a Local Interfacial Field*

1. Correlation between Mobility and Hydrogen Bonding Network of Water at Electrified-Graphite Electrode Using Molecular Dynamics Simulatio
   M. Imai, Y. Yokota, I. Tanabe, K. Inagaki, Y. Morikawa, K. Fukui : Phys. Chem. Chem. Phys.**22** (2020) 1767
2. Ionic-Liquid-Originated Carrier Trapping Dynamics at the Interface in Electric Double-Layer Organic FET Revealed by Operando Interfacial Analyses
   D. Okaue, I. Tanabe, S. Ono, K. Sakamoto, T. Sato, A. Imanishi, Y. Morikawa, J. Takeya, K. Fukui: J. Phys. Chem. C, **124** (2020) 2543

,

FUKUMOTO, Yoshiyuki [B class; 1300 (B), 0 (C)] (317)
— *Effects of Dzyaloshinskii–Moriya interactions and structural distortions on magnetic susceptibilities of spherical-kagome spin-systems*
— *Effects of Dzyaloshinskii-Moriya interactions and exchange randomness on low-temperature specific heats of spherical-kagome spin-systems*

GOHDA, Yoshihiro [C class; 4500 (B), 700 (C)] (99)
— *First-principles calculations of multiferroic interfaces*

1. First-principles study on surface stability and interface magnetic properties of $SmFe_{12}$
   Y. Ainai, T. Shiozawa, Y. Tatetsu, and Y. Gohda: Appl. Phys. Express **13**, 045502 (2020).
2. First-principles study of crystalline Nd-Fe alloys
   Y. Ainai, Y. Tatetsu, A. Terasawa, and Y. Gohda: Appl. Phys. Express **13**, 017006 (2020).
3. Enhancement of magnetoelectric coupling by insertion of Co atomic layer into $Fe_3Si/BaTiO_3(001)$ interfaces identified by first-principles calculations
   Y. Hamazaki and Y. Gohda: J. Appl. Phys. **126**, 233902 (2019).
4. Great Differences between Low-Temperature Grown Co_2FeSi and Co_2MnSi Films on Single-Crystalline Oxides
   K. Kudo, Y. Hamazaki, S. Yamada, S. Abo, Y. Gohda, and K. Hamaya: ACS Appl. Electron. Mater. **1**, 2371 (2019).
5. Efficient Algorithm Based on Liechtenstein Method for Computing Exchange Coupling Constants Using Localized Basis Set
   A. Terasawa, M. Matsumoto, T. Ozaki, and Y. Gohda: J. Phys. Soc. Jpn. **88**, 114706 (2019).

HAGIWARA, Satoshi [B class; 800 (B), 0 (C)] ()
— *Real-time propagated simulation for electron-positron scattering at the surface*

HAMADA, Ikutaro [C class; 5500 (B), 800 (C)] (82)
— *van der Waals density functional study of molecules adsorbed on metal surfaces*

HAMAGUCHI, Satoshi [C class; 4000 (B), 650 (C)] ()
— *Analyses of Surface Reactions in Atomic Layer Etching Processes*

HAMAMOTO, Yuji [C class; 2000 (B), 0 (C)] (141)
— *van der Waals density functional study of image potential states at organic-metal interfaces*

HARADA, KENJI [C class; 2000 (B), 500 (C)] (292)
— *Application of numerical renormalization group method in condensed-matter physics*

1. Entropy Governed by the Absorbing State of Directed Percolation
   K. Harada and N. Kawashima: Phys. Rev. Lett. **123** (2019) 090601.

HARASHIMA, Yosuke [C class; 1500 (B), 0 (C)] (151)
— *First principles study on leaking current at a dislocation in doped semiconductors*

1. Screw dislocation that converts p-type GaN to n-type: Microscopic study on the Mg condensation and the leakage current in p-n diodes
   T. Nakano, Y. Harashima, K. Chokawa, K. Shiraishi, A. Oshiyama, Y. Kangawa, S. Usami, N. Mayama, K. Toda, A. Tanaka, Y. Honda, and H. Amano: arXiv, 2004.06876 (2020).

HARUYAMA, Jun [C class; 5500 (B), 800 (C)] (80)
— *Electrochemical reaction analysis using density functional calculation + implicit solvation model*

HASHIMOTO, Tamotsu [C class; 1500 (B), 450 (C)] (300)
— *Molecular dynamics simulation of ferroelectrics using a shell model V*

1. Structure of Amorphous $BaTiO_3$ by Molecular Dynamics Simulations Using a Shell Model
   T. Hashimoto and H. Moriwake: Physica B: Condens. Matter **579** (2020) 411799.

HASHMI, Arqum [C class; 1000 (B), 0 (C)] (168)
— *2D materials based symmetric and non-symmetric magnetoresistive junctions*

1. Graphene-based Symmetric and Non-Symmetric Magnetoresistive Junctions
   A. Hashmi, K. Nakanishi, T. Ono: J. Phys. Soc. Jpn. 89, 034708 (2020).

HATSUGAI, Yasuhiro [C class; 4000 (B), 700 (C)] (281)
— *Universality of bulk-edge correspondence by numerical methods*

1. Sequential quantum phase transitions in $J_1 - J_2$ Heisenberg chains with integer spins ($S > 1$): Quantized Berry phase and valence
   Shota Fubasami, Tomonari Mizoguchi and Yasuhiro Hatsugai: Phys. Rev. B **100**, 014438 (2019)
2. Many-Body Chern Number without Integration
   Koji Kudo, Haruki Watanabe, Toshikaze Kariyado, and Yasuhiro Hatsugai: Phys. Rev. Lett. **122**, 146601 (2019)
3. Higher-order Topological Mott Insulators
   Koji Kudo, Tsuneya Yoshida, and Yasuhiro Hatsugai : Phys. Rev. Lett. **123**, 196402 (2019)
4. Non-Hermitian fractional quantum Hall states
   Tsuneya Yoshida, Koji Kudo, and Yasuhiro Hatsugai: Scientific Reports **9**, 16895 (2019)
5. Exceptional rings protected by emergent symmetry for mechanical systems
   Tsuneya Yoshida and Yasuhiro Hatsugai: Phys. Rev. B **100**, 054109 (2019)
6. 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 (2019)
7. Z_Q Berry Phase for Higher-Order Symmetry-Protected Topological Phases
   Hiromu Araki, Tomonari Mizoguchi and Yasuhiro Hatsugai: Phys. Rev. Research **2**, 012009(R) (2020)
8. Higher-order topological phases in a spring-mass model on a breathing kagome lattice
   Hiromasa Wakao, Tsuneya Yoshida, Hiromu Araki, Tomonari Mizoguchi, and Yasuhiro Hatsugai:

Phys. Rev. **101**, 094107 (2020)
9. Exceptional band touching for strongly correlated systems in equilibrium
Tsuneya Yoshida, Robert Peters, Norio Kawakami, Yasuhiro Hatsugai: arXiv:2002.11265
10. Mirror skin effect and its electric circuit simulation
Tsuneya Yoshida, Tomonari Mizoguchi, and Yasuhiro Hatsugai: arXiv:1912.12022
11. Non-Analytic Adiabatic Principle for Anyons
Koji Kudo and Yasuhiro Hatsugai : arXiv:2004.00859.

HATTORI, Ken [C class; 1500 (B), 450 (C)] (143)
— *Atomic structure and electronic states for silicide films*

HAYAMI, Satoru [C class; 5500 (B), 0 (C)] (221)
— *Search for new types of skyrmion crystals based on point group symmetry*

1. Magnetic Vortex induced by Nonmagnetic Impurity in Ferromagnets: Magnetic Multipole and Toroidal around the Vacancy
S. Hayami, H.Kusunose, and Y. Motome: J. Phys. Soc. Jpn. **88**, 063702 (2019).
2. Double-Q Chiral Stripe in the d-p Model with Strong Spin-Charge Coupling
R. Yambe and S. Hayami: J. Phys. Soc. Jpn. **89**, 013702 (2020).
3. Electric Toroidal Quadrupoles in Spin-Orbit-Coupled Metal $Cd_2Re_2O_7$
S. Hayami, Y. Yanagi, H. Kusunose, and Y. Motome: Phys. Rev. Lett. **122**, 147602 (2019).
4. Atomic-Scale Magnetic Toroidal Dipole under Odd-Parity Hybridization
M. Yatsushiro and S. Hayami: J. Phys. Soc. Jpn. **88**, 054708 (2019).
5. Multipole expansion for magnetic structures: A generation scheme for symmetry-adapted orthonormal basis set in crystallographic point group
M.-T. Suzuki, T. Nomoto, R. Arita, Y. Yanagi, S. Hayami, and H. Kusunose: Phys. Rev. B **99**, 174407 (2019).
6. Momentum-Dependent Spin Splitting by Collinear Antiferromagnetic Ordering
M. Naka, S. Hayami, H. Kusunose, Y. Yanagi, Y. Motome, and H. Seo: Nat. Commun. **10**, 4305 (2019).
7. Momentum-Dependent Spin Splitting by Collinear Antiferromagnetic Ordering
S. Hayami, Y. Yanagi, and H. Kusunose: J. Phys. Soc. Jpn. **88**, 123702 (2019).
8. Odd-Parity Multipoles by Staggered Magnetic Dipole and Electric Quadrupole Orderings in CeCoSi
M. Yatsushiro and S. Hayami: J. Phys. Soc. Jpn. **89**, 013705 (2020).
9. Dimension transcendence and anomalous charge transport in magnets with moving multiple-Q spin textures
Y. Su, S. Hayami, and S.-Z. Lin: Phys. Rev. Research **2**, 013160 (2020).

HIDA, Kazuo [B class; 700 (B), 90 (C)] (338)
— *Numerical Study of One Dimensional Frustrated Quantum Spin Systems*

1. Ground State Phases of Distorted S=1 Diamond Chains
K. Hida: J. Phys. Soc. Jpn. **88**, 074705 (2019)
2. Exact Thermodynamic Properties of Mixed Diamond Chains with Strong Single-Site Anisotropy
R. Iwazaki and K. Hida: J. Phys. Soc. Jpn. **88**, 095001 (2019)
3. Ground-State Phases of Alternating-Bond S=1 Diamond Chains
K. Hida: J. Phys. Soc. Jpn. **89**, 024709 (2020)

HIGUCHI, Yuji [C class; 9500 (B), 1650 (C)] (244)
— *Brittle structure of crystalline polymers by large-scale coarse-grained molecular dynamics simulation*
— *Creep fracture process of crystalline polymers by large-scale molecular dynamics simulation*

1. Stress Transmitters at the Molecular Level in the Deformation and Fracture Processes of the Lamellar Structure of Polyethylene via Coarse-Grained Molecular Dynamics Simulations
Y. Higuchi: Macromolecules **52** (2019) 6201.

HINOKIHARA, Taichi [C class; 500 (B), 0 (C)] (349)
— *Magnetization reversal process in classical spin systems*

1. Time Quantified Monte Carlo method for Long-range Interacting Systems
   Taichi Hinokihara,Yuta Okuyama, Munetaka Sasaki, and Seiji Miyashita: Journal of Computational Physics, in review

HINUMA, Yoyo [B class; 600 (B), 0 (C)] (188)
— *Calculation of multication oxide surface properties for catalyst informatics*

1. Band alignment at surfaces and heterointerfaces of Al2O3, Ga2O3, In2O3, and related group-III oxide polymorphs: A first-principles study
   Y. Hinuma, T. Gake, and F. Oba: Phys. Rev. Mater., **3** (2019) 084605.

HIRATSUKA, Masaki [B class; 800 (B), 100 (C)] ()
— *Effect of van der Waals interaction on vibrational spectra from ab initio molecular dynamics simulation*

HIYAMA, Miyabi [B class; 600 (B), 80 (C)] (186)
— *Analysis of absorption spectra for caged compounds in aqueous solution*

1. Theoretical study of the wavelength selection for the photocleavage of coumarin-caged D-luciferin
   J. Usukura, M. Hiyama, M. Kurata, Y. Hazama, X-P. Qiu, F. M. Winnik, H. Akiyama, and N. Koga: Photochem. Photobiol. (2020) in press.
2. Photoabsorption Spectra of Aqueous Oxyluciferin Anions Elucidated by Explicit Quantum Solvent
   Y.Noguchi, M. Hiyama, M. Shiga, H. Akiyama, and O. Sugino: J. Chem.Theo. Comput.,**15** (2019) 5474.

HOSHI, Takeo [C class; 6500 (B), 900 (C)] (76)
— *Unification of massively parallel quantum material simulation and data-driven science*

1. Kω –Open-source library for the shifted Krylov subspace method
   Takeo Hoshi, Mitsuaki Kawamura, Kazuyoshi Yoshimi, Yuichi Motoyama, Takahiro Misawa, Youhei Yamaji, Synge Todo, Naoki Kawashima, Tomohiro Sogabe: arXiv:2001.08707
2. Two-stage data-analysis method for total-reflection high-energy positron diffraction (TRHEPD)
   Kazuyuki Tanaka, Izumi. Mochizuki, Takashi Hanada, Ayahiko Ichimiya, Toshio Hyodo, and Takeo Hoshi: Submitted; Preprint:https://arxiv.org/abs/2002.12165
3. Development of data-analysis software for total-reflection high-energy positron diffraction (TRHEPD)
   Kazuyuki Tanaka, Takeo Hoshi, Izumi Mochizuki, Takashi Hanada, Ayahiko Ichimiya, Toshio Hyodo: Acta. Phys. Pol. A 137, 188-192 (2020).
4. An a posteriori verification method for generalized Hermitian eigenvalue problems in large-scale electronic state calculations
   Takeo Hoshi, Takeshi Ogita, Katsuhisa Ozaki, Takeshi Terao: J. Comp. Appl. Math. 376, 112830/1-13 (2020).
5. Charge-Transfer Excited States in the Donor/Acceptor Interface from Large-Scale GW Calculations
   Takatoshi Fujita, Yoshifumi Noguchi, Takeo Hoshi: J. Chem. Phys. 151, 114109/1-8 (2019).
6. EigenKernel - A middleware for parallel generalized eigenvalue solvers to attain high scalability and usability
   Kazuyuki Tanaka, Hiroto Imachi, Tomoya Fukumoto, Akiyoshi Kuwata, Yuki Harada, Takeshi Fukaya, Yusaku Yamamoto, Takeo Hoshi: Japan J. Indust. Appl. Math 36, 719-742 (2019).
7. Numerical aspect of large-scale electronic state calculation for flexible device material
   Takeo Hoshi, Hiroto Imachi, Akiyoshi Kuwata, Kohsuke Kakuda, Takatoshi Fujita, Hiroyuki Matsui: Japan J. Indust. Appl. Math 36, 685-698 (2019).
8. Recent progress in large-scale electronic state calculations and data-driven sciences
   Takeo Hoshi and Satoshi Ito: Chap. 14 of Handbook of Silicon Based MEMS Materials and Technologies 3rd Ed., Elsevier (2020).
9. Numerical methods for large scale electronic state calculation on supercomputer
   Takeo Hoshi, Yusaku Yamamoto, Tomohiro Sogabe, Kohei Shimamura, Fuyuki Shimojo, Aiichiro

Nakano, Rajiv Kalia, Priya Vashishta: Chap. 15 of 21st Century Nanoscience - A Handbook: Nanophysics Sourcebook (Volume One), CRC Press (2019).

HOSHINO, Shintaro [B class; 900 (B), 0 (C)] (230)
— *Dynamical mean-field theory + quantum Monte Carlo approach to strongly correlated electron systems with multi-orbitals*

1. Nickelate superconductors: Multiorbital nature and spin freezing
   P. Werner and S. Hoshino, Phys. Rev. B 101, 041104(R) (2020).
2. Magnetic Field Induced Phase Transition in Superconducting State of Non-Kramers Doublet Kondo Lattice Systems with Semi-Metallic Conduction Bands
   S. Iimura, M. Hirayama, and S. Hoshino: JPS Conf. Proc. 30, 011048 (2020).
3. Fermi-surface anisotropy effects on full-gap superconductivity in non-Kramers doublets coupled to compensated metals
   S. Iimura, M. Hirayama, and S. Hoshino: JPS Conf. Proc. 29, 011003 (2020).

HOTTA, Chisa [B class; 600 (B), 0 (C)] (347)
— *Numerical studies on some new phases of the transverse Ising model*

1. Spin-orbital glass transition in a model of frustrated pyrochlore magnet without quenched disorder
   Kouta Mitsumoto, Chisa Hotta, and Hajime Yoshino: Phys. Rev. Lett. **124** (2020) 087201.
2. Multiple quadrupolar or nematic phases driven by the Heisenberg interactions in a spin-1 dimer system forming a bilayer
   Katsuhiro Tanaka, Chisa Hotta: Phys. Rev. B **101** (2020) 094422.
3. Discovering momentum-dependent magnon spin texture in insulating antiferromagnets: Role of the Kitaev interaction
   Masataka Kawano, Chisa Hotta: Phys. Rev. B **100** (2019) 174402.

HOTTA, Takashi [C class; 7500 (B), 0 (C)] (215, 217)
— *Research of Two-Channel Kondo Effect in Transuranium Systems*
— *Two-Channel Kondo Effect Emerging in a Multiorbital Anderson Model Hybridized with* Γ_7 *and* Γ_8 *Conduction Bands*

1. Two-Channel Kondo Effect Emerging from Np and Pu Ions
   Dai Matsui and Takashi Hotta, JPS Conf. Proc. **30**, 011125 (2020).

HU, Shiqian [C class; 2500 (B), 650 (C)] (125)
— *manipulation of the cross-plane thermal conductivity on the 2D hetero-junction materials*

HUKUSHIMA, Koji [C class; 3500 (B), 0 (C)] (287)
— *Development of data-driven science to materials science*

1. Adjusting the descriptor for a crystal structure search using Bayesian optimization
   Nobuya Sato, Tomoki Yamashita, Tamio Oguchi, Koji Hukushima, and Takashi Miyake: Phys. Rev. Materials **4**, (2020) 033801.

IDO, Kota [C class; 5000 (B), 750 (C)] (262)
— *Numerical studies on magnetization process of the Kitaev spin liquid*

1. Correlation effects on the magnetization process of the Kitaev model
   K. Ido, and T. Misawa: Phys. Rev. B **101** (2020) 045121.
2. Charge dynamics of correlated electrons: Variational description with inclusion of composite fermions
   K. Ido, M. Imada, and T. Misawa: Phys. Rev. B **101** (2020) 075124.

IGARASHI, Ryo [C class; 1000 (B), 500 (C)] ()
— *Full diagonalization using low-rank approximation to Hamiltonian matrices and its application to quantum spin models*

IKEDA, Hiroaki [B class; 400 (B), 0 (C)] (195)
— *Development and application of the first-principles approach*

IKUHARA, Yuichi [C class; 4500 (B), 0 (C)] (111)
— *Ab initio calculations of atomic and electronic structures for functional oxide materials*
— *Study of atomic and electronic structure of hetero interface by first-principles molecular dynamics simulations*

1. Strong metalmetal interaction and bonding nature in metal/oxide interfaces with large mismatches
   H. Li, M. Saito, C. Chen, K. Inoue, K. Akagi, Y. Ikuhara: Acta Mater. **179** (2019) 237.

IMADA, Masatoshi [E class; 34000 (B), 4950 (C)] (197)
— *Development of methodology for analysis of nonequilibrium superconductivity in strongly correlated systems via integration of electronic state theory and time-resolved experimental data*
— *Mechanism of quantum spin liquid and high-Tc superconductivity studied by excitation spectra and nonequilibrium dynamics calculation by variational Monte Carlo methods*

1. Charge dynamics of correlated electrons: Variational description with inclusion of composite fermions
   Kota Ido, Masatoshi Imada, Takahiro Misawa: Phys. Rev. B **101** (2020) 075124.
2. *Ab initio* study of superconductivity and inhomogeneity in a Hg-based cuprate superconductor
   Takahiro Ohgoe, Motoaki Hirayama, Takahiro Misawa, Kota Ido, Youhei Yamaji, Masatoshi Imada: Phys. Rev. B **101** (2020) 045124.
3. Effective Hamiltonian for cuprate superconductors derived from multiscale ab initio scheme with level renormalization
   Motoaki Hirayama, Takahiro Misawa, Takahiro Ohgoe, Youhei Yamaji, Masatoshi Imada: Phys. Rev. B **99** (2019) 245155.
4. *Ab initio* derivation of an effective Hamiltonian for the $La_2CuO_4/La_{1.55}Sr_{0.45}CuO_4$ heterostructure
   Terumasa Tadano, Yusuke Nomura, Masatoshi Imada: Phys. Rev. B **99** (2019) 155148.

INAGAKI, Kouji [C class; 2000 (B), 600 (C)] ()
— *Analysis and Design of reaction process and catalyst material for CARE machining*

INAOKA, Takeshi [B,C class; 1000 (B), 200 (C)] (160)
— *Search and realization of novel electronic properties of solid surfaces and interfaces and of small particles*
— *Search and realization of novel electronic properties of solid surfaces and interfaces and of small particles II*

1. Finite-difference time-domain analysis of scanning tunneling microscope light emission from vibrating molecules
   Y. Uehara, W. Iida, T. Inaoka, S. Iwaoka, H. Aoyagi, and S. Katano: to be submitted.

ISHIBASHI, Shoji [C class; 4500 (B), 0 (C)] (110)
— *Prediction of properties of organic ferroelectrics and piezoelectrics by first-principles calculation*

1. Coexistence of normal and inverse deuterium isotope effects in a phase-transition sequence of organic ferroelectrics
   S. Horiuchi, S. Ishibashi, K. Kobayashi, and R. Kumai: RSC Adv. **9** (2019) 39662.

ISHIDA, Kunio [B class; 1200 (B), 170 (C)] (315)
— *Entanglement in remote electron-phonon systems created by photoirradiation*
— *Ultrafast nonadiabatic dynamics of electron-phonon-photon system*

1. Interplay of electron-phonon nonadiabaticity and Raman scattering in the wavepacket dynamics of electron-phonon-photon systems
   Kunio Ishida: Eur. Phys. J. D73, 117 (2019)
2. Coherent control of nonadiabatic dynamics of electron-phonon systems by quantized light field
   Kunio Ishida: Progress in Ultrafast Intense Laser Science XV, 10.1007/978-3-030-47098-2_6

ISHIHARA, Sumio [B class; 800 (B), 0 (C)] (234)

— *Photoinduced dynamics and high harmonic generation in magnetism*

1. Nonequilibrium susceptibility in photoinduced Floquet states
   Atsushi Ono and Sumio Ishihara, Phys. Rev. B **100**, 075127 (2019).
2. Optical Response in Excitonic Insulating State: Variational Cluster Approach
   Hengyue Li, Junya Otsuki, Makoto Naka, Sumio Ishihara, Phys. Rev. B **101**, 125117 (2020).
3. Photoinduced Ultrafast Phenomena in Correlated Electron Magnets
   Sumio Ishihara, J. Phys. Soc. Jpn. **88**, 023703 (2019).

ISHII, Fumiyuki [C class; 8500 (B), 0 (C)] (70)

— *First-Principles Crystal Structure Prediction of Magnetic Thermoelectric Materials*

— *First-principles study of electric-field effect on magnetic insulator*

1. Realization of Spin-dependent Functionality by Covering a Metal Surface with a Single Layer of Molecules
   H. Isshiki, K. Kondou, S. Takizawa, K. Shimose, T. Kawabe, E. Minamitani, N. Yamaguchi, F. Ishii, A. Shiotari, Y. Sugimoto, S. Miwa and Y. Otani: Nano Lett. **197** (2019) 7119.
2. First-principles Study of Spiral Spin Density Waves in Monolayer MnCl2 Using Generalized Bloch Theorem
   T.B. Prayitno and F. Ishii: J. Phys. Soc. Jpn. **88** (2019) 104705.
3. Intrinsic persistent spin helix state in two-dimensional group-IV monochalcogenide MX monolayers (M=Sn or Ge and X=S, Se, or Te)
   M.A.U. Absor and F. Ishii: Phys. Rev. B. **100** (2019) 115104.
4. Photoinduced Rashba Spin-to-Charge Conversion via an Interfacial Unoccupied State
   J. Puebla, F. Auvray, N. Yamaguchi, M. Xu, S.Z. Bisri, Y. Iwasa, F. Ishii, and Y. Otani: Phys. Rev. Lett. **122** (2019) 256401.
5. Electric-field-induced Z2 topological phase transition in strained single bilayer Bi(111)
   H. Sawahata, Y. Yamaguchi, and F. Ishii: Appl. Phys. Express **12** (2019) 075009.

ISHIZUKA, Jun [C class; 4500 (B), 750 (C)] (223)

— *Multipole and anisotropic superconductivity from first principles*

1. Insulator-Metal Transition and Topological Superconductivity in UTe_2 from a First-Principles Calculation
   Jun Ishizuka, Shuntaro Sumita, Akito Daido, and Youichi Yanase: Phys. Rev. Lett. 123, 217001 (2019).
2. Observation of superconducting diode effect
   Fuyuki Ando, Yuta Miyasaka, Tian Li, Jun Ishizuka, Yoichi Shiota, Takahiro Moriyama, Yoichi Yanase, and Teruo Ono: submitted to Nature.

ISOBE, Masaharu [B class; 600 (B), 0 (C)] (345)

— *Nonequilibrium phase transition and slow dynamics in the dense hard sphere systems*

IYODA, Eiki [C class; 1500 (B), 0 (C)] (309)

— *Numerical analysis on the off-diagonal eigenstate thermalization hypothesis*

1. Characterizing complexity of many-body quantum dynamics by higher-order eigenstate thermalization
   K. Kaneko, E. Iyoda, and T. Sagawa: Phys. Rev. A, in press.

JESCHKE, Harald [C class; 6500 (B), 0 (C)] (257, 258)

— *Doping dependence of electronic structure and superconductivity in FeSe intercalated by organic molecules*

— *Stability of the superconductor $LaFe_2As_2$*

1. Novel Fe-Based Superconductor LaFe2As2 in Comparison with Traditional Pnictides
   I. I. Mazin, M. Shimizu, N. Takemori, and H. O. Jeschke: Phys. Rev. Lett. **123** (2019), 267001.
2. Unusual non-valence-skipping electronic state of Sn in AgSnSe2

Y. Naijo, K. Hada, T. Furukawa, T. Itou, T. Ueno, K. Kobayashi, I. I. Mazin, H. O. Jeschke, and J. Akimitsu: Phys. Rev. B **101** (2020), 075134.

JOUTSUKA, Tatsuya [B class; 1300 (B), 0 (C)] (158, 159)
— *Ab Initio Calculation of High-Rate Deposition of Copper Film by Low-Pressure Chemical Vapor Deposition with CuI on Ru Substrate*
— *Molecular Science at Solid/Liquid Interfaces using Molecular Dynamics Simulation and Ab Initio Calculation*

1. Low-pressure chemical vapor deposition of Cu on Ru substrate using CuI: Ab initio calculations
   T. Joutsuka, S. Yamauchi: Chem. Phys. Lett. **741** (2020) 137108.

JU, Shenghong [C class; 5000 (B), 1200 (C)] (83)
— *Energy Transport in Hybrid Organic-Inorganic Thermoelectric Materials*

KAGESHIMA, Hiroyuki [C class; 500 (B), 0 (C)] (189)
— *Study on structural elementary excitations at semiconductor surfaces and interfaces*

1. First-principles Study of pressure and SiO-incorporation effect on dynamical properties of silicon oxide
   H. Kageshima, Y. Yajima, K. Shiraishi, and T. Endoh: Jpn. J. Appl. Phys. **58** (2019) 111004 (11pages).

KARIYADO, Toshikaze [B class; 1000 (B), 0 (C)] (331)
— *Manipulation of electronic states with nanostructures: model construction and its application*

1. Flat band in twisted bilayer Bravais lattices
   T. Kariyado and A. Vishwanath, Phys. Rev. Research **1** (2019) 033076.

KASAMATSU, Shusuke [C class; 11000 (B), 1750 (C)] (57, 386)
— *Designing doping schemes for $BaZrO_3$-based ion conductors*
— *First-principles configurational sampling of highly-doped ionic conductors*

1. Insights Into Defect Arrangements in Y-Doped BaZrO3 From Large-Scale First-Principles Thermodynamic Sampling: Association, Repulsion, Percolation, and Trapping
   Chemrxiv. Preprint.

KATO, Takeo [D class; 10000 (B), 1000 (C)] (210)
— *Variational Monte Carlo calculation of two-dimensional Wigner crystal under lattice commensurability*

KATO, Yusuke [C class; 5000 (B), 0 (C)] (272)
— *Functional Renormalization Group Study of Quantum Spin Liquids*

KAWAKAMI, Norio [C class; 9500 (B), 1700 (C)] (206)
— *Study of magnetism and superconductivity in strongly correlated quantum systems using approaches including non-equilibrium methods*
— *Study of magnetism topology and transport phenomena in strongly correlated quantum systems*

1. Spin-caloritronic transport in hexagonal graphene nanoflakes
   Thi. Thu Phung, Robert Peters, Andreas Honecker, Guy Trambly de Laissardiere, and Javad Vahedi: arXiv:2003.01139.
2. Equivalence of the effective non-hermitian Hamiltonians in the context of open quantum systems and strongly-correlated electron systems
   Yoshihiro Michishita and Robert Peters: arXiv:2001.09045.
3. Hubbard model on the honeycomb lattice: From static and dynamical mean-field theories to lattice quantum Monte Carlo simulations
   Marcin Raczkowski, Robert Peters, Thi. Thu Phng, Nayuta Takemori, Fakher F. Assaad, Andreas Honecker, and Javad Vahedi: Phys. Rev. B **101** (2020) 125103.
4. Relationship between exceptional points and the Kondo effect in f -electron materials

Yoshihiro Michishita, Tsuneya Yoshida, and Robert Peters: Phys. Rev. B **101** (2020) 085122.
5. Chiral-symmetry protected exceptional torus in correlated nodal-line semimetals
Kazuhiro Kimura, Tsuneya Yoshida, and Norio Kawakami: Phys. Rev. B **100** (2019) 115124.
6. Quantum oscillations in strongly correlated topological Kondo insulators
Robert Peters, Tsuneya Yoshida, and Norio Kawakami: Phys. Rev. B **100** (2019) 085104.
7. Impact of the Rashba Spin Orbit Coupling on f-electron Materials
Yoshihiro Michishita and Robert Peters: Phys. Rev. B **99** (2019) 155141.

KAWAMURA, Hikaru [C class; 11000 (B), 0 (C)] (249)
— *Novel order in frustrated magnets*
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, 1444062-(1-14) (2019)
2. Ripple state in the frustrated honeycomb-lattice antiferromagnet
T. Shimokawa and H. Kawamura, Phys. Rev. Letters 123, 057202(1-6) (2019)
3. Nature of the randomness-induced quantum spin liquids in two dimensions
H. Kawamura and K. Uematsu, J. Phys. Condens. Matter 31, 504003(1-18) (2019)
4. Randomness-induced quantum spin liquid behavior in the s=1/2 random-bond Heisenberg antiferromagnet on the pyrochlore lattice
K. Uematsu and H. Kawamura, Phys. Rev. Letters 123, 087201-(1-6) (2019)
5. Effects of magnetic anisotropy on spin and thermal transport in classical antiferromagnets on the square lattice
K. Aoyama and H. Kawamura, Phys. Rev. B 100, 144416-(1-19) (2019)
6. Multiple-q states of the J1-J2 classical honeycomb-lattice Heisenberg antiferromagnet under a magnetic field
T. Shimokawa and H. Kawamura, Phys. Rev. B 100, 224404-(1-15) (2019)
7. Monte Carlo study of the critical properties of noncollinear Heisenberg magnets: O(3) × O(2) universality class
Y. Nagano, K. Uematsu, and H. Kawamura, Phys. Rev. B 100, 224430(1-15) (2019)
8. Monte Carlo studies of the spin-chirality decoupling in the three-dimensional Heisenberg spin glass
T. Ogawa, K. Uematsu, and H. Kawamura, Phys. Rev. B 101, 014434(1-16) (2020)
9. Spin Current as a Probe of the Z2-Vortex Topological Transition in the Classical Heisenberg Antiferromagnet on the Triangular Lattice
K. Aoyama and H. Kawamura, Phys. Rev. Letters 124, 047202-(1-6) (2020)

KAWAMURA, Mitsuaki [B class; 700 (B), 90 (C)] (176)
— *Benchmark of density functional theory for superconductors*
1. Benchmark of density functional theory for superconductors in elemental materials
M. Kawamura, Y. Hizume, and T. Ozaki Phys. Rev. B **101**, (2020) 134511.

KAWASHIMA, Naoki [E class; 39000 (B), 5450 (C)] (239)
— *Tensor-Ring Decomposition Based on HOSVD and Its Appication*
— *Variational calculation of Kitaev and related models with tensor-network representation*
1. Tensor network wavefunction of S = 1 Kitaev spin liquids
Hyun-Yong Lee, Naoki Kawashima, and Yong Baek Kim:arXiv:1911.07714
2. Boundary conformal spectrum and surface critical behavior of classical spin systems:A tensor network renormalization study
Shumpei Iino, Satoshi Morita, and Naoki Kawashima: Phys. Rev. B **101**, 155418 (2020)
3. Magnetic field induced quantum phases in a tensor network study of Kitaev magnets
Hyun-Yong Lee, Ryui Kaneko, Li Ern Chern, Tsuyoshi Okubo, Youhei Yamaji, Naoki Kawashima and Yong Baek Kim: Nature Communications **11**, 1639 (2020)
4. Abelian and non-Abelian chiral spin liquids in a compact tensor network
Hyun-Yong Lee, Ryui Kaneko, Tsuyoshi Okubo, Naoki Kawashima: Phys. Rev. B **101**, 035140 (2020)
5. Thermal-transport studies of kagom antiferromagnets

Minoru Yamashita, Masatoshi Akazawa, Masaaki Shimozawa, Takasada Shibauchi, Yuji Matsuda, Hajime Ishikawa, Takeshi Yajima, Zenji Hiroi, Migaku Oda, Hiroyuki Yoshida, Hyun-Yong Lee, Jung Hoon Han and Naoki Kawashima: J. Phys: Condens. Matter **32**, 074001(11pp) (2019)

6. Entropy Governed by the Absorbing State of Directed Percolation
   Kenji Harada and Naoki Kawashima: Phys. Rev. Lett. **123**, 090601 (2019)
7. Boundary Tensor Renormalization Group
   Shumpei Iino, Satoshi Morita, and Naoki Kawashima: Phys. Rev. B **100**, 035449 (2019)
8. Gapless Kitaev Spin Liquid to Classical String Gas through Tensor Networks
   Hyun-Yong Lee, Ryui Kaneko, Tsuyoshi Okubo, and Naoki Kawashima: Phys. Rev. Lett. **123**, 087203 (2019)
9. Tensor-Ring Decomposition with Index-Splitting
   Hyun-Yong Lee and Naoki Kawashima: J. Phys. Soc. Jpn. **89**, 054003 (2020)

KITA, Takafumi [C class; 1000 (B), 0 (C)] ()
— *studying the enhancement of the thermal Hall angle in d-wave superconductors*

KITAO, Akio [C class; 5000 (B), 0 (C)] (270)
— *Efficient sampling simulation of the soft modes significantly contribute to protein properties*

1. Kinetic selection and relaxation of the Intrinsically Disordered Region of a Protein upon Binding.
   D.P. Tran and A Kitao: J. Chem. Theory Comput, in press (2020) doi: 10.1021/acs.jctc.9b01203.
2. High pressure inhibits signaling protein binding to the flagellar motor and bacterial chemotaxis through enhanced hydration.
   H. Hata, Y. Nishihara, M. Nishiyama, Y. Sowa, I. Kawagishi, A. Kitao: Sci. rep. **10** (2020) 2351.
3. Molecular dynamics simulation of proteins under high pressure: Structure, function and thermodynamics.
   H. Hata, M. Nishiyama, A. Kitao: Biochimica et Biophysica Acta **1864** (2020) 7.
4. evERdock BAI: Machine-learning-guided selection of protein-protein complex structure.
   K. Terayama, A. Shinobu, K. Tsuda, K. Takemura, and A. Kitao: J. Chem. Phys. **151** (2019) 215104.
5. Impact of key residues within chloroplast thioredoxin-f on recognition for reduction and oxidation of target proteins.
   Y. Yokochi et. al.: J. Biol. Chem. **294** (2019) 17437.
6. Phagocytosis is mediated by two-dimensional assemblies of the F-BAR protein GAS7.
   K. Hanawa-Suetsugu et. al.: Nat. Commun. **10** (2019) 10.
7. Enhancing Biomolecular Sampling with Reinforcement Learning: A Tree Search Molecular Dynamics Simulation Method.
   K. Shin, D.P. Tran, K. Takemura, A. Kitao, K. Terayama, and K. Tsuda: ACS omega **4** (2019) 13853.
8. Cancellation between auto-and mutual correlation contributions of protein/water dynamics in terahertz time-domain spectra.
   Y. Joti and A. Kitao: Biophys. Physicobiol. **16** (2019) 240.
9. More efficient screening of protein-protein complex model structures for reducing the number of candidates.
   K. Takemura and A. Kitao: Biophys. Physicobiol. **16** (2019) 295.

KOBAYASHI, Akito [B class; 1500 (B), 200 (C)] (228)
— *Spin-Charge Separation in Charge Order Phase of Organic Dirac Electron System α-(BEDT-TTF)$_2I_3$*

1. Domain wall conductivity with strong Coulomb interaction of two-dimensional massive Dirac electrons in the organic conductor α-(BEDT-TTF)2I3
   D. Ohki, Y. Omori, and A. Kobayashi, Phys. Rev. **B** 100, 075206 (2019).

KOBAYASHI, Katsuyoshi [B class; 400 (B), 50 (C)] (190)
— *Theoretical study on electronic properties of new nanoscale surfaces and interfaces*

KOBAYASHI, Nobuhiko [C class; 4000 (B), 650 (C)] (108)
— *First-principles study of quantum transport in nanostructures*

1. Second highest occupied molecular orbital effects on the valence band structure of organic semiconductors
   Y. Kuroda, H. Ishii, S. Yoshino, N. Kobayashi, Jpn. J. Appl. Phys. 58 SIIB27 (2019).
2. Carrier transport calculations of organic semiconductors with static and dynamic disorder
   H. Ishii , N. Kobayashi, and K. Hirose, Jpn. J. Appl. Physics 58, 110501 (2019).
3. Electronic Band Structure of TiN/MgO-4×4 and 5×5 Nanostructures
   K. Kobayashi, H. Takaki, M. Shimono, N. Kobayashi, and K. Hirose, Jpn. J. Appl. Phys. 58 SBBH06 (2019).
4. Seebeck coefficients in $CuFeS_2$ thin films by first-principles calculations
   H. Takaki, K. Kobayashi, M. Shimono, N. Kobayashi, K. Hirose, N. Tsujii, and T. Mori Jpn. J. Appl. Phys. 58 SIIB01 (2019).
5. Magnetism-mediated thermoelectric performance of the Cr-doped bismuth telluride tetradymite
   J. B. Vaney, S. A. Yamini, H. Takaki, K. Kobayashi, N. Kobayashi, T. Mori, Mater. Today Phys. 8 (2019) 100090.
6. Sub-molecular structural relaxation at a physisorbed interface with monolayer organic single-crystal semiconductors
   A. Yamamura, H.Fujii, H. Ogasawara, D. Nordlund, O. Takahashi, Y. Kishi, H. Ishii, N. Kobayashi, N. Niitsu, B. Blulle, T. Okamoto, Y. Wakabayashi, S. Watanabe, and J. Takeya, Commun. Phys. 3 20 (2020)
7. Charge mobility calculation of organic semiconductors without use of experimental single-crystal data
   H. Ishii, S. Obata, N. Niitsu, S. Watanabe, H. Goto, K. Hirose, N. Kobayashi, T. Okamoto, and J. Takeya, Sci Rep 10, 2524 (2020)

KOBAYASHI, Riki [B class; 300 (B), 0 (C)] (357)
— *Screening of substitutable non-magnetic element in rare-earth inter-metallic compounds*

KOGA, Akihisa [C class; 9500 (B), 650 (C)] (211, 212)
— *Magnetic and transport properties in double-exchange systems with quasiperiodicity*
— *Numerical analysis for nonequilibrium dynamics in correlated electron systems with orbital degrees of freedom*

1. Majorana-mediated spin transport without spin polarization in Kitaev quantum spin liquids
   T. Minakawa, Y. Murakami, A. Koga and J. Nasu: submitted to PRL.
2. Spin transport in the Quantum Spin Liquid State in the $S = 1$ Kitaev model: role of the fractionalized quasiparticles
   A. Koga, T. Minakawa, Y. Murakami and J. Nasu: J. Phys. Soc. Jpn. **89** (2020) 033701.
3. Excitonic condensation reflecting electronic states in two-band Penrose-Hubbard model
   K. Inayoshi, Y. Murakami and A. Koga: submitted to JPSJ.

KOMATSU, Hisato [B class; 1100 (B), 150 (C)] (321, 323)
— *Competiton between dipolar and Dzyaloshinskii-Moriya interactions on the magnetic thin films*
— *Competiton between dipolar and short-range interactions on the magnetic thin films*

1. Anisotropy-temperature phase diagram for the two-dimensional dipolar Heisenberg model with and without magnetic field
   H. Komatsu, Y. Nonomura, and M. Nishino, Phys. Rev. B **100**, 094407 (2019).

KOMATSU, Yu [C class; 2500 (B), 500 (C)] (291)
— *Constructing the electronic structure database for the molecular design of pigments utilizing near infrared light*

KOTA, Yohei [B class; 400 (B), 0 (C)] (193)
— *Analysis of magnetic properties in Cr and Mn alloys*
— *Analysis of strain effect on magnetism in chromium metals*

1. Perpendicularly magnetized Cu_2Sb type (Mn-Cr)AlGe films onto amorphous SiO_2
   T. Kubota, Y. Kota, K. Ito, R. Y. Umetsu, M. Sun, M. Mizuguchi, and K. Takanashi: Appl. Phys. Express **12** (2019) 103002.

KOU, Sonju [B class; 400 (B), 0 (C)] (191)
— *Development of First-principles calculations method of Seebeck coefficient in the framework of linear response theory*

KOURA, Akihide [C class; 1000 (B), 0 (C)] (167)
— *First principles study on static structure of glass materials*

1. Guidelines for creating artificial neural network empirical interatomic potential from first-principles molecular dynamics data under specific conditions and its application to α-Ag_2Se
   K. Shimamura, S. Fukushima, A. Koura, F. Shimojo, M. Misawa, R. K. Kalia, A. Nakano, P. Vashishta et al.: J. Chem. Phys. 151, (2019) 124303.
2. GGA+U Molecular Dynamics Study of Structural and Dynamic Properties of Superionic Conductor Ag_2Se
   S. Fukushima, M. Misawa, A. Koura, and F. Shimojo: J. Phys. Soc. Jpn. 88, (2019) 115002.
3. Thermodynamic Integration by Neural Network Potentials Based on First-principles Dynamic Calculations
   S. Fukushima, E. Ushijima, H. Kumazoe, A. Koura, F. Shimojo, K. Shimamura, M. Misawa, R. K. Kalia, A. Nakano, and P. Vashishta: Phys. Rev. B 100, (2019) 214108.
4. コンピュータシミュレーションによる永久高密度化ガラスの構造計算
   高良明英, 若林大佑, 下條冬樹: NEW GLASS 35, (2020) 12.
5. Intermediate range structure of amorphous Cu_2GeTe_3: *ab initio* molecular dynamics study
   A. Koura, and F. Shimojo: J. Phys.: Condens. Matter 32, (2020) 244001.
6. Molecular-Dynamics Study of Thermal Conductivity of Silver Chalcogenides
   S. Fukushima, A. Koura, and F. Shimojo: submitted to Phys. Status Solidi B
7. Pressure Dependence of Static Structure of Liquid V_2O_5: *ab initio* Molecular Dynamics Study
   A. Koura, and F. Shimojo: submitted to Phys. Status Solidi B

KUMAZOE, Hiroyuki [C class; 1000 (B), 250 (C)] (320)
— *Establishment of new analysis method for extend X-ray absorption fine structure with sparse modeling*

KUNISADA, Yuji [C class; 8000 (B), 0 (C)] (72)
— *Reduction of Rare Metals in Formic Acid Decomposition Catalysts and Oxygen Storage Materials*

1. 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 **62** (2019) 344.
2. Extraordinarily Large Kinetic Isotope Effect on Alkene Hydrogenation over Rh-based Intermetallic Compounds
   S. Furukawa, P. Yi, Y. Kunisada, K. Shimizu: Science and Technology of Advanced Materials **20** (2019) 805.
3. Co-appearance of superconductivity and ferromagnetism in a Ca_2RuO_4 nanofilm crystal
   SH. Nobukane, K. Yanagihara, Y. Kunisada, Y. Ogasawara, K. Nomura, Y. Asano, S. Tanda: Scientific Reports **10** (2020) 3462.

KUROKI, Kazuhiko [C class; 10500 (B), 1600 (C)] (204)
— *Study on electron correlation and possible superconductivity in mixed-anion systems*
— *Study on the possibility of superconductivity in ladder-type electronic structures constructed from multiple anions*

1. Comparative first-principles study of antiperovskite oxides and nitrides as thermoelectric material: multiple dirac cones, low-dimensional band dispersion, and high valley degeneracy
   M. Ochi, K. Kuroki: Phys. Rev. Applied. **12** (2019) 034009.
2. Strongly enhanced superconductivity due to finite energy spin fluctuations induced by an incipient band : a FLEX study on the bilayer Hubbard model with vertical and diagonal interlayer hoppings
   K. Matsumoto, D. Ogura, and K. Kuroki: J. Phys. Soc. Jpn. **89** (2020) 044709.

3. Many-variable variational Monte-Carlo study of superconductivity in two-band Hubbard models with an incipient band
   D. Kato and K. Kuroki: Phys. Rev. Research, in press (2020) (arXiv:1912.11983)

KUSAKABE, Koichi [C class; 2000 (B), 300 (C)] (140)
— *Transport and reaction properties of nanographene*

1. Spin-current control by induced electric-polarization reversal in Ni/hBN/Ni: A cross-correlation material
   H. Harfah, Y. Wicaksono, M.A. Majidi, and K. Kusakabe: ACS Appl. Elect. Materials, in press.
2. Interplanar stiffness in defect-free monocrystalline graphite
   K. Kusakabe, A. Wake, A. Nagakubo, K. Murashima, M. Murakami, K. Adachi, H. Ogi: Phys. Rev. Materials **4** (2020) 043603.
3. アルカン脱水素触媒，及びこれを用いる水素製造方法
   草部浩一，高井和之，西川正浩，劉明, 特願 2019-135780.
4. Counting the Zero Modes and Magnetic Moment by Topology of a Phenalenyl-Tessellation Molecule with Vacancies
   N. Morishita, K. Kusakabe: J. Phys. Soc. Jpn. **88** (2019) 124707.

MAKINO, Takayuki [B class; 1500 (B), 210 (C)] (149)
— *Ab-initio calculation of phonon density-of-states spectra in cuprous oxides*
— *Calculation of electron-phonon interaction in delafossite-type cuprates*
— *Electronic structure calculation in strongly-correlated electron oxides under presence of static electric field*

1. Temperature dependence of dielectric functions in Yb2O3 and Lu2O3 epitaxial thin films on sapphire (0001)
   T. Makino et al.: Jpn. J. Appl. Phys. (2020) .

MASUDA, Keisuke [B class; 600 (B), 90 (C)] (184)
— *First-principles study of magnetoresistance ratios and magnetic anisotropy in magnetic tunnel junctions*

1. Mechanism of strong enhancement of anomalous Nernst effect in Fe by Ga substitution
   H. Nakayama, K. Masuda, J. Wang, A. Miura, K. Uchida, M. Murata, and Yuya Sakuraba: Phys. Rev. Materials **3** (2019) 114412.
2. Observation of anomalous Ettingshausen effect and large transverse thermoelectric conductivity in permanent magnets
   A. Miura, H. Sepehri-Amin, K. Masuda, H. Tsuchiura, Y. Miura, R. Iguchi, Y. Sakuraba, J. Shiomi, K. Hono, and K. Uchida: Appl. Phys. Lett. **115** (2019) 222403.
3. Contributions of magnetic structure and nitrogen to perpendicular magnetocrystalline anisotropy in antiperovskite $\epsilon - Mn_4N$
   S. Isogami, K. Masuda, and Y. Miura: Phys. Rev. Materials **4** (2020) 014406.
4. Strain-induced enhancement of the Seebeck effect in magnetic tunneling junctions via interface resonant tunneling: *Abinitio* study
   K. Yamamoto, K. Masuda, K. Uchida, and Y. Miura: Phys. Rev. B **101** (2020) 094430.
5. Interface-driven giant tunnel magnetoresistance in (111)-oriented junctions
   K. Masuda, H. Itoh, and Y. Miura: Phys. Rev. B **101** (2020) 144404.

MATSUDA, Yasuhiro [B,C class; 3700 (B), 640 (C)] (227)
— *Estimation of the density of states using Maximum entropy method and Sparse modeling*
— *Study on the high-field-induced phases of low dimensional frustrated quantum spin system*

MATSUKAWA, Hiroshi [C class; 1500 (B), 400 (C)] ()
— *Physics of Friction*

MATSUMOTO, Munehisa [C,D class; 17000 (B), 1350 (C)] (49, 51)

— Ab initio optimization of the champion rare earth magnet compound (Nd R)2(Fe Co)14B (R=rare earth)

— Multiscale data assimilation between ab initio theory at finite temperatures and experiments for rare-earth permanent magnets

— Self-consistent analysis between miroscopic electronic structure calculations and macroscopic data analysis for experimental measurements

1. Calculating Curie temperatures for rare-earth permanent magnets: Ab initio inspection of localized magnetic moments in d-electron ferromagnetism
   Munehisa Matsumoto and Hisazumi Akai: Phys. Rev. B **101** (2020) 144402.
2. Magnetism trends in doped Ce-Cu intermetallics in the vicinity of quantum criticality: realistic Kondo lattice models based on dynamical mean-field theory
   Munehisa Matsumoto: Phys. Rev. Materials 4 (2020) 054401.
3. (Sm,Zr)$Fe_{12-x}M_x$ (M=Zr,Ti,Co) for permanent-magnet applications: Ab initio material design integrated with experimental characterization
   Munehisa Matsumoto, Takafumi Hawai, and Kanta Ono: Phys. Rev. Applied 13 (2020) 064028.

MATSUNAKA, Daisuke [B class; 700 (B), 0 (C)] (183)

— First-principles Study of Defects of Magnesium Alloys

1. Molecular Dynamics Study of Influences of Non-Glide Stress on Slips in Magnesium
   So Yoshikawa, Daisuke Matsunaka: ,Materials Transactions **61** (2019) 127-135.
2. Molecular Dynamics Simulation on Defect Nucleation from Pre-existing I1 Stacking Fault in Magnesium
   S. Yoshikawa and D. Matsunaka: Computational Materials Science, **179** (2020) 109644.

MATSUSHITA, Katsuyoshi [C class; 0 (B), 800 (C)] (333)

— Adhesion Inducing Cell Dynamics in Tissue

— Numerical Study of Cell Guiding Mechanism in Cellular Tissue

1. Crowding-Boosting Polarity and Motion Order of Cells
   K Matsushita, K Horibe, N Kamamoto, S Yabunaka, K Fujimoto Proceedings of the Symposium on Simulation of Traffic Flow 25, 21
2. Curved surface geometry-induced topological change of an excitable planar wavefront
   K Horibe, K Hironaka, K Matsushita, K Fujimoto Chaos: An Interdisciplinary Journal of Nonlinear Science 29 (9), 093120
3. Cell Motion Alignment as a Polarity Memory Effect
   Matsushita, K Horibe, N Kamamoto, K Fujimoto Journal of the Physical Society of Japan 88 (10), 103801

MATSUSHITA, Yu-ichiro [C class; 11500 (B), 1800 (C)] (56)

— Identification of interface-state defects in power semiconductors: Approach from ab-initio calculations

— Relation between defect structures and electronic properties in power semiconductors: Approach from ab-initio calculations

1. Native point defects and carbon clusters in 4H-SiC: A hybrid functional study
   T. Kobayashi, K. Harada, Y. Kumagai, F. Oba, and Y. Matsushita: J. Appl. Phys. **125** (2019) 125701.
2. Energetics and electronic structure of native point defects in α-Ga_2O_3
   T. Kobayashi, T. Gake, Y. Kumagai, F. Oba, and Y. Matsushita: Appl. Phys. Expr. **12** (2019) 091001.
3. Structure and energetics of carbon-related defects in SiC(0001)/SiO_2 systems revealed by first-principles calculations: Defects in SiC, SiO_2, and just at their interface
   T. Kobayashi and Y. Matsushita: J. Appl. Phys. **126** (2019) 145302.
4. Carbon dangling-bond center (carbon P_b center) at 4H-SiC(0001)/SiO_2 interface
   T. Umeda, T. Kobayashi, M. Sometani, H. Yano, Y. Matsushita, and S. Harada: Appl. Phys. Lett. **116** (2020) 071604.

MAYUMI, Koichi [B class; 1400 (B), 180 (C)] (303, 305)
— *Study on Dynamic Mechanical Properties of Slide-Ring Gels using Coarse-Grained MD Simulations*
— *Study on Microscopic Dynamics of Polyrotaxanes using Full-Atomistic MD Simulations*

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, K. Ito: Macromolecules, 2019, 52, 3787.
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, H. Yokoyama, T. Yamada, K. Fujimoto, S. Okazaki, H. Yokoyama, K. Ito: J. Am. Chem. Soc., 2019, 141, 9655.

MINAMITANI, Emi [C class; 6500 (B), 450 (C)] (79)
— *Ab-initio analysis of electron-phonon interaction*

1. Simulating lattice thermal conductivity in semiconducting materials using high-dimensional neural network potential
   E. Minamitani, M. Ogura, S. Watanabe:Appl. Phys. Express, 12 (2019) 095001

MISAWA, Masaaki [B class; 400 (B), 0 (C)] ()
— *First-principles study on the structures and electronic properties of silicates under high pressure*

MISAWA, Takahiro [E class; 19500 (B), 2750 (C)] ()
— *Numerical analysis of quantum transport phenomena in topological materials*

MIURA, Yoshio [B class; 800 (B), 100 (C)] ()
— *A first-principles calculation on finite temperature effects of half-metallic ferromagnets*

MIZUGUCHI, Tomoko [C class; 1000 (B), 0 (C)] (329)
— *Molecular dynamics simulations of water confined in carbon structures with the reactive force field*

1. Hydrogen bond analysis of confined water in mesoporous silica using the reactive force field
   T. Mizuguchi, K. Hagita, S. Fujiwara and T. Yamada: Mol. Sim. **45** (2019) 1437.
2. Icosahedral order in liquid and glassy phases of cyclohexane
   T. Mizuguchi, S. Tatsumi and S. Fujiwara: Mol. Sim. in press.

MIZUKAMI, Wataru [C class; 2500 (B), 150 (C)] (134)
— *Exploration of surface reactions on model real catalyst II*

1. Orbital optimized unitary coupled cluster theory for quantum computer
   W. Mizukami, K. Mitarai, Y.O. Nakagawa, T. Yamamoto, T. Yan, Y.y. Ohnishi: arXiv:1910:11526 (2019)

MOMIDA, Hiroyoshi [C class; 4000 (B), 650 (C)] (106)
— *Electrode properties of novel lithium-ion secondary battery materials: First-principles calculations*

1. 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).
2. Spectral Dependence of the Third-Order Optical Susceptibility of Au Nanostructures: Experiments and First-Principles Calculations
   B. Zhang, R. Sato, H. Momida, T. Ohno, M. Chundak, M. Naito, M. Yoshitake and Y. Takeda: Phys. Rev. B **100**, 035446 (2019).
3. Amorphous xNaF-$FeSO_4$ Systems ($1 \leq x \leq 2$) with Excellent Cathode Properties for Sodium-Ion Batteries
   A. Kitajou, H. Momida, T. Yamashita, T. Oguchi and S. Okada: ACS Appl. Energy Mater. **2**, 5968 (2019).
4. First-Principles Study of X-Ray Absorption Spectra in $NaFeSO_4F$ for Exploring Na-Ion Battery Reactions

H. Momida, A. Kitajou, S. Okada and T. Oguchi: J. Phys. Soc. Jpn. **88**, 124709 (2019).

5. Significant Role of Oxygen Redox Reaction with O_2-Release in Li-Excess Cation-Disordered Rock-Salt Cathodes $Li_{2+2x}Mn_{1-x}Ti_{1-x}O_4$: First-Principles Calculations
   M. Hamaguchi, H. Momida and T. Oguchi: Electrochim. Acta **330**, 135286 (2020).

MORIKAWA, Yoshitada [C class; 5000 (B), 750 (C)] (95)

— *First-principles Theoretical Study of Chemical Reactions in Heterogeneous Catalysts*

1. 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.
2. Vibration-driven reaction of CO_2 on Cu surfaces via EleyRideal-type mechanism
   J. Quan, F. Muttaqien, T. Kondo, T. Kozarashi, T. Mogi, T. Imabayashi, Y. Hamamoto, K. Inagaki, I. Hamada, Y. Morikawa, and J. Nakamura: Nature Chem. **11** (2019) 722.
3. Development of Co supported on Co- Al spinel catalysts from exsolution of amorphous Co- Al oxides for carbon dioxide reforming of methane
   Y. J. Wong, M. K. Koh, N. F. Khairudin, S. Ichikawa, Y. Morikawa, and A. R. Mohamed: Chem. Cat. Chem. **11** (2019) 5593.
4. First-principles theoretical study on carrier doping effects induced by Zn vacancies in Mn-doped in $ZnSnAs_2$
   H. Kizaki and Y. Morikawa: Jpn. J. Appl. Phys. **58** (2019) 110601.
5. Analyses of three-dimensional atomic arrangements of impurities doped in Si relating to electrical activity by spectro-photoelectron holography
   K. Tsutsui and Y. Morikawa: Jpn. J. Appl. Phys. **59** (2020) 010503.
6. Insight into Trimeric Formation of Nitric Oxide on Cu(111): A Density Functional Theory Study
   T. N. Pham, Y. Hamamoto, K. Inagaki, D. N. Son, I. Hamada, and Y. Morikawa: J. Phys. Chem. C **124** (2020) 2968.
7. Atomic and Molecular Adsorption on Single Platinum Atom at the Graphene Edge: A Density Functional Theory Study
   S. A. Wella, Y. Hamamoto, F. Iskandar, Suprijadi, Y. Morikawa, and I. Hamada: J. Chem. Phys. **152** (2020) 104707.

MORITA, Satoshi [B class; 800 (B), 100 (C)] (25)

— *Improvement of higher-order tensor renormalization group method and its applications*

MOTOME, Yukitoshi [C class; 13500 (B), 1900 (C)] (202)

— *Theoretical study of novel quantum properties induced by strong spin-orbit coupling*

— *Theoretical study of quantum properties induced by spin-orbit coupling and electron correlation*

1. Magnetic Vortex Induced by Nonmagnetic Impurity in Ferromagnets: Magnetic Multipole and Toroidal around the Vacancy
   S. Hayami, H. Kusunose, and Y. Motome, J. Phys. Soc. Jpn. **88**, 063702 (2019).
2. Antiferromagnetic Kitaev interaction in f-electron based honeycomb magnets
   S.-H. Jang, R. Sano, Y. Kato, and Y. Motome, Phys. Rev. B **99**, 241106(R) (2019).
3. Nonequilibrium Majorana dynamics by quenching a magnetic field in Kitaev spin liquids
   J. Nasu and Y. Motome, Phys. Rev. Research **1**, 033007 (2019).
4. Hunting Majorana Fermions in Kitaev Magnets
   Y. Motome and J. Nasu, J. Phys. Soc. Jpn. **89**, 012002 (2020).
5. Chiral spin liquids with crystalline $\mathbf{Z}_2$ gauge order in a three-dimensional Kitaev model
   P. A. Mishchenko, Y. Kato, K. O'Brien, T. A. Bojesen, T. Eschmann, M. Hermanns, S. Trebst, and Y. Motome, Phys. Rev. B **101**, 045118 (2020).
6. The range of non-Kitaev terms and fractional particles in α-$RuCl_3$
   Y. Wang, G. B. Osterhoudt, Y. Tian, P. Lampen-Kelley, A. Banerjee, T. Goldstein, J. Yan, J. Knolle, H. Ji, J. Cava, J. Nasu, Y. Motome, S. Nagler, D. Mandrus, and K. S. Burch, npj Quant. Mat. **5**, 14 (2020).
7. Majorana-magnon crossover by a magnetic field in the Kitaev model: Continuous-time quantum

Monte Carlo study
J. Yoshitake, J. Nasu, Y. Kato, and Y. Motome, Phys. Rev. B **101**, 100408(R) (2020).

8. Antiferromagnetic Kitaev interactions in polar spin-orbit Mott insulators
Y. Sugita, Y. Kato, and Y. Motome, Phys. Rev. B **101**, 100410(R) (2020).
9. Spin-current diode with a monoaxial chiral magnet
S.-H. Jang, R. Sano, Y. Kato, and Y. Motome, preprint (arXiv:1912.03422), submitted to Phys. Rev. Materials

MURAGUCHI, Masakazu [B class; 600 (B), 80 (C)] (185)
— *Study on carrier dynamics in nano scale semiconductor devices with machine learning*

MURAI, Naoki [B class; 900 (B), 100 (C)] (327)
— *Lattice dynamics investigation of a charge-density-wave phase in transition metal chalcogenides*

MURASHIMA, Takahiro [E class; 8500 (B), 2100 (C)] (250)
— *Multiscale analysis of polymeric fluids and solids*

1. Coupling Finite Element Method with Large Scale Atomic/Molecular Massively Parallel Simulator(LAMMPS) for Hierarchical Multiscale Simulations
T. Murashima, S. Urata, S. Li: Euro. Phys. J. B **92** (2019) 211.
2. ミクロスケールとマクロスケールのシミュレーション連成による高分子材料系のマルチスケールシミュレーション
村島隆浩: CICSJ Bulletin (日本化学情報化学部会誌) **37** (2019) 87.
3. Multiscale Modeling of Plasticity in Amorphous & Polymeric Materials
S. Li, S. Urata, T. Murashima: IACM Express. **46** (2020) 10.

NADA, Hiroki [C class; 0 (B), 750 (C)] (340)
— *Construction of A New Method for Analysis of Crystallization Mechanism from Amorphous Precursor Using Molecular Dynamics Simulation Method and Unsupervised Machine Learning*

1. 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., **116** (2019) 8679.
2. 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: ACS Omega, **4** (2019) 11014.
3. Transport Mechanisms of Water Molecules and Ions in Sub-Nano Channels of Nanostructured Water Treatment Liquid-Crystalline Membranes: A Molecular Dynamics Simulation Study
H. Nada, T. Sakamoto, M. Henmi, T. Ogawa, M. Kimura and T. Kato: Environ. Sci.: Water Res. & Technol., **6** (2020) 604.
4. Pathways for the Formation of Ice Polymorphs from Water Predicted by a Metadynamics Method
H. Nada: Sci. Rep., **10** (2020) 4708.

NAKAGAWA, Naoko [C class; 3500 (B), 600 (C)] (286)
— *Macroscopic properties characterized by an extended thermodynamic functions to nonequilibrium*

1. Global thermodynamics for heat conduction systems
N. Nakagawa and S.-i. Sasa: J. Stat. Phys. **177** (2019) 825.
2. Multiplicative Langevin Equation to Reproduce Long-time Properties of Nonequilibrium Brownian Motion
Atsumasa Seya, Tatsuya Aoyagi, Masato Itami, Yohei Nakayama and Naoko Nakagawa: J. Stat. Mech. **2020** (2020) 013201

NAKAHARA, Akio [B class; 700 (B), 90 (C)] (337)
— *Transition in the memory effect of paste*

NAKAMURA, Kazuma [C,D class; 8500 (B), 0 (C)] (66, 68)
— *Ab initio calculation for thermodynamic phase diagram*
— *Ab initio calculations for Sr2IrO4 and Ca5Ir3O12*
— *Ab initio phonon calculation for Ca5Ir3O12*

1. GW calculation of plasmon excitations in the quasi-one-dimensional organic compound (TMTSF)2PF6
   Kazuma Nakamura, Shiro Sakai, Ryotaro Arita, and Kazuhiko Kuroki: Physical Review B **88** (2013) 125128.
2. Effect of Electron-Phonon Interactions on Orbital Fluctuations in Iron-Based Superconductors
   Yusuke Nomura, Kazuma Nakamura, and Ryotaro Arita: Phys. Rev. Lett. **112** (2014) 027002.
3. Ab initio GW plus cumulant calculation for isolated band systems: Application to organic conductor (TMTSF)2PF6 and transition-metal oxide
   Kazuma Nakamura, Yoshiro Nohara, Yoshihide Yoshimoto, and Yusuke Nomura: Phys. Rev. B **93** (2016) 085124.
4. Large enhancement of superconducting transition temperature in single-element superconducting rhenium by shear strain
   M. Mito, H. Matsui, K. Tsuruta, T. Yamaguchi, K. Nakamura, H. Deguchi, N. Shirakawa, H. Adachi, T. Yamasaki, H. Iwaoka, Y. Ikoma, and Z. Horita: Scientific reports **6**, (2016) 36337.
5. Uniaxial strain effects on superconducting transition in Re-doped Hg-1223 cuprate superconductors
   M. Mito, K. Ogata, H. Goto, K. Tsuruta, K. Nakamura, H. Deguchi, T. Horide, K. Matsumoto, T. Tajiri, H. Hara, T. Ozaki, H. Takeya, and Y. Takano: Phys. Rev. B **95**, (2017) 064503.
6. Nonlinear Conductivity of Geometrically Frustrated Iridate Ca5Ir3O12
   K. Matsuhira, K. Nakamura, Y. Yasukuni, Y. Yoshimoto, D. Hirai, Z. Hiroi: J. Phys. Soc. Jpn. **87**, (2018) 013703.
7. 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.
8. Hydrostatic Compression Effects on Fifth-Group Element Superconductors V, Nb, and Ta Subjected to High-Pressure Torsion
   M. Mito, S. Shigeoka, H. Kondo, N. Noumi, Y. Kitamura, K. Irie, K. Nakamura, S. Takagi, H. Deguchi, T. Tajiri, M. Ishizuka, T. Nishizaki, K. Edalati, Z. Horita: Mater. Trans. (Overview), **60**, (2019) 1472-1483.
9. Anisotropic compression effects on nanocrystalline crystals of nickel oxide
   M. Mito, T. Tajiri, S. Saisho, H. Deguch, A. Kohno, K. Nakamura: Journal of Magnetism and Magnetic Materials **489**, (2019) 165407.
10. Harmonic voltage response to AC current in the nonlinear conductivity of iridium oxide Ca5Ir3O12
    H. Hanate, K. Nakamura, K. Matsuhira: J. Magn. Magn. Mater. **498**, (2020) 166203.
11. Formation of a two-dimensional single-component correlated electron system and band engineering in the nickelate superconductor NdNiO2
    Y. Nomura, M. Hirayama, T. Tadano, Y. Yoshimoto, K. Nakamura, R. Arita: Phys. Rev. B **100**, (2019) 205138(1-11). [Editors' Suggestion]
12. Raman Scattering Investigation of Structural Transition in Ca5Ir3O12
    T. Hasegawa, W. Yoshida, K. Nakamura, N. Ogita, K. Matsuhira: J. Phys. Soc. Jpn **89** (2020) 054602/1-11.
13. Study of Phonon Dispersion of Iridium Oxide Ca5Ir3O12 with Strong Spin?Orbit Interaction
    H. Hanate, T. Hasegawa, S. Tsutsui, K. Nakamura, Y. Yoshimoto, N. Kishigami, S. Haneta, K. Matsuhira1: J. Phys. Soc. Jpn **89** (2020) 053601/1-5.

NAKANO, Hiroki [C class; 4000 (B), 1050 (C)] (268)
— *Numerical study on low-energy states of quantum spin systems*

1. Haldane Gaps of Large-S Heisenberg Antiferromagnetic Chains and Asymptotic Behavior
   H. Nakano, N. Todoroki, and T. Sakai: J. Phys. Soc. Jpn. **88** (2019) 114702.
2. 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).

3. Two magnetization plateaus in the kagome fluoride $Cs_2LiTi_3F_{12}$
   R. Shirakami, H. Ueda, H. O. Jeschke, H. Nakano, S. Kobayashi , A. Matsuo, T. Sakai, N. Katayama, H. Sawa, K. Kindo, C. Michioka, and K. Yoshimura: Phys. Rev. B **100** (2019) 174401.

NAKAYAMA, Takashi [C class; 5000 (B), 800 (C)] (92)

— *First-principles study on physics of gap-state control at metal/semiconductor interfaces*

1. Effect of electric field on formation energies of point defects around metal/SiC and metal/GaN interfaces: First-principles study
   R. Nagasawa, T. Nakayama: Jpn. J. Appl. Phys. **58** (2019) 091006.
2. Origin of Fermi-level depinning at TiN/Ge(001) interfaces: first-principles study
   T. Nishimoto, T. Nakayama: Jpn. J. Appl. Phys. **58** (2019) 061007.
3. Origin of Fermi-level depinning at metal/Ge interfaces: first-principles study on effect of segregation
   T. Nishimoto, T. Nakayama: Jpn. J. Appl. Phys. **58** (2019) SIIB11.
4. Resonance-enhanced tunneling current through Si-p/n junction with additional dopants; theoretical study
   S. Cho, S. Iizuka, T. Nakayama: Jpn. J. Appl. Phys. **58** (2019) 061004.
5. Theoretical studies on the switching mechanism of VMCO memories
   T. Nakanishi, K. Chokawa, M. Araidai, T. Nakayama, K. Shiraishi: Microelectronic Engineering **215** (2019) 110997.

NASU, Joji [C class; 3500 (B), 1500 (C)] (226)

— *Magnetic state of Kitaev spin liquid under time-dependent field*

— *Time evolution by magnetic-field quench in Kitaev spin liquid*

1. Low temperature properties in the Bilayer Kitaev model
   H. Tomishige, J. Nasu, A. Koga: Phys. Rev. B **99**, 174424 (2019).
2. Ferromagnetic instability for the single-band Hubbard model in the strong-coupling regime
   Y. Kamogawa, J. Nasu, and A. Koga: Phys. Rev. B **99**, 235107 (2019).
3. Residual Entropy and Spin Fractionalizations in the Mixed-Spin Kitaev Model
   A. Koga and J. Nasu: Phys. Rev. B **100**, 100404(R) (2019).
4. Nonequilibrium Majorana Dynamics by Quenching a Magnetic Field in Kitaev Spin Liquids
   J. Nasu, and Y. Motome: Phys. Rev. Research **1**, 033007 (2019).
5. Hunting Majorana Fermions in Kitaev Magnets
   Y. Motome and J. Nasu: J. Phys. Soc. Jpn. **89**, 012002 (2020).
6. Two-step gap opening across the quantum critical point in the Kitaev honeycomb magnet α-$RuCl_3$
   Y. Nagai, T. Jinno, Y. Yoshitake, J. Nasu, Y. Motome, M. Itoh, and Y. Shimizu: Phys. Rev. B **101**, 020414(R) (2020).
7. Spin Transport in the Quantum Spin Liquid State in the $S = 1$ Kitaev Model: Role of the Fractionalized Quasiparticles
   A. Koga, T. Minakawa, Y. Murakami, and J. Nasu: J. Phys. Soc. Jpn. **89**, 033701 (2020).
8. The range of non-Kitaev terms and fractional particles in α-$RuCl_3$
   Y. Wang, G. B. Osterhoudt, Y. Tian, P. Lampen-Kelley, A. Banerjee, T. Goldstein, J. Yan, J. Knolle, H. Ji, R. J. Cava, J. Nasu, Y. Motome, S. Nagler, D. Mandrus, and K. S. Burch: npj Quantum Materials **5**, 14 (2020).
9. Majorana-Magnon Crossover by a Magnetic Field in the Kitaev Model: Continuous-Time Quantum Monte Carlo Study
   J. Yoshitake, J. Nasu, Y. Kato, and Y. Motome: Phys. Rev. B **101**, 100408(R) (2020).

NISHIDATE, Kazume [C class; 3000 (B), 0 (C)] (131)

— *Computational physics and chemistry approach to develop the artificial photosynthesis and fuel cell catalysts*

1. Electronic Properties and Crystal Structures of Double-Perovskites, $Ba_2Bi^{III}Bi^{V}O_6$, Ba_2PrBiO_6, and Ba_2PrSbO_6: First-principles study

K. Nishidate et al.: submitted.

NISHIGUCHI, Kazutaka [B class; 700 (B), 0 (C)] (342)
— *Theoretical study for superconductivity in superstructured strongly correlated materials with two-particle self-consistent approach*

1. Possible Superconductivity Induced by a Large Spin-Orbit Coupling in Carrier Doped Iridium Oxide Insulators: A Weak Coupling Approach
   Kazutaka Nishiguchi, Tomonori Shirakawa, Hiroshi Watanabe, Ryotaro Arita, and Seiji Yunoki: J. Phys. Soc. Jpn. **88** (2019) 094701

NISHINO, Masamichi [B class; 700 (B), 90 (C)] (336)
— *Elucidation of coercivity mechanism by statistical physical approaches*

1. Nontrivial temperature dependence of ferromagnetic resonance frequency for spin reorientation transitions
   M. Nishino, and S. Miyashita: Phys. Rev. B **100** (2019) 020403(R).
2. Multistep spin-crossover transitions induced by the interplay between short- and long-range interactions with frustration on a triangular lattice
   M. Nishino, C. Enachescu, and S. Miyashita:Phys. Rev. B **100** (2019) 134414
3. Anisotropy-temperature phase diagram for the two-dimensional dipolar Heisenberg model with and without magnetic field
   H. Komatsu, Y. Nonomura, and M. Nishino: Phys. Rev. B **100**, (2019) 094407

NOGUCHI, Hiroshi [C class; 11000 (B), 1800 (C)] (243)
— *structure formation of biomembrane*

1. Shape transition from elliptical to cylindrical membrane tubes induced by chiral crescent-shaped protein rods
   H. Noguchi: Sci. Rep. **9**, 11721 (2019).
2. Cup-to-vesicle transition of a fluid membrane with spontaneous curvature
   H. Noguchi: J. Chem. Phys. **51**, 094903 (2019).
3. Detachment of fluid membrane from substrate and vesiculation
   H. Noguchi: Soft Matter **15**, 8741 (2019).
4. Curvature induction and sensing of the F-BAR protein Pacsin1 on lipid membranes via molecular dynamics simulations
   M. I. Mahmood, H. Noguchi, and K. Okazaki: Sci. Rep. **9**, 14557 (2019).
5. Effects of Cavitation on Karman Vortex Behind Circular-Cylinder Arrays: A Molecular Dynamics Study
   Y. Asano, H. Watanabe, and H. Noguchi: J. Chem. Phys. **152**, 034501 (2020).
6. 分子動力学計算による複雑流体中のカルマン渦の解析
   浅野 優太, 渡辺 宙志, 野口 博司: 分子シミュレーション研究会会誌“アンサンブル”**22**, 157 (2020).

NOGUCHI, Yoshifumi [C class; 3500 (B), 600 (C)] (112)
— *GW method without GPP model*

1. Photoabsorption Spectra of Aqueous Oxyluciferin Anions Elucidated by Explicit Quantum Solvent
   Y. Noguchi, M. Hiyama, M. Shiga, H. Akiyama, and O. Sugino: J. Chem. Theory Compt., **15** (2019) 5474.

NOMURA, Yusuke [C class; 9500 (B), 1600 (C)] (207, 209)
— *Study on frustrated magnetism using machine learning*
— *Study on metal-insulator transition in nickel oxides*

1. Strong-coupling formula for momentum-dependent susceptibilities in dynamical mean-field theory
   Junya Otsuki, Kazuyoshi Yoshimi, Hiroshi Shinaoka, and Yusuke Nomura: Phys. Rev. B **99** (2019) 165134.
2. Ab initio derivation of an effective Hamiltonian for the La2CuO4/La1.55Sr0.45CuO4 heterostructure
   Terumasa Tadano, Yusuke Nomura, and Masatoshi Imada: Phys. Rev. B **99** (2019) 155148.

3. Formation of a two-dimensional single-component correlated electron system and band engineering in the nickelate superconductor NdNiO2
   Yusuke Nomura, Motoaki Hirayama, Terumasa Tadano, Yoshihide Yoshimoto, Kazuma Nakamura, and Ryotaro Arita: Phys. Rev. B **100** (2019) 205138.
4. Wannier90 as a community code: new features and applications
   Giovanni Pizzi *et. al.*: J. Phys.: Condens. Matter **32** (2020) 165902.
5. Materials design of dynamically stable d9 layered nickelates
   Motoaki Hirayama, Terumasa Tadano, Yusuke Nomura, and Ryotaro Arita: Phys. Rev. B **101** (2020) 075107.

NONOMURA, Yoshihiko [B,C class; 2700 (B), 490 (C)] (288, 289)
— *Generalization of temperature scaling in early-time nonequilibrium relaxation*
— *Unified understanding of early-time nonequilibrium relaxation in Monte Carlo simulations*

NOZAWA, Kazuki [C class; 1000 (B), 100 (C)] (162)
— *Atomic and electronic structures of intermetallic compound catalysts*

OBATA, Masao [B,C class; 1800 (B), 100 (C)] (145)
— *Analysis on atomic and magnetic structure in magnetic molecular complex crystal and interface and investigation of external electric and magnetic field effect*

1. Noncollinear magnetic structure with spin-dependent van der Waals density functional approach: β-phase solid oxygen
   M. Christivana, M. Obata, and T. Oda: J. Phys. Soc. Jpn. **88** (2019) 104601
2. Density Functional Approach under External Magnetic Field
   A. R. Rio, I. Pardede,A. M. Gani, M. Christivana, M. Obata, T. Oda: J. Phys. Soc. Jpn. **89**, (2020) 035002

ODA, Tatsuki [E class; 25500 (B), 2650 (C)] (47)
— *Analyses on electronic structure and magnetic property in high-performance spintronics and magnetic materials*

1. Noncollinear magnetic structure with spin-dependent van der Waals density functional approach: β-phase solid oxygen
   Mega Christivana, Masao Obata, and Tatsuki Oda: Journal of the Physical Society of Japan, **88** (2019) 104601.
2. Large nonvolatile control of interfacial magnetic anisotropy in CoPt by a ferroelectric ZnO-based tunneling barrier
   Muftah Al-Mahdawi, Mohamed Belmoubarik, Masao Obata, Daiki Yoshikawa, Hideyuki Sato, Tomohiro Nozaki, Tatsuki Oda, Masashi Sahashi: Phys. Rev. B,**100** (2019) 054423.
3. Anatomy of large perpendicular magnetic anisotropy in free-standing Co/Ni (111) multilayer, Journal of Magnetism and Magnetic Materials
   Indra Pardede, Daiki Yoshikawa, Tomosato Kanagawa, Nurul Ikhsan, Itsuki Murata, Masao Obata, Tatsuki Oda: Journal of Magnetism and Magnetic Materials **500**(2020)166357.
4. Density functional approach under external magnetic field
   Afrioni Roma Rio, Indra Pardede, Achmad Maulana Gani, Mega Christivana, Masao Obata, and Tatsuki Oda: Journal of the Physical Society of Japan, 89,(2020) 035002.
5. Finite electric-field approach to evaluate the vertex correction for the screened Coulomb interaction in the quasiparticle self-consistent GW method
   Hirofumi Sakakibara, Takao Kotani, Masao Obata, and Tatsuki Oda: submitted to Physical Review B.

OHGOE, Takahiro [C class; 4500 (B), 700 (C)] (225)
— *Development and applications of continuous-time quantum Monte Carlo method in the thermodynamic limit*

OHMURA, Satoshi [B,C class; 3200 (B), 0 (C)] (122, 123)

— *Ab initio molecular dynamics study of stability of artificial retina molecule*

— *Ab initio molecular dynamics study of structural properties and immiscibility in liquid Fe-Si-O mixtures under high pressure*

1. Selective Reduction Mechanism of Graphene Oxide Driven by the Photon Mode versus the Thermal Mode
   M. Hada, K. Miyata, S. Ohmura, Y. Arashida, K. Ichiyanagi, I. Katayama, T. Suzuki, W. Chen, S. Mizote, T. Sawa, T. Yokoya, T. Seki, J. Matsuo, T. Tokunaga, C. Itoh, K. Tsuruta, R. Fukaya, S. Nozawa, S. Adachi, J. Takeda, K. Onda, S. Koshihara, Y. Hayashi, Y. Nishina: ACS NANO. **13** 2019) 10103.
2. 共有結合にとらわれた原子が液体中でどのように動くのか——共有結合性液体の高圧物性
   大村訓史, 下條冬樹, 土屋卓久: 日本物理学会誌, **74** (2019) 621.
3. Structures of liquid iron-light-element mixtures under high pressure
   S. Ohmura, T. Tsuchiya, and F. Shimojo: Physica Status Solidi B. in press

OHNISHI, Masato [C class; 4500 (B), 700 (C)] (98)

— *Analysis of Thermoelectric Properties of Clathrate Compounds with Ab Initio Calculations*

1. Enhancing thermal boundary conductance of graphite- metal interface by triazine-based molecular bonding
   Aun Ota, Masato Ohnishi, Hisayoshi Oshima, Hisayoshi, Takuma Shiga, Takashi Kodama, Junichiro Shiomi :ACS Applied Materials & Interfaces, 11, 37295-37301 (2019).
2. Spectral control of thermal boundary conductance between copper and carbon crystals by self-assembled monolayers
   Shih-Wei Hung, Shiqian Hu, Junichiro Shiomi: ACS Applied Electronic Materials, 1, 2594-2601 (2019).
3. Disorder Limits the Coherent Phonon Transport in Two- Dimensional Phononic Crystal Structure
   Shiqian Hu, Zhongwei Zhang, Pengfei Jiang, Weijun Ren, Cuiqian Yu, Junichiro Shiomi, Jie Chen: Nanoscale, 11, 11839-11846 (2019).

OHSAWA, Kazuhito [C class; 1000 (B), 0 (C)] (165)

— *Study of interaction between radiation damage and interstitial atom*

OHTO, Tatsuhiko [C class; 9500 (B), 0 (C)] (60, 61)

— *First-principles molecular dynamics simulation of electron-doped graphene/water interfaces*

— *First-principles molecular dynamics simulation of the water/air interface using hybrid functionals*

1. Hydrogen-Bonds and Molecular Orientations of Supramolecular Structure between Barbituric Acid and Melamine Derivative at the Air/Water Interface Revealed by Heterodyne-Detected Vibrational Sum Frequency Generation Spectroscopy
   Masanari Okuno, Shuhei Yamada, Tatsuhiko Ohto, Hirokazu Tada, Waka Nakanishi, Katsuhiko Ariga, and Taka-aki Ishibashi: J. Phys. Chem. Lett. 11, 2422 (2020).
2. Mechanical switching of current-voltage characteristics in spiropyran single-molecule junctions
   Takashi Tamaki, Keigo Minode, Yuichi Numai, Tatsuhiko Ohto, Ryo Yamada, Hiroshi Masai, Hirokazu Tada, and Jun Terao: Nanoscale, in press.
3. Molecular Structure and Modeling of Water-Air and Ice-Air Interfaces Monitored by Sum-Frequency Generation
   Fujie Tang, Tatsuhiko Ohto, Shumei Sun, Jeremy Rouxel, Sho Imoto, Ellen H. G. Backus, Shaul Mukamel, Mischa Bonn, and Yuki Nagata: Chem. Rev. in press.
4. Effect of Graphene Encapsulation of NiMo Alloys on Oxygen Evolution Reaction
   Samuel Jeong, Kailong Hu, Tatsuhiko Ohto, Yuki Nagata, Hideki Masuda, Jun-ichi Fujita, and Yoshikazu Ito: ACS Catal. 10, 792 (2020).
5. Three Sites Molecular Orbital Controlled Single-Molecule Rectifier based on Perpendicularly Linked Porphyrin-Imide Dyads
   Murni Handayani, Hirofumi Tanaka, Shinichi Katayose, Tatsuhiko Ohto, Zhijin Chen, Ryo Yamada, Hirokazu Tada, and Takuji Ogawa: Nanoscale, 11, 22724 (2019).
6. Effects of cis-trans Conformation Between Thiophene Rings on Conductance of Oligothiophenes

Tatsuhiko Ohto, Takuya Inoue, Helen Stewart, Yuichi Numai, Yoshio Aso, Yutaka Ie, Ryo Yamada, and Hirokazu Tada: J. Phys. Chem. Lett. 10, 5292 (2019).

7. Accessing the Accuracy of Density Functional Theory through Structure and Dynamics of the Water-Air Interface
   Tatsuhiko Ohto, Mayank Dodia, Jianhang Xu, Sho Imoto, Fujie Tang, Frederik Zysk, Thomas D. Kuhne, Yasuteru Shigeta, Mischa Bonn, Xifan Wu, and Yuki Nagata: J. Phys. Chem. Lett. 10, 4914 (2019).
8. Impact of intermolecular vibrational coupling effects on the sum-frequency generation spectra of the water/air interface
   Naveen Kumar Kaliannan, Andres Henao Aristizabal, Hendrik Wiebeler, Frederik Zysk, Tatsuhiko Ohto, Yuki Nagata, and Thomas D. Kuhne: Mol. Phys. in press.
9. Highly Planar and Completely Insulated Oligothiophenes: Effects of π-Conjugation on Hopping Charge Transport
   Yutaka Ie, Yuji Okamoto, Takuya Inoue, Saori Tone, Takuji Seo, Yasushi Honda, Shoji Tanaka, See Kei Lee, Tatsuhiko Ohto, Ryo Yamada, Hirokazu Tada, and Yoshio Aso: J. Phys. Chem. Lett. 10, 3197 (2019).
10. Structure and Dynamics of Water at the Water?Air Interface Using First Principles Molecular Dynamics Simulations II: Non-Local vs Empirical van der Waals Corrections
    Mayank Dodia, Tatsuhiko Ohto, Sho Imoto, and Yuki Nagata: J. Chem. Theory Comput. 15, 3836 (2019).
11. 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. 6, 1900119 (2019).

OHTSUKI, Tomi [C class; 4500 (B), 750 (C)] (267)

— *Wave function analyses in disordered electron systems*

1. Ballistic transport in disordered Dirac and Weyl semimetals
   K. Kobayashi, M. Wada, T. Ohtsuki: arXiv:2003.01929
2. Drawing Phase Diagrams of Random Quantum Systems by Deep Learning the Wave Functions
   T. Ohtsuki, T. Mano: Journal of the Physical Society of Japan **89**, 022001 (2020)
3. Critical behavior of Anderson transitions in three-dimensional orthogonal classes with particle-hole symmetries
   X. Luo, B. Xu, T. Ohtsuki, R. Shindou: Physical Review B **101**, 020202(R), (2020)
4. Application of Convolutional Neural Network to Quantum Percolation in Topological Insulators
   T. Mano, T. Ohtsuki: Journal of the Physical Society of Japan **88**, 123704 (2019)
5. Multifractality and the distribution of the Kondo temperature at the Anderson transition
   K. Slevin, S. Kettemann, T. Ohtsuki: The European Physical Journal B **92**, 281, (2019)

OKAMOTO, Yuko [C,E class; 2000 (B), 0 (C)] (353)

— *Study on complex systems by generalized-ensemble algorithms*

— *Study on phase transitions of Lennard-Jones fluid systems by generalized-ensemble algorithms*

1. Efficient simulation protocol for determining the density of states: Combination of replica-exchange Wang-Landau method and multicanonical replica-exchange method
   T. Hayashi and Y. Okamoto: Phys. Rev. E **100** (2019) 043304.
2. Analysis of liquids, gases, and supercritical fluids by a two-dimensional replica-exchange Monte Carlo method in temperature and chemical potential space
   D. Matsubara and Y. Okamoto: J. Chem. Phys. **152** (2020) 194108.

OKITSU, Kouhei [C class; 1500 (B), 0 (C)] (307)

— *Study on an X-ray n-beam method to solve protein crystal structure*

— *Study on crystal structure analysis using the X-ray multiple-beam diffraction theory*

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) 474-482. https://doi.org/10.1107/S205327331900
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) 483-488. https://doi.org/10.1107/S2053273319002936.
3. X 線多波 (n 波) 動力学理論とその数値解法および放射光実験による検証 (X-ray n-beam dynamical diffraction theories, numerical method to solve them and experimental verification)
沖津康平: 日本結晶学会誌 **33** (2020) K. Okitsu: J. Jpn. Soc. Synchrotron Rad. Res. **33** (2020) 61-80 [Invited].

OKUBO, Tsuyoshi [C class; 5500 (B), 800 (C)] (259)
— *Novel phases and dynamics in frustrated spin systems*
1. Anisotropic Tensor Renormalization Group
D. Adachi, T. Okubo and S. Todo: arXiv:1906.02007.
2. Gapless Kitaev Spin Liquid to Classical String Gas through Tensor Networks
H.-Y. Lee, R. Kaneko, T. Okubo and N. Kawashima: Phys. Rev. Lett. **123** (2019) 087203.
3. Multiple–q states of the J_1–J_2 classical honeycomb-lattice Heisenberg antiferromagnet under magnetic fields
T. Shimokawa, T. Okubo and H. Kawamura: Phys. Rev. B **100** (2019) 224404.
4. Abelian and Non-Abelian Chiral Spin Liquids in a Compact Tensor Network Representation
H.-Y. Lee, R. Kaneko, T. Okubo and N. Kawashima: Phys. Rev. B **101** (2020) 035140.
5. Magnetic-field Induced Quantum Phases in Tensor Network Study of Kitaev Magnets
H.-Y. Lee, R. Kaneko, L.-E. Chern, T. Okubo, Y. Yamaji, N. Kawashima, and Y.-B. Kim: Nat. Commun. **11** (2020) 1639.

OKUMURA, Hisashi [C class; 11000 (B), 0 (C)] (248)
— *Aggregation process of full-length amyloid-beta peptides studied by molecular dynamics simulations*
1. Conformational change of amyloid-β 40 in associated with binding to GM1-glycan cluster
Y. Tachi, Y. Okamoto, and H. Okumura: Sci. Rep. **9** (2019) 6853 (11 pages).
2. Dynamic views of the Fc region of immunoglobulin G provided by experimental and computational observations
S. Yanaka, R. Yogo, R. Inoue, M. Sugiyama, S. G. Itoh, H. Okumura, Y. Miyanoiri, H. Yagi, T. Satoh, T. Yamaguchi, and K. Kato: Antibodies **8** (2019) 39 (13pages).
3. Replica sub-permutation method for molecular dynamics and Monte Carlo simulations
M. Yamauchi and H. Okumura: J. Comput. Chem. **40** (2019) 2694-2711.
4. Structural characterization of HypX responsible for CO biosynthesis in the maturation of NiFe-hydrogenase
N. Muraki, K. Ishii, S. Uchiyama, S. G. Itoh, H. Okumura, S. Aono: Commun. Biol. **2** (2019) 385 (12 pages).
5. Molecular dynamics simulations of amyloid-β(16-22) peptide aggregation at air-water interfaces
H. Okumura and S. G. Itoh: J. Chem. Phys. **151** (2020) 095101 (12 pages).

ONISHI, Hiroaki [C class; 2000 (B), 0 (C)] (299)
— *Spin multipole dynamics and spin transport in frustrated magnets*
1. Magnetic excitations and transport properties in frustrated ferromagnetic chain
H. Onishi, J. Magn. Magn. Mater. 479, 88 (2019).

ONO, Shota [B class; 1200 (B), 170 (C)] (313, 314)
— *Femtosecond luminescence dynamics of metals*
— *Ultrafast relaxation of inhomogeneous electron distribution around the Dirac cone in graphene*
1. Ultrafast photoluminescence in metals: Theory and its application to silver
S. Ono and T. Suemoto: submitted to Phys. Rev. B

ONO, Tomoya [C class; 8500 (B), 750 (C)] (62)
— *Development of first-principles electronic-structure and transport calculation code RSPACE and simulations for device*

1. Highly Reproducible Formation of a Polymer Single-Molecule Junction for a Well-Defined Current Signal
   T. Harashima, Y. Hasegawa, S. Kaneko, M. Kiguchi, T. Ono, and T. Nishino: Angewandte Chem. Int. Ed. **58** (2019) 9109.
2. Efficient calculation of self-energy matrices for electron-transport simulations
   Y. Egami, S. Tsukamoto, and T. Ono: Phys. Rev. B, **100** (2019) 075413.
3. Graphene-based Symmetric and Non-Symmetric Magnetoresistive Junctions
   A. Hashmi, K. Nakanishi, and T. Ono: J. Phys. Soc. Jpn. **89** (2019) 034708.
4. DFT calculation for oxidation reaction of SiC(0001)
   T. Ono: Materials Science Forum, Materials Science Forum **963** (2019) 208.a

ONO, Yoshiaki [C class; 5000 (B), 750 (C)] (219)
— *First-principles and quantum many-body calculations for electronic states and superconductivity in the multi-band systems*

1. First-Principles Study and Orbital-Fluctuation Effect on the Superconductivity in Tungsten Bronze A_xWO_3
   Takuya Sekikawa, Rai Watabe, Jun Ishizuka, Yoshihiro Nitta, Kazuhiro Sano and Yoshiaki Ōno: JPS Conf. Proc. **30**, 011043 (2020)
2. RKKY Interaction and Quadrupole Order in PrT_2Al_{20} (T=Ti, V) Based on Effective 196 Orbital Model Extracted from First-Principles Calculation
   Yuto Iizuka, Takemi Yamada, Katsurou Hanzawa and Yoshiaki Ōno: JPS Conf. Proc. **30**, 011152 (2020)
3. Dynamical Mean-Field Study of Excitonic Phase in the Spinless Two-Band Hubbard Model for Electron-Hole System
   Kento Sasaki, Takemi Yamada, Kaoru Domon and Yoshiaki Ōno: JPS Conf. Proc. **30**, 011070 (2020)
4. FFLO Superconductivity Mediated by Excitonic Fluctuation in Semimetallic Ta_2NiSe_5
   Takemi Yamada, Kaoru Domon and Yoshiaki Ōno: Journal of the Physical Society of Japan **88**, 064701 (2019)

OSHIKAWA, Masaki [B class; 700 (B), 0 (C)] (180)
— *A data-driven investigation of topological materials based on symmetry*

OSHIYAMA, Atsushi [E class; 43500 (B), 5550 (C)] (44)
— *Mechanisms of Semiconductor Interface Formation and its Electronic Properties based on Quantum Theory*

1. Microscopic Identification of Surface Steps on SiC by Density-Functional Calculations
   K. Seino and A. Oshiyama: Proc. ICSRM2019
2. Energetics of the surface step and its morphology on the 3C-SiC(111) surface clarified by the density-functional theory
   K. Seino and A. Oshiyama: Appl. Phys. Exp. **13** (2020) 015506.
3. Density-Functional Calculations for Structures and Energetics of Atomic Steps and their Implication for Surface Morphology on Si-face SiC Polar Surfaces
   K. Seino and A. Oshiyama: Phys. Rev. B (2020) to be published
4. A two-dimensional liquid-like phase on Ga-rich GaN (0001) surfaces evidenced by first principles molecular dynamics
   K. M. Bui, M. Boero, K. Shiraishi and A. Oshiyama: Jpn. J. Appl. Phys. **59** (2020) SGGK04.
5. Computational study of oxygen stability in vicinal m(10-10)-GaN growth by MOVPE
   F. Shintaku, D. Yosho, Y. Kangawa, J.-I. Iwata, A. Oshiyama, K. Shiraishi, A. Tanaka aand H. Amano: Appl. Phys. Exp. **13** (2020) 055507.
6. Oxygen incorporation kinetics in vicinal m(10-10)-GaN growth by MOVPE
   D. Yosho, F. Shintaku, Y. Inatomi, Y. Kangawa, J.-I. Iwata, A. Oshiyama, K. Shiraishi, A. Tanaka and H. Amano: Phys. Sta. Solidi - Rapid Res. Lett. (2020) 2000142.

OTOMO, Junichiro [C class; 1500 (B), 950 (C)] (138)
— *Analysis of ion conduction in materials of proton-conducting solid electrolyte and application to catalytic surface reaction with proton conductors*

OZEKI, Yukiyasu [C class; 8000 (B), 0 (C)] (254)
— *Dynamical scaling analysis applied to studies on critical universality for topological phase transitions*
— *Dynamical scaling analysis applied to studies on critical universality for topological phase transitions II*

1. Dynamical scaling analysis on critical universality class for fully frustrated XY models in two dimensions
   Y. Ozeki, Y. Yajima and Y. Nakamura: Phys. Rev B **101** (2020) 094437

RAEBIGER, Hannes [C class; 6000 (B), 0 (C)] (87)
— *First principles calculation of quantum phase transitions*

1. Supercomputer System at ISSP
   S. Tsuneyuki: J. Phys. Soc. Jpn. **32** (1996) 41.
2. First principles methods for defects: state of the art and emerging methods
   E. Ertekin and H. Raebiger: Characterisation and Control of Defects in Semiconductors, ed. F. Tuomisto (IET, United Kingdom 2019) pp. 289–343; ISBN-10: 1-78561-655-2, ISBN-13: 978-1-78561-655-6
3. Electronic mechanism for resistive Switching in metal/insulator/metal nanodevices
   H. Raebiger, A. C. M. Padilha, A. R. Rocha, and G. M. Dalpian: Journal of Physics D: Applied Physics, accepted (2020); DOI: 10.1088/1361-6463/ab7a58
4. Modulation of the optical absorption edge of ϵ- and κ-Ga2O3 due to Co impurities caused by band structure changes: Work function measurements and first-principle calculations
   K. Yamanaka, H. Raebiger, K. Mukai, and K. Shudo: Journal of Applied Physics **127** (2020) 065701.
5. Carrier mediated ferromagnetism in Ga_2O_3:Cr
   K. Ichihashi, H. Shinya, and H. Raebiger: Applied Physics Express **13** (2020) 021002.

SAITO, Mineo [C class; 7500 (B), 0 (C)] (75)
— *First-principles study for widening the potential of spin-polarized positron experiments*

1. First-principles calculation of anomalous muonium in silicon: origin of the negative Fermi contact interaction constant
   Muhamad Nasruddin Manaf, Susumu Minami, Fumiyuki Ishii and Mineo Saito: J. J. Appl. Phys. **58** (2019) 081008.

SAKAGUCHI, Norihito [C class; 7000 (B), 0 (C)] (78)
— *Reduction of Rare Metals in Fuel Cell Catalysts and Hydrogen Permeable Membrane*

1. 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 **62** (2019) 344.
2. Extraordinarily Large Kinetic Isotope Effect on Alkene Hydrogenation over Rh-based Intermetallic Compounds
   S. Furukawa, P. Yi, Y. Kunisada, K. Shimizu: Science and Technology of Advanced Materials **20** (2019) 805.
3. Co-appearance of superconductivity and ferromagnetism in a Ca_2RuO_4 nanofilm crystal
   SH. Nobukane, K. Yanagihara, Y. Kunisada, Y. Ogasawara, K. Nomura, Y. Asano, S. Tanda: Scientific Reports **10** (2020) 3462.

SAKAI, Toru [C class; 9500 (B), 1600 (C)] (245, 247)
— *Numerical Diagonalization Study on Spin Nematic Phase of Low-Dimensional Systems*
— *Topological Magnetization Plateau of Quantum Antiferromagnetic Spin Chain with Anisotropies*

1. 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.
2. 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).

3. Magnetization plateau of the S=2 antiferromagnetic Heisenberg chain with anisotropies
T. Sakai, K. Okamoto and T. Tonegawa: Phys. Rev. B 100 (2019) 054407.
4. Two magnetization plateaus in the kagome fluoride $Ce_2LiTi_3F_{12}$
R. Shirakami, H. Ueda, H. O. Jeschke, H. Nakano, S. Kobayashi, A. Matsuo, T. Sakai, N. Katayama, H. Sawa, K. Kindo, C. Michioka and K. Yoshimura: Phys. Rev. B 100 (2019) 174401.
5. Properties of the H-T phase diagram of the 3-K phase in eutectic Sr2RuO4-Ru: Evidence for chiral superconductivity
H. Kaneyasu, Y. Enokida, T. Nomura, Y. Hasegawa, T. Sakai and M. Sigrist: Phys. Rev. B 100 (2019) 21451.
6. Spin Nematic Phase of the Quantum Spin Nanotube
T. Sakai: JPS Conference Proceedings 29 (2020) 014004.
7. Field-Induced Spin Nematic Phase in the S=1 Anisotropic Spin Ladder
R. Yamanokuchi, K. Okamoto and T. Sakai: Proceedings of 2018 16th International Conference on Megagauss Magnetic Field Generation and Related Topics (MEGAGAUSS) (2019) 8722674.
8. Haldane Gaps of Large-S Heisenberg Antiferromagnetic Chains and Asymptotic Behavior
H. Nakano, N. Todoroki and T. Sakai: J. Phys. Soc. Jpn. 88 (2019) 114702.
9. Spin Nematic Liquids of the S = 1 Spin Ladder in Magnetic Field
T. Sakai and K. Okamoto: JPS Conference Proceedings 30 (2020) 011083.
10. Ground-State Phase Diagram of an Anisotropic S = 1 Ferromagnetic-Antiferromagnetic Bond-Alternating Chain
K. Okamoto, T. Tonegawa, M. Kaburagi and T. Sakai: JPS Conference Proceedings 30 (2020) 011024.
11. Quantum Phase Transition of the Twisted Spin Tube
Y. Tachibana, Y. Ueno, T. Zenda, K. Okamoto and T. Sakai: JPS Conference Proceedings 30 (2020) 011082.
12. Quantum Phase Transitions of the Distorted Diamond Spin Chain
T. Zenda, Y. Tachibana, Y. Ueno, K. Okamoto and T. Sakai: JPS Conference Proceedings 30 (2020) 011084.
13. Magnetization Plateau of the Distorted Diamond Spin Chain
Y. Ueno, T. Zenda, Y. Tachibana, K. Okamoto and T. Sakai: JPS Conference Proceedings 30 (2020) 011085.
14. Features of Chirality Generated by Paramagnetic Coupling to Magnetic Fields in the 3K-Phase of Sr_2RuO_4
H. Kaneyasu, Y. Enokida, T. Nomura, Y. Hasegawa, T. Sakai and M. Sigrist: JPS Conference Proceedings 30 (2020) 011039.

SAKAKIBARA, Hirofumi [B class; 800 (B), 0 (C)] (171)
— *Developments of a derivation method of a low-energy models in first-principles*

1. Model-mapped random phase approximation to evaluate superconductivity in the fluctuation exchange approximation from first principles
H. Sakakibara, T. Kotani: Phys. Rev. B **99**, 195141(2019).
2. Finite electric-field approach to evaluate the vertex correction for the screened Coulomb interaction in the quasiparticle self-consistent GW method
H. Sakakibara, T. Kotani, M. Obata, T. Oda: Phy. Rev. B (2020) in press.

SAKURAGI, Shunsuke [C class; 1000 (B), 0 (C)] (163)
— *Controlling of magnetism in Pd(100) ultrathin films by modification of quantum-well states via adsorption of transition metals*

1. Switching of magnetism via modifying phase shift of quantum-well states by tailoring the interface electronic structure
S. Sakuragi, H. Kageshima, and T. Sato: Phys. Rev. B **101** (2020) 014410.

SASAKI, Kazuo [B class; 700 (B), 90 (C)] (335)
— *Simulation analysis of collision of two filaments driven by protein molecular motors*

SASAKI, Takehiko [C class; 3000 (B), 200 (C)] (120)
— *Reaction processes of polyalcohols in high temperature water by First Principles Calculations*

SATO, Tetsuya [C class; 1000 (B), 350 (C)] (157)
— *Study of appearance of ferromagnetism by electric field application to Pt thin film*

SHAO, Cheng [C class; 2000 (B), 650 (C)] (132)
— *Multiscale computational design of thermoelectric materials*

SHIGA, Takuma [B,C class; 2200 (B), 0 (C)] (293, 295, 296)
— *Clarification of thermal transport spectra in hierarchical structured organic bulk materials*
— *Compherensive study on transition between heat conduction and radiative heat transfer*
— *Heat conduction analysis for phononic crystal*

SHIMADA, Toshihiro [B class; 800 (B), 0 (C)] (170)
— *First principle simulation on ultrahigh pressure synthesis of new material from organic molecules*

1. Sugar-assisted Mechanochemical Exfoliation of Graphitic Carbon Nitride for Enhanced Visible-light Photocatalytic Performance
   Wei Liu, Takashi Yanase, Nobuhiro Iwasa, Hitoshi Koizumi, Shin Mukai, Shinichiro Iwamura, Taro Nagahama, and Toshihiro Shimada: International J. of Hydrogen Enegry **44** (2020) 8444.
2. Porous Graphitic Carbon Nitride Nanoplates Obtained by A Combined Exfoliation Strategy for Enhanced Visible Light Photocatalytic Activity
   Wei Liu, Nobuhiro Iwasa, Shinichiro Fujita, Hitoshi Koizumi, Makoto Yamaguchi and Toshihiro Shimada: Applied Surface Science **499** (2020) 143901.
3. Synthesis and Enhanced Room-temperature Ferromagnetic Properties of Carbon-doped Boron Nitride Nanosheets
   Wei Liu, Takashi Yanase, Taro Nagahama and Toshihiro Shimada: J. Alloys and Compounds **792** (2019) 1206.

SHIMAMURA, Kohei [C class; 2500 (B), 650 (C)] (124)
— *Construction of neural network force field for molecular dynamics simulation in multicomponent system*

1. Guidelines for Creating Artificial Neural Network Empirical Interatomic Potential from First-Principles Molecular Dynamics Data under Specific Conditions and Its Application to α-Ag_2Se
   K. Shimamura, S. Fukushima, A. Koura, F. Shimojo, M. Misawa, R. K. Kalia, A. Nakano, P. Vashishta, T. Matsubara, and S. Tanaka: J. Chem. Phys. **151** (2019) 124303.

SHIMOJO, Fuyuki [C class; 5000 (B), 0 (C)] (103)
— *First-Principles Molecular-Dynamics Study of Structural and Electronic Properties of Covalent Liquids and Glasses under Pressure*

1. Structural studies on fluid sulfur at high temperatures and high pressures: II. Molecular structure obtained by *ab initio* molecular dynamics simulations
   S. Munejiri, F. Shimojo, K. Hoshino, and M. Inui: J. Non-Cryst. Solids **510**, 15 (2019).
2. Structural change in liquid sulphur from chain polymeric liquid to atomic simple liquid under high pressure
   S. Ohmura and F. Shimojo,: J. Phys.: Condens. Matter **31**, 215101 (2019).
3. Guidelines for Creating Artificial Neural Network Empirical Interatomic Potential from First-Principles Molecular Dynamics Data under Specific Conditions and Its Application to α-Ag_2Se
   K. Shimamura, S. Fukushima, A. Koura, F. Shimojo, M. Misawa, R. K. Kalia, A. Nakano, P. Vashishta, T. Matsubara, and S. Tanaka: J. Chem. Phys. **151**, 124303 (2019).
4. GGA+U Molecular Dynamics Study of Structural and Dynamic Properties of Superionic Conductor Ag_2Se

S. Fukushima, M. Misawa, A. Koura and F. Shimojo: J. Phys. Soc. Jpn. **88**, 115002 (2019).

5. Thermodynamic Integration by Neural Network Potentials Based on First-principles Dynamic Calculations
   S. Fukushima, E. Ushijima, H. Kumazoe, A. Koura, F. Shimojo, K. Shimamura, M. Misawa, R. K. Kalia, A. Nakano, and P. Vashishta: Phys. Rev. B **100**, 214108 (2019).

SHIMOKAWA, Tokuro [C class; 4500 (B), 1250 (C)] (261)
— *Thermal effect on the quantum frustrated magnetism*

SHINAOKA, Hiroshi [B class; 800 (B), 0 (C)] (232)
— *Exploring low-rank tensor representation of Matsubara Green's functions*

1. Sparse sampling and tensor network representation of two-particle Green's functions
   H. Shinaoka, D. Geffroy, M. Wallerberger, J. Otsuki, K. Yoshimi, E. Gull, J. Kuneš, SciPost Phys. **8**, (2020) 012 .

SHINODA, Wataru [E class; 24000 (B), 3000 (C)] (355)
— *Molecular basis analysis of Soft Materials using All-Atom and Coarse-Grained Molecular Dynamics Simulations*

1. Free energy analysis of membrane pore formation process in the presence of multiple melittin peptides
   Y. Miyazaki, S. Okazaki, and W. Shinodai: BBA - Biomembranes **1861** (2019) 1409-1419.
2. Cholesterol-Induced Conformational Change in the Sphingomyelin Headgroup
   S. Hanashima, K. Murakami, M. Yura, Y. Yano, Y. Umegawa, H. Tsuchikawa, N. Matsumori, S. Seo, W. Shinoda, and M. Murata: Biophys. J. **117** (2019) 307-318.
3. Hydrogen Permeation in Hydrated Perfluorosulfonic Acid Polymer Membranes: Effect of Polymer Crystallinity and Equivalent Weight
   K. Takeuchi, A. Kuo, T. Hirai, T. Miyajima, S. Urata, S. Terazono, S. Okazaki, and W. Shinoda: J. Phys. Chem. C **123**, (2019) 20628-20638.
4. Average Conformation of Branched Chain Lipid PGP-Me That Accounts for the Thermal Stability and High-Salinity Resistance of Archaeal Membranes
   M. Yamagami, H. Tsuchikawa, J. Cui, Y. Umegawa, Y. Miyazaki, S. Seo, W. Shinoda, and M. Murata: Biochemistry **58**, (2019) 3869-3879.
5. Effects of Packing Density and Chain Length on the Surface Hydrophobicity of Thin Films Composed of Perfluoroalkyl Acrylate Chains: A Molecular Dynamics Study
   H. O. S. Yadav, A. Kuo, S. Urata, and W. Shinoda: Langmuir **35**, (2019) 14316-14323.
6. Large-scale molecular dynamics simulation of perfluorosulfonic acid T membranes: Remapping coarse-grained to all-atomistic simulations
   A. Kuo, Y. Miyazaki, C. Jang, T. Miyajima, S. Urata, S. O. Nielsen, S. Okazaki, and W. Shinoda: Polymer **181**, (2019) 121766.
7. Heteroaryldihydropyrimidines Alter Capsid Assembly By Adjusting the Binding Affinity and Pattern of the Hepatitis B Virus Core Protein
   H. Liu, S. Okazaki, and W. Shinoda: J. Chem. Inf. Model. **59**, (2019) 5104-5110.
8. pSPICA: A Coarse-Grained Force Field for Lipid Membranes Based on a Polar Water Model
   Y. Miyazaki, S. Okazaki, and W. Shinoda: J. Chem. Theory Comput. **16**, (2020) 782-793.

SHINOHARA, Yasushi [C class; 4000 (B), 0 (C)] (113)
— *First-principles calculations for nonlinear light absorption of insulators*

1. Asymmetric nonlinear optics of a polar chemical bond
   Yuya Morimoto, Yasushi Shinohara, Mizuki Tani, Bo-Han Chen, Kenichi L. Ishikawa, Peter Baum: arXiv:1910.11821, submitted.
2. Detecting electron-phonon couplings during photo-induced phase transition
   Takeshi Suzuki, Yasushi Shinohara, Yangfan Lu, Mari Watanabe, Jiadi Xu, Kenichi L. Ishikawa, Hide Takagi, Minoru Nohara, Naoyuki Katayama, Hiroshi Sawa, Masami Fujisawa, Teruto Kanai, Jiro Itatani, Takashi Mizokawa, Shik Shin, Kozo Okazaki: arXiv:2002.10037, submitted.
3. Strong-Field Electron Dynamics in Solids

Kenichi L. Ishikawa, Yasushi Shinohara, Takeshi Sato, Tomohito Otobe: arXiv:2003.14090, appeared as a chapter in a book.

SHIOMI, Junichiro [C class; 4500 (B), 750 (C)] (265)
— *Screening for Thermal Functional Materials using Materials Informatics*

1. Design of highly-selective radiative-cooling structure accelerated by materials informatics
   Jiang Guo, Shenghong Ju, Junichiro Shiomi: Optics Letters, 45, 343-346(2020).
2. Enhancing thermal boundary conductance of graphite- metal interface by triazine-based molecular bonding
   Aun Ota, Masato Ohnishi, Hisayoshi Oshima, Hisayoshi, Takuma Shiga, Takashi Kodama, Junichiro Shiomi: ACS Applied Materials & Interfaces, 11, 37295-37301 (2019).
3. Spectral control of thermal boundary conductance between copper and carbon crystals by self-assembled monolayers
   Shih-Wei Hung, Shiqian Hu, Junichiro Shiomi: ACS Applied Electronic Materials, 1, 2594-2601 (2019).
4. Scalable multi- nanostructured silicon for room-temperature thermoelectrics
   Makoto Kashiwagi, Yuxuan Liao, Shenghong Ju, Asuka Miura, Shota Konishi, Takuma Shiga, Takashi Kodama, and Junichiro Shiomi: ACS Applied Energy Materials, 2, 7083-7091 (2019).
5. Disorder Limits the Coherent Phonon Transport in Two- Dimensional Phononic Crystal Structure
   Shiqian Hu, Zhongwei Zhang, Pengfei Jiang, Weijun Ren, Cuiqian Yu, Junichiro Shiomi, Jie Chen: Nanoscale, 11, 11839-11846 (2019).
6. Monte Carlo tree search for materials design and discovery
   Thaer Dieb, Shenghong Ju, Junichiro Shiomi, Koji Tsuda: MRS Communications, 9, 532-536 (2019).
7. Anomalously low thermal conductivity in superhard cubic-Si3N4
   Jing Liu, Shenghong Ju, Norimasa Nishiyama, Junichiro Shiomi: Physical Review B, 100, 064303 (2019).
8. Materials informatics for heat transfer: Recent progresses and perspectives
   Shenghong Ju, Junichiro Shiomi: Nanoscale and Microscale Thermophysical Engineering, 23, 157172 (2019).
9. Quantifying phonon particle and wave transport in nanostructures–The unexpectedly strong particle effect in silicon nanophononic metamaterial with cross junction, Materials Today Physics, 8, 56-61 (2019). cooling structure accelerated by materials informatics
   Dengke Ma, Anuj Arora, Shichen Deng, Junichiro Shiomi, Nuo Yang: Optics Letters, 45, 343-346 (2020).

SHIRAI, Tatsuhiko [B class; 700 (B), 0 (C)] (341)
— *The analysis of the dynamical response to the optical bistability*

1. Dynamical phase transition in Floquet optical bistable systems: An approach from finite-size quantum systems
   T. Shirai, S. Todo, and S. Miyashita: Phys. Rev. A **101** (2020) 013809.
2. Thermalization in open many-body systems based on eigenstate thermalization hypothesis
   T. Shirai and T. Mori: Phys. Rev. E **101** (2020) 042116.
3. A guiding principle for embedding in simulated-annealing based Ising machines
   T. Shirai, S. Tanaka and N. Togawa: Submitted to IEEE Transactions on Computers: Special Issue of Quantum Computing

SHIRAISHI, Kenji [C class; 5500 (B), 0 (C)] (97)
— *Theoretical Design of Gate Dielectrics of Future GaN Power Devices*

SHUDO, Ken-ichi [C class; 500 (B), 50 (C)] ()
— *Impurity effects on electronic states of PbS nano-particles*

SUGINO, Osamu [E class; 13000 (B), 2000 (C)] (52)
— *Physics of electrode interfaces*

1. Nuclear quantum effect for hydrogen adsorption on Pt(111)
   L. Yan, Y. Yamamoto, M. Shiga, and O. Sugino: Phys. Rev. B 101, 165414 (2020).
2. Scaling Relation of Oxygen Reduction Reaction Intermediates at Defective TiO2 Surfaces
   Y. Yamamoto, S. Kasamatsu, and O. Sugino: J. Phys. Chem. C 123, 19486-19492 (2019).

SUWA, Hidemaro [C class; 9500 (B), 0 (C)] (251)
— *Dynamical spin structure factor of spin-orbit insulator*
— *Dynamics of Slater-Mott crossover materials*

SUZUKI, Takafumi [C class; 4000 (B), 650 (C)] (285)
— *Quantum spin liquids in extended Kitaev models on a honeycomb lattice*

1. Quantized Δ S=2 Excitation Spectra by Confinement in an S=1 Spin Chain
   Takafumi Suzuki and Seiichiro Suga:J. Phys. Soc. Jpn. **88**, 053702 (2019).
2. Temperature Dependence of Heat Capacity in the Kitaev-Heisenbeg Model on a Honeycomb Lattice
   Takafumi Suzuki and Youhei Yamaji:J. Phys. Soc. Jpn. **88**, 115001 (2019).

SUZUKI, Yuji [C class; 6000 (B), 0 (C)] (85)
— *Development of High-performance Polymer Electret*
— *Development of High-performance Polymer Electret Using Quantum Chemical Analysis*

1. Solid State Quantum Chemical Investigation of a High-performance Fluorinated Amorphous Polymer Electret
   S. Kim, K.Suzuki, and Y. Suzuki: Invited talk, IEEE 17th Int. Symp. Electrets (ISE17), Limerick, p.23 (2019)
2. Investigation of Charge Stability in Amorphous Fluorinated Polymer Using Quantum Chemical Analysis
   S. Kim, Y. Zhang, K.Suzuki, and Y. Suzuki: IEEE Conf. on Electr. Insul. Dielectr. Phenom. (CEIDP), Richland, 8-1 (2019)

TADANO, Terumasa [C class; 6000 (B), 1000 (C)] (15)
— *Predicting and understanding structural phase transition of solids from finite-temperature phonon calculations*

1. First-principles study of phonon anharmonicity and negative thermal expansion in ScF_3
   Y. Oba, T. Tadano, R. Akashi and S. Tsuneyuki: Phys. Rev. Mater. **3** (2019) 033601.
2. Quantum crystal structure in the 250-kelvin superconducting lanthanum hydride
   I. Errea, F. Belli, L. Monacelli, A. Sanna, T. Koretsune, T. Tadano, R. Bianco, M. Calandra, R. Arita, F. Mauri and J. A. Flores-Livas: Nature **578** (2020) 66.
3. Materials design of dynamically stable d9 layered nickelates
   M. Hirayama, T. Tadano, Y. Nomura and R. Arita: Phys. Rev. B **101** (2020) 075107.
4. Anharmonicity Explains Temperature Renormalization Effects of the Band Gap in $SrTiO_3$.
   Y. Wu, W. A. Saidi, J. K. Wuenschell, T. Tadano, P. Ohodnicki, B. Chorpening and Y. Duan: J. Phys. Chem. Lett. **11** (2020) 2518.
5. Enargite Cu_3PS_4: A CuS-Based Thermoelectric Material with a Wurtzite-Derivative Structure
   T. Tanimoto, K. Suekuni, T. Tanishita, H. Usui, T. Tadano, T. Kamei, H. Saito, H. Nishiate, C. H. Lee, K. Kuroki and M. Ohtaki: Adv. Funct. Mater. **2020** (2020) 2000973.

TAKAHASHI, Osamu [C,D class; 1000 (B), 750 (C)] (148)
— *Electronic state of water and ethanol in aqueous solution*
— *Electronic state of water under various environments*

1. Si $1s^{-1}$, $2s^{-1}$ and $2p^{-1}$ lifetime broadening of SiX_4 (X = F, Cl, Br, CH_3) molecules: SiF_4 anomalous behaviour reassessed
   R. Pttner, T. Marchenko, R. Guillemin, L. Journel, G. Goldsztejn, D. Colin, O. Takahashi, K. Ueda, A. F. Lago, M. N. Piancastelli, and M. Simon: Phys. Chem. Chem. Phys., 21(17), 8827 -

8836 (2019)
2. Electronic States of Acetic Acid in a Binary Mixture of Acetic Acid and 1-Methylimidazole Depend on the Environment
N. Yoshimura, O. Takahashi, M. Oura, and Y. Horikawa: J. Phys. Chem. B 123 (6), 1332 - 1339(2019)
3. pH dependence of aqueous oxalic acid observed by X-ray absorption and emission spectroscopy
R. Yamamura, T. Suenaga, M. Oura, T. Tokushima, and O. Takahashi, Chem. Phys. Lett. 738, 136895 (2020).

TAKETSUGU, Tetsuya [C class; 3500 (B), 600 (C)] ()
— *Ab initio study on the structure and functions of nanomaterials*

TAMURA, Ryo [C class; 1000 (B), 250 (C)] (318)
Effective model estimation using experimental results
1. Efficient recommendation tool of materials by an executable file based on machine learning
K. Terayama, K. Tsuda, and R. Tamura: Japanese Journal of Applied Physics **58** (2019) 098001.
2. Quantum Phase Transition in Fully Connected Quantum WajnflaszPick Model
Y. Seki, S. Tanaka, and S. Kawabata: J. Phys. Soc. Jpn. **88** (2019) 054006.
3. Application of Ising Machines and a Software Development for Ising Machines
K. Tanahashi, S. Takayanagi, T. Motohashi, and S. Tanaka: J. Phys. Soc. Jpn. **88** (2019) 061010.
4. 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 on Information and Systems, **E102.D** (2019) 1696.
5. Designing metamaterials with quantum annealing and factorization machines
K. Kitai, J. Guo, S. Ju, S. Tanaka, K. Tsuda, J. Shiomi, and R. Tamura: Physical Review Research **2** (2019) 013319.
6. Data Integration for Accelerated Materials Design via Preference Learning
X. Sun, Z. Hou, M. Sumita, S. Ishihara, R. Tamura, and K. Tsuda: New Journal of Physics in press.
7. A guiding principle for embedding in simulated-annealing based Ising machines
T. Shirai, S. Tanaka, and N. Togawa: submitted to IEEE Journal
8. Data-driven determination of a spin Hamiltonian of $KCu_4P_3O_{12}$ with uncertainty
R. Tamura, K. Hukushima, A. Matsuo, K. Kindo, and M. Hase: submitted.

TANAKA, Hajime [B,D class; 4900 (B), 0 (C)] (273, 275, 277, 279)
— *Coarsening mechanism of network-forming phase separation in colloidal suspensions*
1. Influence of Hydrodynamic Interactions on Colloidal Crystallization
M. Tateno ,T. Yanagishima ,J. Russo and H. Tanaka: Phys. Rev. Lett. **123** (2019) 258002.

TANAKA, Shu [C class; 500 (B), 100 (C)] (344)
— *Study on Ising machines from a viewpoint of statistical mechanics*
1. Quantum Phase Transition in Fully Connected Quantum WajnflaszPick 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. **88** (2019) 061010.
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 on Information and Systems, **E102.D** (2019) 1696.
4. Efficient recommendation tool of materials by an executable file based on machine learning
K. Terayama, K. Tsuda, and R. Tamura: Japanese Journal of Applied Physics **58** (2019) 098001.
5. Designing Metamaterials with Quantum Annealing and Factorization Machines
K. Kitai, J. Guo, S. Ju, S. Tanaka, K. Tsuda, J. Shiomi, and R. Tamura: Phys. Rev. Research **2** (2020) 013319.

6. Data Integration for Accelerated Materials Design via Preference Learning
   X. Sun, Z. Hou, M. Sumita, S. Ishihara, R. Tamura, and K. Tsuda: New Journal of Physics in press.
7. A guiding principle for embedding in simulated-annealing based Ising machines
   T. Shirai, S. Tanaka, and N. Togawa: submitted to IEEE Journal.
8. Data-driven determination of a spin Hamiltonian of $KCu_4P_3O_{12}$ with uncertainty
   R. Tamura, K. Hukushima, A. Matsuo, K. Kindo, and M. Hase: submitted.

TATENO, Masaru [C class; 5000 (B), 0 (C)] ()
— *Multi-scale Hybrid Molecular Dynamics Simulations of Biological Catalysis*

TATETSU, Yasutomi [C class; 4000 (B), 750 (C)] (105)
— *First-principles study on grain boundaries of permanent magnets*
1. First-principles study on surface stability and interface magnetic properties of $SmFe_{12}$
   Y. Ainai, T. Shiozawa, Y. Tatetsu, and Y. Gohda: Appl. Phys. Exp. **13** (2020) 045502.
2. First-principles study of crystalline NdFe alloys
   Y. Ainai, Y. Tatetsu, A. Terasawa, and Y. Gohda, Appl. Phys. Exp. **13** (2020) 017006.

TATEYAMA, Yoshitaka [C class; 12500 (B), 900 (C)] (54)
— *DFT sampling analysis of interfaces and electrolytes in novel batteries*
— *DFT-MD sampling analysis of interfaces and electrolytes in novel batteries*
1. Li+ Transport Mechanism at Heterogeneous Cathode / Solid Electrolyte Interface in All-Solid-State Battery via First-Principles Structure Prediction Scheme
   B. Gao, R. Jalem, Y. Ma, Y. Tateyama, Chem. Mater. **32** (2020) 85.
2. Reaction Energy Benchmarks of Hydrocarbon Combustion by Gaussian Basis and Plane Wave Basis Approaches
   A. Ishikawa, Y. Tateyama, J. Comp. Chem. **40** (2019) 1866.
3. Electrochemical properties of fluorinated boron-doped diamond electrodes via fluorine-containing plasma treatmen
   C. Yamaguchi, K. Natsui, S. Iizuka, Y. Tateyama, Y. Einaga, Phys. Chem. Chem. Phys. **21** (2019) 13788.
4. Theoretical picture of positive electrode / solid electrolyte interface in all-solid-state battery from electrochemistry and semiconductor physics viewpoints
   Y. Tateyama, B. Gao, R. Jalem, J. Haruyama, Curr. Opin. Electrochem. **17** (2019) 149.
5. Surface-Dependent Stability of Interface between the Garnet Li7La3Zr2O12 and the Li Metal in the All-Solid-State Battery from First-Principles Calculations
   B. Gao, R. Jalem, Y. Tateyama, ACS Appl. Mater. Interfaces, **12** (2020) 16350.
6. Possible high-potential ilmenite type Na1MO3 (M = VNi) cathodes realized by dominant oxygen redox reaction
   M. H. N. Assadi, M. Okubo, A. Yamada, Y. Tateyama, Phys. Rev. Mater. **4** (2020) 015401.
7. Machine learning prediction of coordination energies for alkali group elements in battery electrolyte solvents
   A. Ishikawa, K. Sodeyama, Y. Igarashi, T. Nakayama, Y. Tateyama, M. Okada, Phys. Chem. Chem. Phys. **21** (2019) 26339.
8. What Is the Active Site for the Oxidative Coupling of Methane Catalyzed by MgO? A Metadynamics-Biased Ab Initio Molecular Dynamics Study
   A. Ishikawa, Y. Tateyama, J. Phys. Chem. C **124** (2020) 6054.

TERAO, Takamichi [B class; 1200 (B), 160 (C)] (316)
— *Molecular simulation of patchy particles*
1. Numerical method to study three-dimensional metamaterial composites
   T. Terao: Proceedings of 13th international congress on artificial materials for novel wave phenomena (2019) X426.

TERASAWA, Asako [C class; 3000 (B), 550 (C)] (115)

— *First principles calculations and analysis on relationship between exchange coupling constants and local structures for magnetic alloys and amorphous grain boundary phases in permanent magnets*

1. Efficient Algorithm Based on Liechtenstein Method for Computing Exchange Coupling Constants Using Localized Basis Set
   A. Terasawa, M. Matsumoto, T. Ozaki, and Y. Gohda: J. Phys. Soc. Jpn., vol. 88, no. 11, p. 114706, Oct. 2019, doi: 10.7566/JPSJ.88.114706.

TODO, Synge [C class; 6000 (B), 850 (C)] (256)

— *Entanglement Quantum Phase Transition and Quantum Dynamics in Quantum Many-body Systems*

1. Machine learning for molecular dynamics with strongly correlated electrons
   Hidemaro Suwa, Justin S. Smith, Nicholas Lubbers, Cristian D. Batista, Gia-Wei Chern, Kipton Barros, Phys. Rev. B **99**, 161107 (5pp) (2019)
2. Gapless Kitaev Spin Liquid to Classical String Gas through Tensor Networks
   Hyun-Yong Lee, Ryui Kaneko, Tsuyoshi Okubo, Naoki Kawashima, Phys. Rev. Lett. 123, 087203 (6pp) (2019)
3. Subspace-search variational quantum eigensolver for excited states
   Ken M. Nakanishi, Kosuke Mitarai, Keisuke Fujii, Phys. Rev. Research 1, 033062 (7pp) (2019)
4. Characterization of localized effective spins in gapped quantum spin chains
   Hayate Nakano, Seiji Miyashita, Phys. Rev. B **100**, 195105 (11pp) (2019)
5. Multiple-q states of the J_1-J_2 classical honeycomb-lattice Heisenberg antiferromagnet under magnetic fields
   Tokuro Shimokawa, Tsuyoshi Okubo, Hikaru Kawamura, Phys. Rev. B 100, 224404 (15pp) (2019)
6. Dynamical phase transition in Floquet optical bistable systems: An approach from finite-size quantum systems
   Tatsuhiko Shirai, Synge Todo, Seiji Miyashita, Phys. Rev. A 101, 013809 (7pp) (2020)
7. Abelian and Non-Abelian Chiral Spin Liquids in a Compact Tensor Network Representation
   Hyun-Yong Lee, Ryui Kaneko, Tsuyoshi Okubo, Naoki Kawashima, Phys. Rev. B 101, 035140 (9pp) (2020)
8. Spin-lattice coupling in a ferrimagnetic spinel: Exotic $H - T$ phase diagram of $MnCr_2S_4$ up to 110 T
   A. Miyata, H. Suwa, T. Nomura, L. Prodan, V. Felea, Y. Skourski, J. Deisenhofer, H.-A. Krug von Nidda, O. Portugall, S. Zherlitsyn, V. Tsurkan, J. Wosnitza, A. Loidl, Phys. Rev. B 101, 054432 (8pp) (2020)

TOHYAMA, Takami [C class; 2500 (B), 550 (C)] (290)

— *Finite-Temperature Properties and Spin Dynamics in Kagome Kitaev-Heisenberg Model*

1. Finite-temperature properties of the Kitaev-Heisenberg models on kagome and triangular lattices studied by improved finite-temperature Lanczos methods
   K. Morita and T. Tohyama: Phys. Rev. Research **2**, (2020) 013205.
2. Magnetic orders induced by RKKY interaction in Tsai-type quasicrystalline approximant Au-Al-Gd
   H. Miyazaki, T. Sugimoto, K. Morita, and T. Tohyama: Phys. Rev. Materials **4**, (2020) 024417.
3. Vanishing Wilson ratio as the hallmark of quantum spin-liquid models
   P. Prelovsek, K. Morita, T. Tohyama, and J. Herbrych: Phys. Rev. esearch **2**, (2020) 023024.

TOMITA, Yusuke [C class; 5500 (B), 0 (C)] (264)

— *Study of relaxor ferroelectrics by using a minimal model*

TONEGAWA, Takashi [B,C class; 2100 (B), 0 (C)] (297)

— *Numerical Study of the One-Dimensional Quantum Spin Systems with Spatial Structures*

— *Numerical Study of the One-Dimensional Quantum Spin Systems with Spatial Studies*

1. Mgnetization Plateau of the $S = 2$ Antiferromagnetic Heisenberg Chain with Anisotropies
   T. Sakai, K. Okamoto, and T. Tonegawa: Phys. Rev. B **100**, 054407 (2019).
2. Ground-State Phase Diagram of an Anisotropic $S = 1$ Ferromagnetic-Antiferromagnetic Bond-

Alternating Chain
K. Okamoto, T. Tonegawa, M. Kaburagi, and T. Sakai: JPS Conf. Proc. **30**, 011024 (2020).

TSUKAHARA, Noriyuki [B class; 400 (B), 0 (C)] ()
— *Theoretical study of spin detection in lanthanoid atoms and molecules by adsorption on superconducting substrate*

TSUNEYUKI, Shinji [C class; 7000 (B), 950 (C)] (73)
— *Material exploration by advanced first-principles simulation*

1. 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., **127** (2019) 404.
2. 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. **241** (2019) 92.
3. X 線回折実験とシミュレーションのデータ同化による結晶構造解析
   藤堂 眞治, 常行 真司, 日本結晶学会誌 **62** (2020) 51.

TSURUTA, Kenji [C class; 2500 (B), 0 (C)] (137)
— *Hybrid Ab-Initio/Machine-Learning Computation for Designing Dynamical Properties of Nano/Molecular Structures*

1. First-principles Study on Water Dissociation in Grain Boundary of MAPbI3 Perovskite
   M.A.A. Asad, K. Sato, and K. Tsuruta: MRS Adv. **4** (2019) 1965.
2. Optimization of Molecular Characteristics via Machine Learning based on Continuous Representation of Molecules
   K. Sato and K. Tsuruta: Mater. Sci. Forum, in press.

UCHIDA, Takashi [B class; 500 (B), 90 (C)] (348)
— *Magnetic structures of multiple-Q states in frustrated itinerant magnets*

WAKABAYASHI, Daisuke [B class; 700 (B), 0 (C)] ()
— *Inhomogeneous structure of silica glass during the structural transformations under high pressure*

WATANABE, Hiroshi [B class; 900 (B), 100 (C)] (326)
— *Molecular dynamics study of the properties of near-critical fluids*

WATANABE, Hiroshi [B class; 700 (B), 0 (C)] (236)
— *Calculation for ground and excited states in strongly-correlated electron systems by variational Monte Carlo method*

1. Mechanism of superconductivity and electron-hole doping asymmetry in κ-type molecular conductors
   H. Watanabe, H. Seo, and S. Yunoki: Nat. Commun. **10** (2019) 3167.

WATANABE, Kazuyuki [C class; 8000 (B), 700 (C)] (64)
— *First-Principles Study of Excited Electron Positron and Atom Dynamics and Optical and Thermoelectric Properties of Nanostructures*

1. Angle-resolved photoemission spectroscopy in low-dimensional periodic structures: a real-time first-principles simulation
   K. Uchida, Y. Akimoto, K. Einaga, and K. Watanabe, Jpn. J. Appl. Phys. **58**, 128001 (2019).
2. Excitons in two-dimensional atomic layer materials from time-dependent density functional theory : mono-layer and bi-layer hexagonal boron nitride and transition-metal dichalcogenides
   Y. Suzuki and K. Watanabe, Phys. Chem. Chem. Phys. **22**, 2908 (2020).
3. Simulation of a hydrogen atom in a laser field using the time-dependent variational principle
   K. Rowan, L. Schatzki, T. Zaklama, Y. Suzuki, K. Watanabe, and K. Varga, Phys. Rev. E **101**, 023313 (2020).

4. Stationary-state electron scattering using a complex injecting potential
   T. Yamaguchi, K. Uchida, K. Varga, and K. Watanabe, J. Phys. Soc. Jpn. **89**,044002(2020).

WATANABE, Satoshi [C class; 10500 (B), 1700 (C)] (58)
— *Analyses of atomic structures and atom dynamics at surfaces interfaces and defects*

1. 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. **1** (2019) 585.
2. Simulating lattice thermal conductivity in semiconducting materials using high-dimensional neural network potential
   E Minamitani, M Ogura, and S Watanabe: Appl. Phys. Express **12** (2019) 095001.
3. Low-Energy-Consumption Three-Valued Memory Device Inspired by Solid-State Batteries
   Y. Watanabe, S. Kobayashi, I. Sugiyama, K. Nishio, W. Liu, S. Watanabe, R. Shimizu, and T. Hitosugi: ACS Appl. Mater. interfaces **11** (2019) 45150.
4. 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: J. Phys. Chem. C **124** (2019) 2008.
5. Moisture effect on the diffusion of Cu ions in $Cu/Ta_2O_5/Pt$ and $Cu/SiO_2/Pt$ resistance switches: a first-principles study
   B. Xiao and S. Watanabe: Sci. Technol. Adv. Mater. **20** (2019) 580.
6. 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: Phys. Rev. Mater. **4** (2020) 015402.
7. The effect of phonon anharmonicity on the lattice thermal conductivity of rare-earth pyrochlores: A first-principles study
   Z. Li, Y. Xing, S. Watanabe,and W. Pan: Ceram. Int'l **46** (2020) 9947.
8. Atomistic Simulations for Understanding Microscopic Mechanism of Resistive Switches
   S. Watanabe and B. Xiao: in M. Aono (Ed.) "Atomic Switch: From Invention to Practical Use and Future Prospects" (Springer, 2020), p. 95.

YAMADA, Atsuo [C class; 5000 (B), 750 (C)] (94)
— *First-principles analyses on the cathode materials for rechargeable batteries*

1. Sodium- and Potassium- Hydrate Melts Containing Asymmetric Imide Anions for High- Voltage Aqueous Batteries
   Q. Zheng, S. Miura, K. Miyazaki, S. Ko, E. Watanabe, M. Okoshi, C.- P. Chou, Y. Nishimura, H. Nakai, T. Kamiya, T. Honda, J. Akikusa, Y. Yamada, A. Yamada: Angew. Chem. Int. Ed. **58** (2019) 2358.

YAMADA, Atsushi [C class; 500 (B), 300 (C)] (231)
— *Superconductivity and magnetic properties of the Hubbard model*

YAMAJI, Youhei [E class; 15000 (B), 2300 (C)] (200)
— *Numerical studies on energy current correlations in frustrated quantum spin systems*

1. Possible Kitaev Quantum Spin Liquid State in 2D Materials with S=3/2
   C. Xu, J. Feng, M. Kawamura, Y. Yamaji, Yousra Nahas, S. Prokhorenko, Y. Qi, H. Xiang, L. Bellaiche: Phys. Rev. Lett. **124**(2020) 087205.

YAMAMOTO, Kaoru [B class; 500 (B), 80 (C)] ()
— *First-principles calculation of thermoelectric properties for magnetic tunneling junctions and giant magneto-resistance devices*

YAMAMOTO, Norifumi [B class; 700 (B), 90 (C)] (175)
— *Theoretical Study on the Aggregation-Induced Emission*

YAMASHITA, Koichi [C class; 3000 (B), 0 (C)] (129)
— *Large scale ab initio calculations on the fundamental processes of solar energy convergence devices and on designing principles for new materials*

1. Simulation of Conductive Atomic Force Microscopy of Organic Photovoltaics by Dynamic Monte Carlo Method
   E. Kawashima, M. Fujii, and K. Yamashita: Chem. Lett. **48** (2019) 513.
2. Laser-induced fluorescence of the CHFCHO radical and reaction of OH radicals with halogenated ethylenes
   I. Masumoto, N. Washida, S. Inomata, A. Muraoka, and K. Yamashita: J. Chem. Phys. **150** (2019) 174302.
3. A route for minimizing emissions: sun-mediated processes & clean batteries
   G. Giorgi, K. Yamashita, M. Palummo, and S. Fabris: Curr. Opin. Green. Sustain. Chem. **17** (2019) A1.
4. Entropy Promotes Charge Separation in Bulk Heterojunction Organic Photovoltaics
   E. Kawashima, M. Fujii, and K. Yamashita: J. Photochem. Photobiol. A: Chem. **382** (2019) 111875.
5. Importance of Side-Chains on Molecular Characteristics of Interacting Organic Molecules
   K. Mishima, K. Yamashita: ACS Omega **4** (2019) 10396.
6. Application of accelerated long-range corrected exchange functional [LC-DFT(2Gau)] to periodic boundary condition systems: CO adsorption on Cu(111) surface
   K. Mishima, M. Kaneko, J.-W. Song, H. Kawai, K. Yamashita, and K. Hirao: J. Chem. Phys. **152** (2020) 104105.

YAMASHITA, Tomoki [C class; 2500 (B), 600 (C)] (127)
— *Development of algorithms in crystal structure prediction*

YAMAUCHI, Kunihiko [C class; 5000 (B), 0 (C)] (102)
— *First-principles density functional calculations of transition-metal magnetic oxides*

1. Bulk Rashba effect in multiferroics: A theoretical prediction for BiCoO3
   Kunihiko Yamauchi, Paolo Barone, Silvia Picozzi: Phys. Rev. B **100** (2019) 245115.
2. Conversion of a conventional superconductor into a topological superconductor by topological proximity effect
   C.X. Trang, N. Shimamura, K. Nakayama, S. Souma, K. Sugawara, I. Watanabe, K. Yamauchi, T. Oguchi, K. Segawa, T. Takahashi, Yoichi Ando, and T. Sato: Nat. Commun. **11** (2020) 159.
3. Dimensionality reduction and band quantization induced by potassium intercalation in 1T-HfTe2
   Y. Nakata, K. Sugawara, A. Chainani, K. Yamauchi, K. Nakayama, S. Souma, P.-Y. Chuang, C.-M. Cheng, T. Oguchi, K. Ueno, T. Takahashi, and T. Sato: Phys. Rev. Materials **3** (2019) 071001(R).
4. Evidence for bulk nodal loops and universality of Dirac-node arc surface states in ZrGeXc (Xc = S, Se, Te)
   Takechika Nakamura, Seigo Souma, Zhiwei Wang, Kunihiko Yamauchi, Daichi Takane, Hikaru Oinuma, Kosuke Nakayama, Koji Horiba, Hiroshi Kumigashira, Tamio Oguchi, Takashi Takahashi, Yoichi Ando, and Takafumi Sato: Phys. Rev. B **99** (2019) 245105.
5. Topology analysis for anomalous Hall effect in the noncollinear antiferromagnetic states of Mn3AN (A = Ni, Cu, Zn, Ga, Ge, Pd, In, Sn, Ir, Pt)
   Vu Thi Ngoc Huyen, Michi-To Suzuki, Kunihiko Yamauchi, and Tamio Oguchi: Phys. Rev. B **100** (2019) 094426.
6. Possible emergence of a skyrmion phase in ferroelectric GaMo4S8
   Hui-Min Zhang, Jun Chen, Paolo Barone, Kunihiko Yamauchi, Shuai Dong, and Silvia Picozzi: Phys. Rev. B **99** (2019) 214427.

YANAGISAWA, Susumu [C class; 5000 (B), 0 (C)] (100)
— *Implementation of the phonon analysis for organic semiconductor crystals*
— *Structural distortion or defect in organic molecular thin film: theoretical study*

1. Determination of the ionization energy and the electron affinity of organic molecular crystals from

first-principles: dependence on the molecular orientation at the surface
S. Yanagisawa: Jpn. J. Appl. Phys. **59** (2020) 031002.

2. Nanoscale First-Principles Electronic Structure Simulations of Materials Relevant to Organic Electronics
S. Yanagisawa and I. Hamada: In: T. Onishi (eds) Theoretical Chemistry for Advanced Nanomaterials. Springer, Singapore (2020) 89.
3. Enhancement of the GW space-time program code for accurate prediction of the electronic properties of organic electronics materials
S. Yanagisawa, T. Yamashita, and R. Egawa: Sustained Simulation Performance 2018 and 2019. Springer (2020) 225.

YANAGISAWA, Takashi [B class; 1100 (B), 150 (C)] (229)
— *Study of strongly correlated electron systems based on optimization Monte Carlo method and first-principles calculations*

1. Antiferromagnetism, Superconductivity and phase diagram in the two-dimensional Hubbard model
T. Yanagisawa: J. Phys. Soc. Jpn. 88 (2019) 054702.a
2. Mechanism of high-temperature superconductivity in correlated electron systems
T. Yanagisawa: Condensed Matter 2019 (2019) 57.a
3. Fractional Skyrmion and Absence of Low-lying Andreev Bound States in a Micro Fractional-flux Quantum Vortex
T. Yanagisawa: J. Phys. Soc. Jpn. 88 (2019) 104704.
4. Flat-band in Pyrochlore Oxides: A First-Principles Study
I. Hase, T. Yanagisawa, K. Kawashima: Nanomaterials 2019 (2019) 876.
5. Renormalization group analysis of the hyperbolic sine-Gordon model
T. Yanagisawa: Prog. Theor. Exp. Phys. 2019 (2019) 023A01.
6. Antiferromagnetism, Superconductivity and phase diagram in the three-band model of high-temperature superconductors
T. Yanagisawa: J. Phys. Conf. Ser. 1293 (2019) 012027.a
7. Electronic Structure of Novel Non-centrosymmetric Superconductor Mg_2Rh_3P
I. Hase, T. Yanagisawa, A. Iyo, H. Fujihisa, Y. Goto, H, Eisaki, K. Kawashima: J. Phys. Conf. Ser. 1293 (2019) 012028.
8. Flattened remnant-field distribution in superconducting bilayer
Y. Tanaka, H. Yamamori, T. Yanagisawa, S. ooi, M. Tachiki, S. Arisawa: Physica C 567 (2019) 1253489.
9. Phase diagram of cuprate high-temperature superconductors based on the optimization Monte Carlo method
T. Yanagisawa, M. Miyazaki, K. Yamaji: Modern Phys. Lett. (2019) in press.a
10. Phase diagram and mechanism of superconductivity in strongly correlated electrons
T. Yanagisawa, M. Miyazaki, K. Yamaji: J. Super. Novel Magne. (2019) in press.a
11. Electronic structure of novel superconductor doped ZrPSe
I. Hase, T. Yanagisawa, H. Kito et al.: J. Phys. Conf. Ser. (2019) in press.

YASUDA, Chitoshi [B class; 700 (B), 90 (C)] (334)
— *Magnetism in the system with the multiple-spin exchange interactions*

YOKO, Akira [B class; 1400 (B), 180 (C)] (150)
— *Theoretical calculation of solvation and reaction in supercritical fluids*
— *Theoretical study for structure and property of organic modified metal oxide nanoparticles*

YOKOI, Tatsuya [C class; 3000 (B), 500 (C)] (117)
— *Machine-learning-driven molecular simulations for grain-boundary atomic dynamics*

YOSHIDA, Tsuneya [C class; 7500 (B), 0 (C)] (213)
— *Non-Hermitian topological phenomena in strongly correlated systems*
— *Novel topological phenomena induced by strongly correlated dynamics*

1. Exceptional band touching for strongly correlated systems in equilibrium
   Tsuneya Yoshida, Robert Peters, Norio Kawakami, Yasuhiro Hatsugai: arXiv:2002.11265
2. Antiferromagnetic Topological Insulator in Three-Dimensional Heavy-Fermion Systems
   Kazuhiro Kimura, Tsuneya Yoshida, and Norio Kawakami: JPS Conf. Proc. **30**, 011012 (2020).
3. Relationship between exceptional points and the Kondo effect in f-electron materials
   Yoshihiro Michishita, Tsuneya Yoshida, and Robert Peters: Phys. Rev. B **101**, 085122 (2020).
4. Mirror skin effect and its electric circuit simulation
   Tsuneya Yoshida, Tomonari Mizoguchi, and Yasuhiro Hatsugai: arXiv:1912.12022
5. Non-Hermitian fractional quantum Hall states
   Tsuneya Yoshida, Koji Kudo, and Yasuhiro Hatsugai: Scientific Reports **9**, 16895 (2019).
6. Higher-Order Topological Mott Insulators
   Koji Kudo, Tsuneya Yoshida, and Yasuhiro Hatsugai: Phys. Rev. Lett. **123**, 196402(2019).
7. Chiral-symmetry protected exceptional torus in correlated nodal-line semimetals
   Kazuhiro Kimura, Tsuneya Yoshida, and Norio Kawakami: Phys. Rev. B **100**, 115124 (2019)
8. Efficient method to compute Z_4-indices with glide symmetry and applications to Möbius materials, CeNiSn and UCoGe
   Tsuneya Yoshida, Akito Daido, Norio Kawakami, and Youichi Yanase: Phys. Rev. B **99**, 235105 (2019).
9. Exceptional rings protected by emergent symmetry for mechanical systems
   Tsuneya Yoshida and Yasuhiro Hatsugai: Phys. Rev. B **100**, 054109 (2019).

YOSHIDOME, Takashi [C class; 500 (B), 550 (C)] (325)
— *Investigation of dynamics of a supercooled liquid and proteins using the free-energy landscape*

1. Effects of a Low-Pass Filter on the Classification of Protein Electron-Density Maps in terms of Structural Polymorphism using Manifold Learning: A Simulation Study for Cryo-Electron Microscopy Experiments
   N. Takano and T. Yoshidome: J. Phys. Soc. Jpn. **88** (2019) 094801.

YOSHINO, Hajime [C class; 9000 (B), 0 (C)] (35)
— *Phase transitions of an antiferromagnetic Heisenberg spin model with a dynamical Jahn-Teller effect on a pyrochlore lattice*
— *Simultaneous spin and Jahn-Teller glass transitions in a model frustrated system on pyrochlore lattice*

1. Spin-Orbital Glass Transition in a Model of a Frustrated Pyrochlore Magnet without Quenched Disorder
   Kota Mitsumoto, Chisa Hotta and Hajime Yoshino: Phys. Rev. Lett. 124, 087201 (2020).

YUKAWA, Satoshi [B class; 800 (B), 100 (C)] (332)
— *Statistical Properties in a Branching Network*

□ SCCMS Projects

FUJITA, Takatoshi [7000 (B), 0 (C)] (371)

— Development of Fragment-Based GW/BSE Method and Application to Organic Optoelectronic Materials

— Large-scale GW+BSE excited-state calculations for organic optoelectronic materials

1. Charge-transfer excited states in the donor/acceptor interface from large-scale GW calculations
   T. Fujita, Y. Noguchi, T. Hoshi, J. Chem. Phys. **151** (2019) 114109.
2. Numerical aspect of large-scale electronic state calculation for flexible device material
   T. Hoshi, H. Imachi, A. Kuwata, K. Kakuda, T. Fujita, H Matsui, Japan J. Indust. Appl. Math. **36** (2019) 685.

FUKUSHIMA, Tetsuya [5000 (B), 500 (C)] (372)

— Data-driven materials design for new functional high entropy alloys

1. Theoretical prediction of maximum Curie temperatures of Fe-based dilute magnetic semiconductors by first-principles calculations
   T. Fukushima, H. Shinya, A. Masago, K. Sato and H. Katayama-Yoshida: Appl. Phys. Exp. **12** (2019) 063006
2. Experimental verification of the origin of positive linear magnetoresistance in CoFe(V1 − xMnx)Si Heusler alloys
   S. Yamada, S. Kobayashi, A. Masago, L. S. R. Kumara, H. Tajiri, T. Fukushima, S. Abo, Y. Sakuraba, K. Hono, T. Oguchi, and K. Hamaya: Phys. Rev. B **100** (2019) 195137
3. High Curie temperature in Eu-doped GaN caused by volume-compensated Ga-vacancy
   A. Masago, H. Shinya, T. Fukushima, K. Sato, and H. Katayama-Yoshida: AIP Advances **10** (2020) 025216
4. Valence states and the magnetism of Eu ions in Eu-doped GaN
   T. Nunokawa, Y. Fujiwara, Y. Miyata, N. Fujimura, T. Sakurai, H. Ohta, A. Masago, H. Shinya, T. Fukushima, K. Sato, and H. Katayama-Yoshida: J. Appl. Phys. **127** (2020) 083901

GOHDA, Yoshihiro [5000 (B), 500 (C)] (99)

— First-principles study of magnetic-material interfaces

1. First-principles study on surface stability and interface magnetic properties of $SmFe_{12}$
   Y. Ainai, T. Shiozawa, Y. Tatetsu, and Y. Gohda: Appl. Phys. Express **13**, 045502 (2020).
2. First-principles study of crystalline Nd-Fe alloys
   Y. Ainai, Y. Tatetsu, A. Terasawa, and Y. Gohda: Appl. Phys. Express **13**, 017006 (2020).
3. Enhancement of magnetoelectric coupling by insertion of Co atomic layer into $Fe_3Si/BaTiO_3(001)$ interfaces identified by first-principles calculations
   Y. Hamazaki and Y. Gohda: J. Appl. Phys. **126**, 233902 (2019).
4. Great Differences between Low-Temperature Grown Co_2FeSi and Co_2MnSi Films on Single-Crystalline Oxides
   K. Kudo, Y. Hamazaki, S. Yamada, S. Abo, Y. Gohda, and K. Hamaya: ACS Appl. Electron. Mater. **1**, 2371 (2019).
5. Efficient Algorithm Based on Liechtenstein Method for Computing Exchange Coupling Constants Using Localized Basis Set
   A. Terasawa, M. Matsumoto, T. Ozaki, and Y. Gohda: J. Phys. Soc. Jpn. **88**, 114706 (2019).

HOSHI, Takeo [10000 (B), 1000 (C)] (76)

— Massively parallel electronic structure calculation and data-driven science for next-generation supercomputers

1. Kω –Open-source library for the shifted Krylov subspace method
   Takeo Hoshi, Mitsuaki Kawamura, Kazuyoshi Yoshimi, Yuichi Motoyama, Takahiro Misawa, Youhei Yamaji, Synge Todo, Naoki Kawashima, Tomohiro Sogabe: arXiv:2001.08707
2. Two-stage data-analysis method for total-reflection high-energy positron diffraction (TRHEPD)

Kazuyuki Tanaka, Izumi. Mochizuki, Takashi Hanada, Ayahiko Ichimiya, Toshio Hyodo, and Takeo Hoshi: Submitted; Preprint:https://arxiv.org/abs/2002.12165

3. Development of data-analysis software for total-reflection high-energy positron diffraction (TRHEPD)
   Kazuyuki Tanaka, Takeo Hoshi, Izumi Mochizuki, Takashi Hanada, Ayahiko Ichimiya, Toshio Hyodo: Acta. Phys. Pol. A 137, 188-192 (2020).
4. An a posteriori verification method for generalized Hermitian eigenvalue problems in large-scale electronic state calculations
   Takeo Hoshi, Takeshi Ogita, Katsuhisa Ozaki, Takeshi Terao: J. Comp. Appl. Math. 376, 112830/1-13 (2020).
5. Charge-Transfer Excited States in the Donor/Acceptor Interface from Large-Scale GW Calculations
   Takatoshi Fujita, Yoshifumi Noguchi, Takeo Hoshi: J. Chem. Phys. 151, 114109/1-8 (2019).
6. EigenKernel - A middleware for parallel generalized eigenvalue solvers to attain high scalability and usability
   Kazuyuki Tanaka, Hiroto Imachi, Tomoya Fukumoto, Akiyoshi Kuwata, Yuki Harada, Takeshi Fukaya, Yusaku Yamamoto, Takeo Hoshi: Japan J. Indust. Appl. Math 36, 719-742 (2019).
7. Numerical aspect of large-scale electronic state calculation for flexible device material
   Takeo Hoshi, Hiroto Imachi, Akiyoshi Kuwata, Kohsuke Kakuda, Takatoshi Fujita, Hiroyuki Matsui: Japan J. Indust. Appl. Math 36, 685-698 (2019).
8. Recent progress in large-scale electronic state calculations and data-driven sciences
   Takeo Hoshi and Satoshi Ito: Chap. 14 of Handbook of Silicon Based MEMS Materials and Technologies 3rd Ed., Elsevier (2020).
9. Numerical methods for large scale electronic state calculation on supercomputer
   Takeo Hoshi, Yusaku Yamamoto, Tomohiro Sogabe, Kohei Shimamura, Fuyuki Shimojo, Aiichiro Nakano, Rajiv Kalia, Priya Vashishta: Chap. 15 of 21st Century Nanoscience - A Handbook: Nanophysics Sourcebook (Volume One), CRC Press (2019).

IITAKA, Toshiaki [10000 (B), 1000 (C)] (379)
— *Order-disorder transition in the superhigh-pressure phase of Mg2SiO4*

IMADA, Masatoshi [20000 (B), 2000 (C)] (197)
— *Studies on Quantum Spin Liquids in Materials with Strong Spin-Orbit Interaction*
— *Studies on quantum spin liquids in molecular conductors based on first-principles Hamiltonian*

1. Charge dynamics of correlated electrons: Variational description with inclusion of composite fermions
   Kota Ido, Masatoshi Imada, Takahiro Misawa: Phys. Rev. B **101** (2020) 075124.
2. *Ab initio* study of superconductivity and inhomogeneity in a Hg-based cuprate superconductor
   Takahiro Ohgoe, Motoaki Hirayama, Takahiro Misawa, Kota Ido, Youhei Yamaji, Masatoshi Imada: Phys. Rev. B **101** (2020) 045124.
3. Effective Hamiltonian for cuprate superconductors derived from multiscale ab initio scheme with level renormalization
   Motoaki Hirayama, Takahiro Misawa, Takahiro Ohgoe, Youhei Yamaji, Masatoshi Imada: Phys. Rev. B **99** (2019) 245155.
4. *Ab initio* derivation of an effective Hamiltonian for the $La_2CuO_4/La_1.55Sr_0.45CuO_4$ heterostructure
   Terumasa Tadano, Yusuke Nomura, Masatoshi Imada: Phys. Rev. B **99** (2019) 155148.

KAWAKATSU, Toshihiro [20000 (B), 2000 (C)] (378)
— *Multiscale simulations on complex multiphase flows*

1. Coupling Finite Element Method with Large Scale Atomic/Molecular Massively Parallel Simulator (LAMMPS) for Hierarchical Multiscale Simulations
   T. Murashima, S. Urata, S. Li: Euro. Phys. J. B **92** (2019) 211.
2. ミクロスケールとマクロスケールのシミュレーション連成による高分子材料系のマルチスケールシミュレーション
   村島隆浩: 日本化学会情報化学部会誌 **37** (2019) 87.

3. Multiscale Modeling of Plasticity in Amorphous & Polymeric Materials
   S. Li, S. Urata, T. Murashima: IACM Expressions **46** (2020) 10.
4. Lagrangian Multiscale SImulation of Complex Fluids. I.
   Y. Morii, T. Kawakatsu: to be submitted.

KAWASHIMA, Naoki [20000 (B), 2000 (C)] (239)
— *Application of Tensor Network Method to Condensed Matter Physics*

1. Tensor network wavefunction of S = 1 Kitaev spin liquids
   Hyun-Yong Lee, Naoki Kawashima, and Yong Baek Kim:arXiv:1911.07714
2. Boundary conformal spectrum and surface critical behavior of classical spin systems:A tensor network renormalization study
   Shumpei Iino, Satoshi Morita, and Naoki Kawashima: Phys. Rev. B **101**, 155418 (2020)
3. Magnetic field induced quantum phases in a tensor network study of Kitaev magnets
   Hyun-Yong Lee, Ryui Kaneko, Li Ern Chern, Tsuyoshi Okubo, Youhei Yamaji, Naoki Kawashima and Yong Baek Kim: Nature Communications **11**, 1639 (2020)
4. Abelian and non-Abelian chiral spin liquids in a compact tensor network
   Hyun-Yong Lee, Ryui Kaneko, Tsuyoshi Okubo, Naoki Kawashima: Phys. Rev. B **101**, 035140 (2020)
5. Thermal-transport studies of kagom antiferromagnets
   Minoru Yamashita, Masatoshi Akazawa, Masaaki Shimozawa, Takasada Shibauchi, Yuji Matsuda, Hajime Ishikawa, Takeshi Yajima, Zenji Hiroi, Migaku Oda, Hiroyuki Yoshida, Hyun-Yong Lee, Jung Hoon Han and Naoki Kawashima: J. Phys: Condens. Matter **32**, 074001(11pp) (2019)
6. Entropy Governed by the Absorbing State of Directed Percolation
   Kenji Harada and Naoki Kawashima: Phys. Rev. Lett. **123**, 090601 (2019)
7. Boundary Tensor Renormalization Group
   Shumpei Iino, Satoshi Morita, and Naoki Kawashima: Phys. Rev. B **100**, 035449 (2019)
8. Gapless Kitaev Spin Liquid to Classical String Gas through Tensor Networks
   Hyun-Yong Lee, Ryui Kaneko, Tsuyoshi Okubo, and Naoki Kawashima: Phys. Rev. Lett. **123**, 087203 (2019)
9. Tensor-Ring Decomposition with Index-Splitting
   Hyun-Yong Lee and Naoki Kawashima: J. Phys. Soc. Jpn. **89**, 054003 (2020)

KOHYAMA, Masanori [20000 (B), 2000 (C)] (360)
— *First-Principles Phase Field Mapping*

1. A first-principles phase field method for quantitatively predicting multi-composition phase separation without thermodynamic empirical parameter
   Swastibrata Bhattacharyya, Ryoji Sahara, and Kaoru Ohno: Nature Communications **10** (2019) 3451.
2. Clear evidence of element partitioning effects in a Ti-6Al-4V alloy by the first-principles phase field method
   Thi Nu Pham, Kaoru Ohno, Riichi Kuwahara, and Swastibrata Bhattacharyya: J. Phys.: Cond. Mat. ¥bf 32 (2020) 264001.

MATUBAYASI, Nobuyuki [5000 (B), 500 (C)] (381)
— *Development of calculation method of chemical potential for long-chain polymer melt using all-atom molecular dynamics simulation*

1. Chain-Increment Method for Approaching the Chemical Potential of a Polymer with All-Atom Model
   K. Yamada and N. Matubayasi: Macromolecules **53** (2020) 775.

MISAWA, Takahiro [10000 (B), 1000 (C)] (366)
— *Numerical Study of Quantum Spin Liquid in Organic Conductors using Ab initio Calculation*
— *Development of numerical method for calculating dynamical structure factors based on many-variable variational Monte Carlo method*

1. Effective Hamiltonian for cuprate superconductors derived from multi-scale ab initio scheme with

level renormalization
Motoaki Hirayama, Takahiro Misawa, Takahiro Ohgoe, Youhei Yamaji, and Masatoshi Imada: Phys. Rev. B **99**, 245155 (2019).

2. Real-time evolution and quantized charge pumping in magnetic Weyl semimetals
Takahiro Misawa, Ryota Nakai, and Kentaro Nomura : Phys. Rev. B **100**, 155123 (2019).
3. Spin nematics in frustrated spin-dimer systems with bilayer structure
Toshiya Hikihara, Takahiro Misawa, and Tsutomu Momoi : Phys. Rev. B **100**, 214414 (2019).
4. Semi-quantized Spin pumping and Spin-orbit torques in topological Dirac Semimetals
Takahiro Misawa and Kentaro Nomura : Scientific Reports **9**, 19659 (2019).
5. Ab initio study of superconductivity and inhomogeneity in a Hg-based cuprate superconductor
Takahiro Ohgoe, Motoaki Hirayama, Takahiro Misawa, Kota Ido, Youhei Yamaji and Masatoshi Imada : Phys. Rev. B **101**, 045124 (2020).
6. Charge dynamics of correlated electrons: Variational description with inclusion of composite fermions
Kota Ido, Masatoshi Imada, and Takahiro Misawa : Phys. Rev. B **101**, 075124 (2020).
7. Correlation effects on the magnetization process of the Kitaev model
Kota Ido and Takahiro Misawa : Phys. Rev. B **101**, 045121 (2020).

MIYAKE, Takashi [6000 (B), 0 (C)] (376)
— *High performance permanent magnets and magnetic materials*

1. Cerium as a possible stabilizer of ThMn12-type iron-based compounds: A first-principles studya Yosuke Harashima, Taro Fukazawa, and Takashi Miyake: Scripta Materialia **179** (2020) 12.
2. Adjusting the descriptor for a crystal structure search using Bayesian optimizationa Nobuya Sato, Tomoki Yamashita, Tamio Oguchi, Koji Hukushima and Takashi Miyake: Phys. Rev. Mater. **4** (2020) 033801.
3. Thermal decomposition of $ThMn_{12}$-type phase and its optimum stabilizing elements in SmFe12-based alloys I. Dirba, Y. Harashima, H. Sepehri-Amin, T. Ohkubo, T. Miyake, S. Hirosawa, K. Hono: J. Alloy Compounds **813** (2020) 152224.
4. Bayesian optimization of chemical composition: a comprehensive framework and its application to RFe_{12}-type magnet compounds
Taro Fukazawa, Yosuke Harashima, Zhufeng Hou and Takashi Miyake: Phys. Rev. Mater. **3** (2019) 053807.
5. Ensemble learning reveals dissimilarity between rare-earth transition-metal binary alloys with respect to the Curie temperature
Duong-Nguyen Nguyen, Tien-Lam Pham, Viet-Cuong Nguyen, Hiori Kino, Takashi Miyake, Hieu-Chi Dam: J. Phys. Materials **2** (2019) 034009.

NOGUCHI, Hiroshi [10000 (B), 1000 (C)] (241)
— *Molecular Dynamics Simulation of Complex Fluids*

1. Effects of Cavitation on Karman Vortex Behind Circular-Cylinder Arrays: A Molecular Dynamics Study
Y. Asano, H. Watanabe, and H. Noguchi: J. Chem. Phys. **152**, 034501 (2020).
2. 分子動力学計算による複雑流体中のカルマン渦の解析
浅野 優太, 渡辺 宙志, 野口 博司: 分子シミュレーション研究会会誌“アンサンブル”**22**, 157 (2020).

OGUCHI, Tamio [5000 (B), 0 (C)] (374)
— *Electron Theory on Secondary-Battery Materials*

1. First-Principles Study of Na-Ion Battery Performance and Reaction Mechanism of Tin Sulfide as Negative Electrode
Hiroki Kotaka, Hiroyoshi Momida, Ayuko Kitajou, Shigeto Okada, and Tamio Oguchi, Chem. Rec. **19**, 811 (2019).
2. First-Principles Study of X-Ray Absorption Spectra in $NaFeSO_4F$ for Exploring Na-Ion Battery Reactions
Hiroyoshi Momida, Ayuko Kitajou, Shigeto Okada, and Tamio Oguchi, J. Phys. Soc. Jpn. **88**, 124709 (2019).

3. Amorphous xNaF-$FeSO_4$ Systems ($1 \leq x \leq 2$) with Excellent Cathode Properties for Sodium Ion Batteries
   A. Kitajou, H. Momida, T. Yamashita, T. Oguchi, and S. Okada, ACS Appl. Energy Mater. **2**, 5968 (2019).
4. Significant Role of Oxygen Redox Reaction with O_2-Release in Li-Excess Cation-Disordered Rock-Salt Cathodes $Li_{2+2x}Mn_{1-x}Ti_{1-x}O_4$: First-Principles Calculations
   Motoyuki Hamaguchi, Hiroyoshi Momida, and Tamio Oguchi, Electrochimica Acta **330**, 135286 (2020).

OKAZAKI, Susumu [10000 (B), 1000 (C)] (370)
— Conversion and storage of energy - Fuel cells and secondary batteries: Research and development of fundamental technologies of battery simulators

1. Hydrogen Permeation in Hydrated Perfluorosulfonic Acid Polymer Membranes: Effect of Polymer Crystallinity and Equivalent Weight
   K. Takeuchi, A. Kuo, T. Hirai, T. Miyajima, S. Urata, S. Terazono, S. Okazaki, and W. Shinoda: J. Phys. Chem. C, 123, 20628-20638 (2019)
2. Structure of Hydrated Crystal (Lc), Tilted Gel (Lβ'), and Liquid Crystal (Lα) Phases of Linear Alkylbenzene Sulfonate (LAS) Studied by X-ray Diffraction and Molecular Dynamics Simulation
   K. Takeda, Y. Andoh, S. Shinoda, and S. Okazaki: Langmuir, 35, 9011-9019 (2019).
3. Molecular Behavior of Linear Alkylbenzene Sulfonate in Hydrated Crystal, Tilted Gel, and Liquid Crystal Phases Studied by Molecular Dynamics Simulation
   K. Takeda, Y. Andoh, S. Shinoda, and S. Okazaki: Langmuir, 35, 10877-10884 (2019).
4. Molecular dynamics study of solubilization of cyclohexane, benzene, and phenol into mixed micelles composed of sodium dodecyl sulfate and octaethylene glycol monododecyl ether
   K. Takeda, K. Fujimoto, N. Yoshii, and S. Okazaki: J. Comput. Chem., 40, 2722-2729 (2019).
5. Fast multipole method for three dimensional systems with periodic boundary condition in two directions
   N. Yoshii, Y. Andoh, S. Okazaki: J. Comput. Chem., 41, 940-948 (2020).
6. Extension of the fast multipole method for the rectangular cells with an anisotropic partition tree structure
   Y. Andoh, N. Yoshii, S. Okazaki: J. Comput. Chem., 41, 1353-1367 (2020).

OSHIYAMA, Atsushi [20000 (B), 2000 (C)] (44)
— Exploration of new-functionality and high-performance semiconductor devices

1. Microscopic Identification of Surface Steps on SiC by Density-Functional Calculations
   K. Seino and A. Oshiyama: Proc. ICSRM2019
2. Energetics of the surface step and its morphology on the 3C-SiC(111) surface clarified by the density-functional theory
   K. Seino and A. Oshiyama: Appl. Phys. Exp. **13** (2020) 015506
3. Density-Functional Calculations for Structures and Energetics of Atomic Steps and their Implication for Surface Morphology on Si-face SiC Polar Surfaces
   K. Seino and A. Oshiyama: Phys. Rev. B (2020) to be published
4. A two-dimensional liquid-like phase on Ga-rich GaN (0001) surfaces evidenced by first principles molecular dynamics
   K. M. Bui, M. Boero, K. Shiraishi and A. Oshiyama: Jpn. J. Appl. Phys. **59** (2020) SGGK04
5. Computational study of oxygen stability in vicinal m(10-10)-GaN growth by MOVPE
   F. Shintaku, D. Yosho, Y. Kangawa, J.-I. Iwata, A. Oshiyama, K. Shiraishi, A. Tanaka aand H. Amano: Appl. Phys. Exp. **13** (2020) 055507
6. Oxygen incorporation kinetics in vicinal m(10-10)-GaN growth by MOVPE
   D. Yosho, F. Shintaku, Y. Inatomi, Y. Kangawa, J.-I. Iwata, A. Oshiyama, K. Shiraishi, A. Tanaka and H. Amano: Phys. Sta. Solidi - Rapid Res. Lett. (2020) 2000142

OZAKI, Taisuke [10000 (B), 1000 (C)] (383)
— Study on thermodynamic properties and NOx redox reactions of ternary alloy nanoclusters by O(N) density functional calculations

1. Study on thermodynamic properties and NO_x redox reactions of ternary alloy nanoclusters by O(N) density functional calculations
   S.-H. Hung, A. Hiroshi, Y. Osamu, and T. Ozaki, RSC Advances, in press.

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

SHIBA, Hayato [10000 (B), 1000 (C)] (363)
— *Molecular dynamics study of long-ranged fluctuation and transport properties of electrolyte and glassy liquids*
— *Simulation of electrolyte liquids under constant potential bias*

1. Local Density Fluctuation Governs the Divergence of Viscosity Underlying Elastic and Hydrodynamic Anomalies in a 2D Glass-Forming Liquid
   H. Shiba, T. Kawasaki, and K. Kim: Phys. Rev. Lett. 123, 2655 (2019).

SUGINO, Osamu [10000 (B), 1000 (C)] (361)
— *Priority project 5— energy conversion (chemical energy)*

1. Nuclear quantum effect for hydrogen adsorption on Pt(111)
   L. Yan, Y. Yamamoto, M. Shiga, and O. Sugino: Phys. Rev. B 101, 165414 (2020)
2. Scaling Relation of Oxygen Reduction Reaction Intermediates at Defective TiO2 Surfaces
   Y. Yamamoto, S. Kasamatsu, and O. Sugino: J. Phys. Chem. C 123, 19486 (2019)

TAKETSUGU, Tetsuya [5000 (B), 500 (C)] (375)
— *Ab initio study toward abundant element nanocatalysts with less precious metals*

1. Photo-Induced Pyramidal Inversion Behavior of Phosphines Involved with the Aggregation-Induced Emission (AIE) Behavior
   T. Machida, T. Iwasa, T. Taketsugu, K. Sada, and K. Kokado, Chemistry A European J., in press.
2. Single-molecule resonance Raman effect in a plasmonic nanocavity
   R. B. Jaculbia, H. Imada, K. Miwa, T. Iwasa, M. Takenaka, B. Yang, E. Kazuma, N. Hayazawa, T. Taketsugu, and Y. Kim, Nature Nanotechnology, **15**, (2020) 105.
3. Observations and theories of quantum effects in proton transfer electrode processes
   K. Sakaushi, A. Lyalin, and T. Taketsugu, Current Opinion in Electrochemistry, **19**, (2020) 96.
4. Surface adsorption model calculation database and its application to activity prediction of heterogeneous catalysts
   M. Kobayashi, H. Onoda, Y. Kuroda, and T. Taketsugu, J. Comput. Chem. Jap. **18**, (2019) 251.
5. Single-Phase Borophene on Ir(111): Formation, Structure and Decoupling from the Support
   N. A. Vinogradov, A. Lyalin, T. Taketsugu, A. S. Vinogradov, and A. Preobrajenski, ACS Nano, **13**, (2019) 14511.
6. Roles of silver nanoclusters in surface-enhanced Raman spectroscopy
   T. Tsuneda, T. Iwasa, and T. Taketsugu, J. Chem. Phys. **151**, (2019) 094102.
7. Anharmonic Vibrational Computations with a Quartic Force Field for Curvilinear Coordinates
   Y. Harabuchi, R. Tani, N. DeSilva, B. Njegic, M. S. Gordon, and T. Taketsugu, J. Chem. Phys. **151**,(2019) 064104.
8. Additive-Dependent Iptycene Incorporation in Polyanilines: Insights into the Pentiptycene Clipping Effect and the Polymerization Mechanism
   W. S. Tan, T.-Y. Lee, S.-F. Tseng, Y.-F. Hsu, M. Ebina, T. Taketsugu, S.-J. Huang, and J.-S. Yang, J. Chin. Chem. Soc. **66**, (2019) 1141.
9. Synthesis of polyaminophosphonic acid-functionalized poly(glycidyl methacrylate) for the efficient sorption of La(III) and Y(III)
   A. A. Galhoum, E. A. Elshehy, D. A. Tolan, A. M. El-Nahas, T. Taketsugu, K. Nishikiori, T. Akashi, A. S. Morshedy, and E. Guibal, Chem. Eng. J. **375**, (2019) 121932.
10. Suppression of Pyrite Oxidation by Ferric-catecholate Complexes: An Electrochemical Study
    X. Li, M. Gao, N. Hiroyoshi, C. B. Tabelin, T. Taketsugu, and M. Ito, Minerals Eng. **138**, (2019) 226.

TOHYAMA, Takami [5000 (B), 500 (C)] (369)
— *Cooperation Research with Big Experimental Facilities*

1. Magnetic excitations in magnetization plateaus of a frustrated spin ladder
   K. Sasaki, T. Sugimoto, T. Tohyama, and S. Sota: Phys. Rev. B **101**, (2020) 144407.
2. Spin dynamics in the t-t'-J model: Dynamical density-matrix renormalization group study
   T. Tohyama, S. Sota, and S. Yunoki: submitted to Phys. Rev. B

YABANA, Kazuhiro [10000 (B), 1000 (C)] (368)
— *Unified Photonic-Electronic Devices*

YAMADA, Atsuo [5000 (B), 500 (C)] (94)
— *Dynamical analyses on electrolytes for Na-ion batteries*

1. Sodium- and Potassium- Hydrate Melts Containing Asymmetric Imide Anions for High- Voltage Aqueous Batteries
   Q. Zheng, S. Miura, K. Miyazaki, S. Ko, E. Watanabe, M. Okoshi, C.- P. Chou, Y. Nishimura, H. Nakai, T. Kamiya, T. Honda, J. Akikusa, Y. Yamada, A. Yamada: Angew. Chem. Int. Ed. **58** (2019) 2358.

YOSHIMI, Kazuyoshi [10000 (B), 1000 (C)] (364, 388)
— *Development of accuracy verification method on analytic continuation results using cross validation*

1. SpM: Sparse modeling tool for analytic continuation of imaginary-time Green ' s function
   K. Yoshimi J. Otsuki, Y. Motoyama, M. Ohzeki, and H. Shinaoka: Comput. Phys. Commun. **244** (2019) 319.

□ Doctor Theses

1. **ADACHI, Daiki**
   High-accuracy tensor renormalization group algorithms and their applications
   The University of Tokyo, 2020-03

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□ Master Theses

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Theoretical study of electronic and magnetic properties in thin films of Weyl semimetals
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Aridity dependence of the characteristic bifurcation angle in a model drainage network.
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Magnetism in the double exchange model on the quasiperodic lattice
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Theoretical study on electrical conduction properties of higher-order topological insulators
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First-Principles Calculations on Defects in Fe Based Sueprconductor LiFeAs
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