4 PUBLICATION LIST

Example:

LASTNAME, Firstname [project class; # points (B), # points (C)] (Page #)
— *Project title*
1. First paper
   Names of Authors, etc.
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□ ISSP Joint Research Projects

○ B–E classes

ADACHI, Kyosuke [B class; 700 (B), 100 (C)] (311)
— *Multi-component phase separation dynamics of proteins*

AKASHI, Ryosuke [B class; 600 (B), 100 (C)] (312)
— *Solution of the Eliashberg equation with the electron-electron Coulomb interaction*
1. Revisiting homogeneous electron gas in pursuit of properly normed ab initio Eliashberg theory
   R. Akashi Physical Review B **105**, 104510 (2022).
   DOI:10.1103/PhysRevB.105.104510

AOYAMA, Kazushi [B class; 900 (B), 180 (C)] (291)
— *Magnetic field effect on a topological chiral order in breathing-kagome antiferromagnets*
— *Topological chirality order and its stability in breathing-kagome antiferromagnets*
1. Zero-Field Miniature Skyrmion Crystal and Chiral Domain State in Breathing-Kagome Antiferromagnets
   K. Aoyama and H. Kawamura, J. Phys. Soc. Jpn. **92**, (2023) 033701.
   DOI:10.7566/JPSJ.92.033701

2. Spin and thermal transport and critical phenomena in three-dimensional antiferromagnets
   K. Aoyama, Phys. Rev. B **106**, (2022) 224407.
   DOI:10.1103/PhysRevB.106.224407

3. Hedgehog lattice and field-induced chirality in breathing-pyrochlore Heisenberg antiferromagnets
   K. Aoyama and H. Kawamura, Phys. Rev. B **106**, (2022) 064412.
   DOI:10.1103/PhysRevB.106.064412

ARAI, Munehito [C class; 6600 (B), 0 (C)] (230)
— *Theoretical design of novel antibodies that inhibit disease-related protein-protein interactions*
— *Theoretical design of novel proteins for medical and industrial applications*

ARAI, Toyoko [B class; 500 (B), 80 (C)] (170)
— *RSDFT calculation of the force acting between a tip and a sample detected by noncontact atomic force microscope*

ARAKI, Takeaki [B class; 900 (B), 170 (C)] (293, 294)
— *Aggregation of polyelectrolytes in mixed solvents*
— *Molecular modeling of ferroelectric nematic phase*

ARIMA, Kenta [B class; 700 (B), 170 (C)] (305)
— *Calculation of electronic structures of graphene nanoribbons with wrinkles*
— *Understanding electronic structures and reactivity of functional graphene sheets toward machining catalyst*

ARUGA, Tetsuya [B class; 500 (B), 160 (C)] (160, 162)
— *In-plane interaction of conjugated molecules*
— *Interaction of magnetic metal phthalocyanines with metal surfaces*

BIN, Xu [C class; 3400 (B), 400 (C)] (108)
— *Machine learning based optimized polymer for thermal function materials*

BUERKLE, Marius [B,C class; 5600 (B), 550 (C)] ()
— *Combining first-principles quantum transport and deep learning to create a virtual experimental environment*
— *First-principles computational study of nanocrystals for photovoltaic applications*

BUI, VANPHO [C class; 1400 (B), 0 (C)] (130)
— *Study on the catalytic mechanism of RuTi alloy in catalyst referred etching method*

DEKURA, Shun [C,D class; 5200 (B), 640 (C)] (79, 80, 81)
— *Elucidation of the mechanism of fast proton conduction based on proton tautomerism in molecular crystals by using first-principles calculations*
— *First-principles calculations of electron correlation parameters to elucidate pi-electron-proton coupled physical properties of the unconventional molecular conductors Cat-TTF analogues*
— *Systematic elucidation of structure and electronic state of pi-electron-proton coupled molecular conductors under pressure*

1. Conjugation Length Effect on the Conducting Behavior of Single-crystalline Oligo(3,4-ethylenedioxythiophene) (nEDOT) Radical Cation Salts
   R. Kameyama, T. Fujino, S. Dekura, H. Mori, Phys. Chem. Chem. Phys. **24**, 9130 (2022).
   DOI:10.1039/D2CP00250G

2. Band-filling effects in single-crystalline oligomer models for doped PEDOT: 3,4-ethylenedioxythiophene (EDOT) dimer salt with hydrogen-bonded infinite sulfate anion chains
   R. Kameyama, T. Fujino, S. Dekura, S. Imajo, T. Miyamoto, H. Okamoto, H. Mori, J. Mater. Chem. C **10**, 7543 (2022).
   DOI:10.1039/D2TC01216B

3. Molecular Arrangement Control of [1]Benzothieno[3,2-b][1]benzothiophene (BTBT) via Charge-Assisted Hydrogen Bond
   R. Akai, K. Oka, S. Dekura, H. Mori, N. Tohnai, Bull. Chem. Soc. Jpn. **95**, 1178 (2022).
   DOI:10.1246/bcsj.20220134

4. Neutral Radical Molecular Conductors Based on a Gold Dimethoxybenzenedithiolene Complex with and without Crystal Solvent
   S. Yokomori, S. Dekura, A. Ueda, T. Higashino, H. Mori, Chem. Lett. **52**, 25 (2023).
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EGAMI, Yoshiyuki [C class; 11400 (B), 950 (C)] (55)
— *First-principles electron-transport study on 2D layered material-based heterostructures*
— *First-principles study on electron-transport properties of large scale atomic layered materials*

1. Unique Electrical Signature of Phosphate for Specific Single-Molecule Detection of Peptide Phosphorylation
   T. Harashima, Y. Egami, K. Homma, Y. Jono, S. Kaneko, S. Fujii, T. Ono, and T. Nishino, J. Am. Chem. Soc. **144**, 17449 (2022).
   DOI:10.1021/jacs.2c05787

FUCHIZAKI, Kazuhiro [C class; 2600 (B), 0 (C)] (269)
— *Kinetics of phase transition and polyamorphism*

1. Can weight hysteresis in a neural network judge the continuity/discontinuity of a phase transition?
   K. Nakamura and K. Fuchizaki, submitted to J. Phys. A.

FUJI, Yohei [B class; 700 (B), 180 (C)] (303)
— *Numerical investigation of universality classes in measurement-induced phase transitions*

1. Charge fluctuation and charge-resolved entanglement in a monitored quantum circuit with $U(1)$ symmetry
   H. Oshima and Y. Fuji, Phys. Rev. B **107**, 014308 (2023).
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FUJII, Susumu [C class; 2800 (B), 0 (C)] (267)
— *Systematic searches for grain boundary structures and structure-based prediction of multiple properties*

FUJIMOTO, Yoshitaka [C class; 600 (B), 0 (C)] (164)
— *Atomic structures and electronic properties of nanocarbon-based materials*

1. Theoretical study on quantum transport of carbon nanotubes for detecting toxic molecules: The role of dopants
   Y. Fujimoto, Journal of Electrochemical Science and Engineering **12**, 431 (2022).

2. First-Principles Theoretical Design of Graphene-Based Field Effect Transistors
   Y. Fujimoto, Advanced Nanoscale MOSFET architectures: Current Trends and Future Perspectives, Accepted.

FUJINO, Tomoko [C class; 1200 (B), 0 (C)] (204)
— *Electronic structures of EDXT oligomers in charge transfer salts: estimation of intramolecular and intermolecular Coulomb repulsion energy*

1. Ambipolar Nickel Dithiolene Complex Semiconductors: from One- to Two-dimensional Electronic Structures based upon Alkoxy Chain Lengths
   M. Ito, T. Fujino*, L. Zhang, S. Yokomori, T. Higashino, R. Makiura, K. J. Takeno, T. Ozaki, H. Mori*, J. Am. Chem. Soc. 145, 2127 (2023).
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2. Band-filling Effects in Single-crystalline Oligomer Models for Doped PEDOT: 3,4-Ethylenedioxythiophene (EDOT) Dimer Salt with Hydrogen-bonded Infinite Sulfate Anion Chains
   R. Kameyama, T. Fujino*, S. Dekura, S. Imajo, T. Miyamoto, H. Okamoto, H. Mori*, J. Mater. Chem. C 10, 7543 (2022).
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FUJISHIRO, Hiroki [C class; 2800 (B), 0 (C)] ()
— *Strained Band-Structure Engineering for Antimonide-Based Terahertz Transistors*

FUKUDA, Jun-ichi [B class; 800 (B), 80 (C)] (302)
— *Calculation of ordered structures dynamics and optical properties of soft materials*

1. Simulation of a cholesteric blue phase cell with large but finite thickness
   J. Fukuda, Front. Soft Matter **2**, 1011618 (2022).
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FUKUDA, Masahiro [B class; 400 (B), 80 (C)] (176)
— *AB type 2D materials database construction by DFT*

1. Prediction of quaternary hydrides based on densest ternary sphere packings
   Ryotaro Koshoji, Masahiro Fukuda, Mitsuaki Kawamura, and Taisuke Ozaki, Phys. Rev. Materials **6**, 114802 (2022).
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2. Atomic arrangement of Si adatom on the Silicene/Ag(111) surface
   Yuuki Adachi, Zhang Runnan, Wang Xinbo, Masahiro Fukuda, Taisuke Ozaki, Yoshiaki Sugimoto, Applied Surface Science, 157336 (2023).
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https://isspns-gitlab.issp.u-tokyo.ac.jp/masahiro.fukuda/openmx-database-of-bulks-using-standard-basis-set

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FUKUDA, Tuneo [C class; 400 (B), 0 (C)] (184)
— *First-principles study of stability of Cu-Ni two-dimensional alloy*

FUKUMOTO, Yoshiyuki [B class; 800 (B), 0 (C)] (306, 308)
— *Numerical studies on thermodynamics and excitation spectra in Heisenberg antiferromagnets on the triangular and kagome lattices*
— *Numerical study of the effect of large bond randomness on the magnetization process and magnetic susceptibility in the spherical Kagome system {W72V30}*

1. Effects of bond-randomness and Dzyaloshinskii-Moriya interactions on the specific heat at low temperatures of a spherical kagome cluster in $\{W_{72}V_{30}\}$
   M. Motohashi, K. Inoue, K. Morita, Y. Fukumoto, and H. Nakano, Prog. Theor. Exp. Phys. 2022, 113I01, (2022).

GOHDA, Yoshihiro [C class; 6000 (B), 450 (C)] (74)
— *Control of magnetic anisotropy by strain and electric polarization at interfaces*

1. Giant converse magnetoelectric effect in a multiferroic heterostructure with polycrystalline Co_2FeSi
   S. Fujii, T. Usami, Y. Shiratsuchi, A.M. Kerrigan, A.M. Yatmeidhy, S. Yamada, T. Kanashima,

R. Nakatani, V.K. Lazarov, T. Oguchi, Y. Gohda, and K. Hamaya, NPG Asia Mater. **14**, 43 (2022).
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2. Superconductivity in a two monolayer thick indium film on Si(111)$\sqrt{3} \times \sqrt{3}$-B
T. Ogino, I. Seo, H. Tajiri, M. Nakatake, S. Takakura, Y. Sato, Y. Hasegawa, Y. Gohda, K. Nakatsuji, and H. Hirayama, Phys. Rev. B **106**, 045423 (2022).
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S. Tsuna, R. Costa-Amaral, and Y. Gohda, J. Appl. Phys. **132**, 234101 (2022).
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4. First-principles phonon calculations of neodymium-magnet compounds
S. Tsuna and Y. Gohda, J. Appl. Phys. **133**, 115103 (2023).
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5. Structures of Sm-Cu intermetallics with Fe as subphase candidates in $SmFe_{12}$-based permanent magnets studied by first-principles thermodynamics
S. Nishino and Y. Gohda, Jpn. J. Appl. Phys. **62**, 030902 (2023).
DOI:10.35848/1347-4065/acc0b8

GOHLKE, Matthias [C class; 3000 (B), 150 (C)] (263)
— *Ground state and dynamical properties of the J_1J_2K-Heisenberg model on the square lattice*

GONOME, Hiroki [C class; 3800 (B), 550 (C)] (104)
— *Study of the principle of photothermal conversion by ab initio calculations*

HAGITA, Katsumi [C class; 1000 (B), 150 (C)] (286)
— *Effect of chain crossing prohibition on phase-separated structure of block copolymers*

1. Ring-Filling Effect on StressStrain Curves of Randomly End-Linked Tetra-Arm Prepolymers
K. Hagita, T. Murashima, T. Ohkuma, H. Jinnai, Macromolecules **55**, 6547 (2022).
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2. Topological transition in multicyclic chains with structural symmetry inducing stress-overshoot phenomena in multicyclic/linear blends under biaxial elongational flow
T. Murashima, K. Hagita, T. Kawakatsu, Macromolecules **55**, 9358 (2022).
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3. Practical compatibility between self-consistent field theory and dissipative particle dynamics
K. Hagita, T. Murashima, Polymer **269**, 125733 (2023).
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4. Lamellar Domain Spacing of Symmetric Linear, Ring, and Four-Arm-Star Block Copolymer Blends
K. Hagita, T. Murashima, and T. Kawakatsu Macromolecules **55**, 8021 (2022).
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5. 分子シミュレーションを用いたフェノール樹脂の構造-物性相関解析
首藤靖幸, 和泉篤士, 萩田克美, 柴山充弘ネットワークポリマー **43**, 246 (2022).
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6. Molecular Dynamics of Topological Barriers on the Crystallization Behavior of Ring Polyethylene

Melts with Trefoil Knots
K. Hagita, T. Murashima, N. Sakata, K. Shimokawa, T. Deguchi, E. Uehara, and S. Fujiwara Macromolecules **56**, 15 (2023).
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HAMADA, Ikutaro [C class; 8200 (B), 0 (C)] (67)
— *Density functional theory study of adsorption and reaction of molecules on metal surfaces*
— *Density functional theory study of molecule/metal interfaces*

1. Interaction of water with nitrogen-doped graphene
   A. F. Z. Abidin and I. Hamada, Phys. Rev. B **105**, 075416 (2022).
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2. Comparative density functional theory study for predicting oxygen reduction activity of single-atom catalyst
   A. F. Z. Abidin and I. Hamada, Surf. Sci. **724**, 122144 (2022).
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3. Phonon dispersion of the organic semiconductor rubrene
   K. Takada, K. Yoshimi, S. Tsutsui, K. Kimura, K. Hayashi, I. Hamada, S. Yanagisawa, N. Kasuya, S. Watanabe, J. Takeya, and Y. Wakabayashi, Phys. Rev. B **105**, 205205 (2022).
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HAMAGUCHI, Satoshi [C class; 8600 (B), 800 (C)] ()
— *Study on plasma resistance of metal oxides*

HAMAMOTO, Yuji [C,D class; 4400 (B), 0 (C)] (99, 100)
— *First principles study of the adsorption structure of helicene on the Ag(111) surface*
— *Global search for metastable structures of silicene on the Ag(111) surface by Gaussian process regression*

1. Hybridization-Induced Image Potential States with Large Effective Mass in Lead Phthalocyanine Overlayers on Graphene
   Y. Hamamoto, H. Sawada, S. A. Wella, K. Inagaki, I. Hamada, and Y. Morikawa, J. Phys. Chem. C **126**, 10855 (2022).
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HARADA, KENJI [C class; 1200 (B), 600 (C)] (275)
— *Tensor data analysis by tensor network*

HARASHIMA, Yosuke [C class; 1000 (B), 0 (C)] (150)
— *Exponent puzzle for metal-insulator transition in doped semiconductors*

1. Systematic search for stabilizing dopants in ZrO_2 and HfO_2 using first-principles calculations
   Y. Harashima, H. Koga, Z. Ni, T. Yonehara, M. Katouda, A. Notake, H. Matsui, T. Moriya, M. K. Si, R. Hasunuma, A. Uedono, and Y. Shigeta, IEEE Trans. Semicon. Man., accepted.
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HARUYAMA, Jun [C class; 3200 (B), 400 (C)] (110)

— *Electrochemical reaction analysis using density functional calculation + implicit solvation model 4*

1. First-Principles Study for Water Adsorption Layers on Platinum Surface
   J. Haruyama, T. Sugimoto, and O. Sugino Vacuum and Surface Science **65**, 355 (2022).
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2. Effect of Nitrogen Doping and Oxygen Vacancy on the Oxygen Reduction Reaction on the Tetragonal Zirconia(101) Surface
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HASHIMOTO, Tamotsu [C class; 1200 (B), 200 (C)] (276)

— *Molecular dynamics simulation of $BaTiO_3$ nano structure II*

1. Domain structures in dielectric polarization vortex of $BaTiO_3$ nanoclusters: A shell model molecular dynamics study
   T. Hashimoto and H. Moriwake, Physica B, **656**, 414768 (2023).
   DOI:10.1016/j.physb.2023.414768

2. Domain structures of rhombohedral $BaTiO_3$ by a shell model
   T. Hashimoto and H. Moriwake, submitted

HATSUGAI, Yasuhiro [C class; 4400 (B), 350 (C)] (249)

— *Numerical studies for science of bulk-edge correspondence and topological phases*

1. Machine Learning Study on the Flat-Band States Constructed by Molecular-Orbital Representation with Randomness
   T. Kuroda, T. Mizoguchi, H. Araki, and Y. Hatsugai J. Phys. Soc. Jpn. 91, 044703 (2022).
   DOI:10.7566/JPSJ.91.044703

2. Adiabatic continuity of the spinful quantum Hall states
   K. Kudo and Y. Hatsugai Phys. Rev. B 106, 075120 (2022).
   DOI:10.1103/PhysRevB.106.075120

3. Observation of bulk-edge correspondence in topological pumping based on a tunable electric circuit
   K. Yatsugi, T. Yoshida, T. Mizoguchi, Y. Kuno, H. Iizuka, Y. Tadokoro, and Y. Hatsugai Commun. Phys. 5, 180 (2022).
   DOI:10.1038/s42005-022-00957-5

4. Higher-Order Topological Insulator on a Martini Lattice and Its Square Root Descendant
   D. Matsumoto, T. Mizoguchi, and Y. Hatsugai J. Phys. Soc. Jpn. 92, 034705 (2023).
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5. Molecular-orbital representation with random U(1) variables

T. Mizoguchi and Y. Hatsugai Phys. Rev. B 107, 094201 (2023).
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6. Reduction of one-dimensional non-Hermitian point-gap topology by interactions
T. Yoshida and Y. Hatsugai Phys. Rev. B 106, 205147 (2022).
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7. Discriminant indicator with generalized rotational symmetry
H. Wakao, T. Yoshida, and Y. Hatsugai Phys. Rev. B 105, 214103 (2022).
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8. Unconventional gapless semiconductor in an extended martini lattice in covalent honeycomb materials
T. Mizoguchi, Y. Gao, M. Maruyama, Y. Hatsugai, and S. Okada Phys. Rev. B 107, L121301 (2023).
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9. Fate of exceptional points under interactions: Reduction of topological classifications
T. Yoshida and Y. Hatsugai Phys. Rev. B 107, 075118 (2023).
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10. A symmetry-protected exceptional ring in a photonic crystal with negative index media
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11. Topological pump of SU(Q) quantum chain and Diophantine equation
Y. Hatsugai and Y. Kuno, arXiv:2210.11646

HAYAMI, Satoru [C class; 5600 (B), 450 (C)] (236)
— Numerical simulations combined with machine learning to search for magnetic skyrmion in frustrated magnets

1. Spin Conductivity Based on Magnetic Toroidal Quadrupole Hidden in Antiferromagnets
S. Hayamia and M. Yatsushiro, J. Phys. Soc. Jpn. **91**, 063702 (2022).
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2. Multifarious skyrmion phases in centrosymmetric trilayer magnets
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3. Rectangular and square skyrmion crystals on a centrosymmetric square lattice with easy-axis anisotropy
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J. Nasu and S. Hayami, Phys. Rev. B **105**, 245125 (2022).
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5. Skyrmion crystal with integer and fractional skyrmion numbers in a nonsymmorphic lattice structure with the screw axis
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6. Skyrmion crystal under D3h point group: Role of out-of-plane Dzyaloshinskii-Moriya interaction
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S. Hayami, J. Phys.: Condens. Matter **34**, 365802 (2022).
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8. Nonlinear spin Hall effect in PT-symmetric collinear mag- nets
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9. Nonlinear nonreciprocal transport in antiferromagnets free from spin-orbit coupling
S. Hayami and M. Yatsushiro, Phys. Rev. B **106**, 014420 (2022).
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10. Stability of Skyrmion Crystal Phase in Centrosymmetric Distorted Triangular-Lattice Antiferromagnets
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11. Magnetic Hedgehog Lattice in a Centrosymmetric Cubic Metal
S. Okumura, S. Hayami, Y. Kato, and Y. Motome, J. Phys. Soc. Jpn. **91**, 093702 (2022).
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12. Nonreciprocal Transport in Noncoplanar Magnetic Systems without Spin-Orbit Coupling, Net Scalar Chirality, or Magnetization
S. Hayami and M. Yatsushiro, J. Phys. Soc. Jpn. **91**, 094704 (2022).
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13. Engineering a skyrmion crystal in ferromagnetic/antiferromagnetic bilayers based on magnetic frustration mechanism
K. Okigami, R. Yambe, and, S. Hayami, J. Phys. Soc. Jpn. **91**, 103701 (2022).
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14. Ferroaxial moment induced by vortex spin texture
S. Hayami, Phys. Rev. B **106**, 144402 (2022).
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15. Electric Ferro-Axial Moment as Nanometric Rotator and Source of Longitudinal Spin Current
S. Hayami, R. Oiwa, and H. Kusunose, J. Phys. Soc. Jpn. **91**, 113702 (2022).
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16. Skyrmion and vortex crystals in the Hubbard model
K. Kobayashi and S. Hayami, Phys. Rev. B **106**, L140406 (2022).
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17. Zero-field skyrmion, meron, and vortex crystals in centrosymmetric hexagonal magnets
S. Hayami, J. Magn. Magn. Mater. **564**, 170036 (2022).
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18. Magnetic Toroidal Moment under Partial Magnetic Order in Hexagonal Zigzag-Chain Compound Ce_3TiBi_5
S. Hayami and H. Kusunose, J. Phys. Soc. Jpn. **91**, 123701 (2022).
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19. Effective spin model in momentum space: Toward a systematic understanding of multiple-Q

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R. Yambe and S. Hayami, Phys. Rev. B **106**, 174437 (2022).
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20. Orthorhombic distortion and rectangular skyrmion crystal in a centrosymmetric tetragonal host
S. Hayami, J. Phys.: Mater. **6**, 014006 (2023).
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21. Stacking-dependent nonreciprocal transport in magnetic skyrmions
S. Hayami, J. Magn. Magn. Mater. **568**, 170420 (2023).
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22. Ferrochiral, antiferrochiral, and ferrichiral skyrmion crystals in an itinerant honeycomb magnet
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23. Multiple-Q instability under fourth-order inplane single-ion anisotropy
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24. Widely-sweeping magnetic fieldtemperature phase diagrams for skyrmion-hosting centrosymmetric tetragonal magnets
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— *Numerical Study of One Dimensional Frustrated Quantum Spin Systems*

HIGUCHI, Yuji [C class; 10200 (B), 900 (C)] (219)
— *Correlation between the structure of charged phospholipid bilayer membrane and ion distribution by multi-scale simulation*
— *Structure and dynamics of charged phospholipid bilayer membrane and water molecules*

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HIYAMA, Miyabi [B class; 400 (B), 80 (C)] (327)
— *Theoretical study for firefly bioluminescence substrate analogs and related molecules*

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— *HPC-based fusion of experiment analysis simulation and data-driven science*

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— *Tensor renormalization-group study of random spin systems*

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— *Stability of quantum spin liquids in frustrated quantum spin systems*

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— *Finite temperature calculation of quantum manybody system using random phase product state and neural network wavefunction*

IKEDA, Hiroaki [B class; 400 (B), 80 (C)] ()
— *first principles calculations in quantum liquid crystals*

IKUHARA, Yuichi [C class; 5800 (B), 0 (C)] (82)
— *Exploring singular atomic arrangements via first-principles calculations*
— *Molecular dynamics simulation of grain boundaries in perovskite oxide*

IMADA, Masatoshi [E class; 32000 (B), 2550 (C)] (23)
— *Integrated spectroscopic studies by combining experimental data and high precision large-scale computation for strongly correlated electrons*
— *Systematic ab initio studies on high temperature superconductivity of transition metal oxides*

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INAOKA, Takeshi [B class; 300 (B), 60 (C)] (185)
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1. Formation of an iodine metallic band in the x-form phthalocyanine crystal
   T. Inaoka, to be submitted.

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— *Thermal conductivity calculation for high thermal conductive insulator*

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— *Loop-gas representation of classical and quantum statistical-mechanical models and its tensor-network calculation*

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— *Theoretical study on electronic properties of new nanoscale surfaces and interfaces*

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— *Development of Efficient Oxygen Storage Materials and Hydrogen Permeation Barrier Materials*

KUROKI, Kazuhiko [C class; 5400 (B), 0 (C)] (194)
— *Theoretical studies on cuprate superconductors with quasi-one-dimensional electronic structure*

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LI, Hao [C class; 4400 (B), 0 (C)] (97)
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— *Development and applications of scaling analysis for critical phenomena*
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— *Theoretical stuidies on dynamics in biomolecular and liquid systems*

SAKAGUCHI, Norihito [C class; 7800 (B), 0 (C)] (70)
— *Reduction of Rare Metals in Fuel Cell and Formic Acid Decomposition Catalysts*

SAKAI, Masatoshi [B class; 300 (B), 70 (C)] (338)
— *Charge distribution in low excitation state of organic charge order materials*

SAKAI, Toru [C class; 6600 (B), 700 (C)] (223, 225)
— *Magnetization Plateau with Spontaneous Symmetry Breaking*
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SAKAKIBARA, Hirofumi [B class; 500 (B), 0 (C)] (172)
— *A study of nickelate superconductors in first-principles*

SAKASHITA, Tatsuya [B class; 200 (B), 60 (C)] (347)
— *Development of integrated interface of eigensolvers Rokko and application to quantum spin systems*

SASAKI, Takehiko [C class; 1200 (B), 200 (C)] (127)
— *Study on oxidation and sulfurization of platinum nanoparticles*

SATO, Masahiro [D class; 6000 (B), 250 (C)] (75)
— *Discovery of Super-Composite Electrical Insulating Materials Based on Multiscale Physics and Deep Learning of Polymers*

1. Extrapolative molecular property prediction using quantum chemistry-assisted machine learning for accelerated materials discovery
   H. Shimakawa, A. Kumada, and M. Sato, Nature Communications, in preparation

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— *the study on super ionic conduction and phase transition by disordering of complex hydride*

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SEKI, Yuya [B class; 400 (B), 70 (C)] (328)
— *Analysis of Ising model in statistical-mechanical informatics*

1. Black-box optimization for integer-variable problems using Ising machines and factorization machines
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SHAO, Cheng [C class; 3200 (B), 350 (C)] ()
— *Machine-learning optimization of ionic liquids for energy storage application*

SHIMADA, Toshihiro [B class; 400 (B), 80 (C)] (174)
— *Computational search for narrow bandgap organic charge transfer complex*

1. Molecular Dynamics Simulation of Poly(Ether Ether Ketone) (PEEK) Polymer to Analyze Intermolecular Ordering by Low Wavenumber Raman Spectroscopy and X-ray Diffraction
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— *Thermal effects on quantum frustrated magnetisms*
— *Thermal effects on the frustrated magnets*

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SHINODA, Wataru [E class; 29500 (B), 1300 (C)] (216)
— *Large-scale Molecular Simulation of Soft Materials using All-Atom and Coarse-Grained Model*

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— *Dynamical properties of the extended Kitaev-Γ model on a honeycomb lattice*

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— *Ab-initio research on nano structures of materials' surfaces and grain boundaries with magnetic elements*

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— *Theoretical study of point defects in visible-light-driven semiconductor photocatalysts using first-principles calculations*

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— *Simulation of quantum many-body systems by tensor network and sampling*

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

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   H. B. Tran, and Y. Matsushita Appl. Mater. Today 32, 101825 (2023).
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5. Skyrmions in van der Waals centrosymmetric materials with Dzyaloshinskii-Moriya interactions
   H. B. Tran, and Y. Matsushita under review
   DOI:10.48550/arXiv.2209.02333

TSUKAHARA, Noriyuki [B class; 200 (B), 60 (C)] (187)
— *DFT calculations of organic halogen molecules and their reaction products on metal surfaces*

1. Substrate-Selective Intermolecular Interaction and the Molecular Self-Assemblies: 1,3,5-Tris(4-bromophenyl)benzene Molecules on the Ag(111) and Si(111) ($\sqrt{3} \times \sqrt{3}$)-Ag Surfaces
   N. Tsukahara, and J. Yoshinobu, Langmuir **38**, 8881 (2022).
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2. Surface-supported 2D metal-organic framework as a template to arrange metal clusters
   N. Tsukahara, R. Arafune, and J. Yoshinobu, submitted to Langmuir

TSUNEYUKI, Shinji [C class; 6200 (B), 0 (C)] (76)
— *First-principle study of photoresponsive functional materials*

1. Lattice Dielectric Properties of Rutile TiO_2: First-Principles Anharmonic Self-Consistent Phonon Study
   T. Amano, T. Yamazaki, R. Akashi, T. Tadano, and S. Tsuneyuki, Phys. Rev. B **107**, 094305 (2023).
   DOI:10.1103/PhysRevB.107.094305

2. A noise-robust data assimilation method for crystal structure determination using powder diffraction intensity
   S. Yoshikawa, R. Sato, R. Akashi, S. Todo and S. Tsuneyuki, J. Chem. Phys. **157**, 224112 (2022).
   DOI:10.1063/5.0125553

3. First-Principles Study of the Optical Dipole Trap for Two-Dimensional Excitons in Graphane
   H. Katow, R. Akashi, Y. Miyamoto, and S. Tsuneyuki, Phys. Rev. Lett. **129**, 047401 (2022).
   DOI:110.1103/PhysRevLett.129.047401

4. Anharmonic phonon renormalization and thermal transport in the type-I $Ba_8Ga_{16}Sn_{30}$ clathrate from first principles
   M. Ohnishi, T. Tadano, S. Tsuneyuki, and J. Shiomi, Phys. Rev. B **106**, 024303 (2022).
   DOI:10.1103/PhysRevB.106.024303

UCHIDA, Ken [C class; 2800 (B), 400 (C)] ()
— *Calculation of thermal and electrical properties of tungsten bronze*

UCHIDA, Takashi [B class; 200 (B), 60 (C)] (346)
— *Magnetic structures of multiple-Q orders in inversion-symmetric Hubbard models*

UJIHARA, Toru [C class; 5200 (B), 0 (C)] ()
— *Analysis of the behavior of third elements to the solvent in the SiC solution method*

USUI, Hidetomo [B class; 500 (B), 90 (C)] (168)
— *First principles study on the band structures of high entropy compounds*

WAKABAYASHI, Daisuke [B class; 400 (B), 0 (C)] (331)
— *Large-scale molecular-dynamics simulation of pressure-induced coordination change in silica glass with ANN potentials*

WATANABE, Hiroshi [C class; 12200 (B), 950 (C)] (218)
— *Molecular dynamics study of dynamic properties of interface structure*
— *Non-equilibrium relaxation analysis on J1-J2 frustrated Ising model*

1. Effect of surfactants on the elasticity of the liquidliquid interface
   S. Kikuchi and H. Watanabe, J. Chem. Phys. 158, 124901 (2023).
   DOI:10.1063/5.0138733

2. Non-monotonic behavior of the Binder parameter in discrete spin systems
   H. Watanabe, Y. Motoyama, S. Morita, N. Kawashima, Prog. Theor. Exp. Phys. 2023, 033A02 (2023).
   DOI:10.1093/ptep/ptad022

WATANABE, Hiroshi [B class; 400 (B), 80 (C)] (207)
— *Unified description of cuprate high-temperature superconductors using multiband models*

1. Monte Carlo study of cuprate superconductors in a four-band *d-p* model: Role of orbital degrees of freedom
H. Watanabe, T. Shirakawa, K. Seki, H. Sakakibara, T. Kotani, H. Ikeda, and S. Yunoki, J. Phys.: Condens. Matter **35**, 195601 (2023).
DOI:10.1088/1361-648X/acc0bf

WATANABE, Satoshi [C class; 10800 (B), 900 (C)] (56)
— Analyses on local properties at complex structures such as surfaces interfaces and defects via machine-learning potentials
— Analyses related to atomic structures and atom dynamics at complex structures such as surfaces interfaces and defects

1. Using neural network potentials to study defect formation and phonon properties of nitrogen vacancies with multiple charge states in GaN
K. Shimizu, Y. Dou, E.F. Arguelles, T. Moriya, E. Minamitani, and S. Watanabe, Phys. Rev. B **106**, 054108 (2022).
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2. Realistic simulation of thermoelectric characteristics of organic semiconductors based on electronic structure calculations
M. Ohno, K. Shimizu, and S. Watanabe, Appl. Phys. Express **16**, 011005 (2023).
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YAMADA, Atsuo [C class; 3200 (B), 350 (C)] (111)
— Theoretical Analysis on Structure/Electronic State of Novel Energy Storage Materials

1. Kinetic Square Scheme in Oxygen-Redox Battery Electrodes
K. Kawai, X. M. Shi, N. Takenaka, J. Jang, B. M. de Boisse, A. Tsuchimoto, D. Asakura, J. Kikkawa, M. Nakayama, M. Okubo, and A. Yamada, Energy Environ. Sci. **15**, 2591 (2022).
DOI:10.1039/D1EE03503G

2. Anhydrous Fast Proton Transport Boosted by the Hydrogen Bond Network in a Dense Oxide-Ion Array of α-MoO3
Z. Ma, X. M. Shi, S. Nishimura, S. Ko, M. Okubo, and A. Yamada, Adv. Mater. **34**, 2203335 (2022).
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3. Electrode Potential Influences the Reversibility of Lithium-Metal Anodes
S. Ko, T. Obukata, T. Shimada, N. Takenaka, M. Nakayama, A. Yamada, and Y. Yamada Nat. Energy **7**, 1217 (2022).
DOI:10.1038/s41560-022-01144-0

YAMADA, Atsushi [C class; 800 (B), 200 (C)] ()
— Studies of the superconductivity and magnetic states in the strongly correlated electron systems using Hubbard models.

YAMADA, Masahiko [E class; 4000 (B), 850 (C)] (246)
— Density matrix renormalization group study of SU(N) Heisenberg models

1. Matrix Product Renormalization Group: Potential Universal Quantum Many-Body Solver
M. G. Yamada, T. Sanno, M. O. Takahashi, Y. Akagi, H. Suwa, S. Fujimoto, and M. Udagawa, submitted to Phys. Rev. Lett.

YAMAGUCHI, Naoya [B class; 700 (B), 100 (C)] (156)
— *Development of Efficient Evaluation Methods of Berry-phase-mediated Physical Properties for Large Scale Systems Using the First-principles LCPAO Method*

1. First-principles LCPAO approach for insulators under finite electric fields with forces
   N. Yamaguchi and F. Ishii, Comput. Phys. Commun. **280**, 108487 (2022).
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2. First-principles calculation of anomalous Hall and Nernst conductivity by local Berry phase
   H. Sawahata, N. Yamaguchi, S. Minami, and F. Ishii, Phys. Rev. B **107**, 024404 (2023).
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3. First-principles study of anomalous Hall effect and anomalous Nernst effect in Fe_2Si
   Y. Morishima, N. Yamaguchi, H. Sawahata, and F. Ishii, Jpn. J. Appl. Phys. **62**, SD1019 (2023).
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4. Persistent spin helix on a diamond surface
   H. P. Kadarisman, N. Yamaguchi, and F. Ishii, Appl. Phys. Express **16**, 023001 (2023).
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5. Seebeck-induced anomalous Nernst effect in van der Waals $MnBi_2Te_4$ layers
   Y. Morishima, N. Yamaguchi, H. Sawahata, and F. Ishii, Appl. Phys. Express **16**, 043003 (2023).
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6. Prediction of wide-gap topological insulating phase in metastable BiTeI
   Y. Zhang, N. Yamaguchi, H. Sawahata, and F. Ishii, Appl. Phys. Express, in press
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YAMAJI, Youhei [E class; 15000 (B), 1150 (C)] (189)
— *Phase competition induced by long-range Coulomb interactions in candidate materials of Kitaev's quantum spin liquid*

1. Superconductivity in Bilayer tt' Hubbard Models
   A. Iwano and Y. Yamaji, J. Phys. Soc. Jpn. **91**, 094702 (2022).
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YAMAMOTO, Tsuyoshi [D class; 1000 (B), 0 (C)] (297)
— *Theory of microwave scattering in a dissipative superconducting circuit element*

YAMASHITA, Tomoki [C class; 4000 (B), 350 (C)] (103)
— *Development of crystal structure prediction method and material search*

1. Hybrid algorithm of Bayesian optimization and evolutionary algorithm in crystal structure prediction
   T. Yamashita, H. Kino, K. Tsuda, T. Miyake, and T. Oguchi, Sci. Technol. Adv. Mater. Meth **2**, 67 (2022).
   DOI:10.1080/27660400.2022.2055987

2. Improvement of look ahead based on quadratic approximation for crystal structure prediction
   T. Yamashita and H. Sekine, Sci. Technol. Adv. Mater. Meth **2**, 84 (2022).
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YAMAUCHI, Kunihiko [C class; 3200 (B), 0 (C)] (112)
— *First-principles design of novel topological materials and evaluation of anomalous Hall conductivity*

1. Microscopic origin of magnetism in monolayer 3d transition metal dihalides

K. Riedl, D. Amoroso, S. Backes, A. Razpopov, T. P. T. Nguyen, K. Yamauchi, P. Barone, S. M. Winter, S. Picozzi, and R. Valenti Phys. Rev. B **106**, 035156 (2022).
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2. Rhombic Fermi surfaces in a ferromagnetic MnGa thin film with perpendicular magnetic anisotropy
M. Kobayashi, N. H. D. Khang, T. Takeda, K. Araki, R. Okano, M. Suzuki, K. Kuroda, K. Yaji, K. Sugawara, S. Souma, K. Nakayama, K. Yamauchi, M. Kitamura, K. Horiba, A. Fujimori, T. Sato, S. Shin, M. Tanaka, and P. N. Hai, Phys. Rev. Mater. **6**, 074403 (2022).
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3. Influence of Orbital Character on the Ground State Electronic Properties in the van Der Waals Transition Metal Iodides VI_3 and CrI_3
a) A. De Vita, T. T. P. Nguyen, R. Sant, G. M. Pierantozzi, D. Amoroso, C. Bigi, V. Polewczyk, G. Vinai, L. T. Nguyen, T. Kong, J. Fujii, I. Vobornik, N. B. Brookes, G. Rossi, R. J. Cava, F. Mazzola, K. Yamauchi, S. Picozzi, and G. Panaccione, Nano Lett. **22**, 7034 (2022).
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4. Ab initio prediction of anomalous Hall effect in antiferromagnetic $CaCrO_3$
T. P. T. Nguyen and K. Yamauchi, Phys. Rev. B **107**, 155126 (2023).
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YANAGISAWA, Susumu [C class; 8000 (B), 0 (C)] (68)
— *First-principles band structure calculation with the electron-phonon coupling at finite temperature*
— *First-principles bandstructure calculation of organic crystals with the electron-phonon coupling*

1. Phonon dispersion of the organic semiconductor rubrene
K. Takada, K. Yoshimi, S. Tsutsui, K. Kimura, K. Hayashi, I. Hamada, S. Yanagisawa, N. Kasuya, S. Watanabe, J. Takeya, and Y. Wakabayashi, Phys. Rev. B **105**, 205205 (2022).
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YANAGISAWA, Takashi [B class; 700 (B), 140 (C)] (205)
— *Numerical study of electronic states in strongly correlated electron systems*
— *Numerical study of electronic states of strongly correlated electron systems*

1. Ferromagnetic diagonal stripe states in the two-dimensional Hubbard model with $U \leq \infty$
M. Miyazaki, T Yanagisawa Phys. Lett. A 446 (2022) 128276

2. Quasi-flat-band in s1/s2 pyrochlore oxides and the effect of spin-orbit interaction
I. Hase, Y. Higashi, T. Yanagisawa J. Phys. Conf. Ser. 2164 (2022) 012063

3. Field resilient superconductivity in atomic layer crystalline materials
Y. Higashi, S. Yoshizawa, T. Yanagisawa et al. unpublished

YASUDA, Chitoshi [C class; 2400 (B), 0 (C)] (271)
— *Numerical study of magnetism in the honeycomb-lattice spin systems*

YASUDA, Yusuke [B class; 900 (B), 160 (C)] (295, 296)
— *Rheology Simulation of Dynamically Cross-linked Elastomers*
— *Structural Analysis and Mechanical Properties Simulations of Polymer Networks with Various Network Structures*

1. Coarse-grained Molecular Dynamics Simulations of Dynamic Bond Elastomers using Inter-bead Potentials for Entropy- and Enthalpy-driven Mechanisms in Their Dynamics and Mechanical Properties
Y. Yasuda, S. Nakagawa, H. Houjou, N. Yoshie and H. Morita, under review

YOKO, Akira [C class; 8600 (B), 800 (C)] (64)
— *Hydrogen production by water splitting on CeO2 (100) facet*
— *Theoretical study for structure and property of metal oxide nanoclusters*

YOKOI, Tatsuya [C class; 4000 (B), 350 (C)] (101)
— *High-accuracy machine-learning interactomic potential and massively large-scale molecular simulation for miscroscopic mechanisms of grain-boundary-dislocation interactions*

YOKOMORI, So [B class; 500 (B), 90 (C)] (166)
— *Study of effects of modulation of molecular arrangement for electronic structure of single-component molecular conductors with canted antiferromagnetism*

YOSHIMOTO, Yuta [C class; 8600 (B), 800 (C)] (220)
— *Constructing a dataset of frequency-dependent dielectric properties of polymeric materials*
— *Constructing a dataset of thermal and dielectric properties of fluoropolymers*

YUAN, Zhicheng [C class; 200 (B), 100 (C)] ()
— *Numerical study of the contact line dynamics on a hybrid hydrophilic surface*

○ A class

Since this class is for trial use, research reports are not required.
When other classes are also used, their publications are shown in the list of B–E classes.
Then, the pages of their reports and publications are given in ( ).

AKIYAMA, Ryota [A class; 100 (B), 50 (C)] ()
— *Band calculations of atomic-layer α-Sn on SnTe*

BUERKLE, Marius [A class; 100 (B), 50 (C)] (383)
— *First-principles computational study of nanocrystals for photovoltaic applications*

FUKUI, Kiyu [A class; 100 (B), 50 (C)] ()
— *Program development of functional renormalization group for spin models with nondiagonal interactions*

HASEGAWA, Taisuke [A class; 100 (B), 50 (C)] ()
— *Analyzing the pump-probe spectra by molecular dynamics simulations*

HATANO, Naomichi [A class; 100 (B), 50 (C)] ()
— *Dynamics of Quantum Walks in Higher Dimensions*

1. Proposal of multidimensional quantum walks to explore Dirac and Schrdinger systems
   M. Yamagishi, N. Hatano, K.-I. Imura, and H. Obuse Phys. Rev. A **107**, 042206 (2023).
   DOI:10.1103/PhysRevA.107.042206

HOSONO, Nobuhiko [A class; 100 (B), 50 (C)] ()
— *Molecular Dynamics Simulation of Molecular Diffusion in Metal-Organic Frameworks*

JESCHKE, Harald [A class; 100 (B), 50 (C)] (247, 248, 394)
— *FLEX computation of susceptibility and superconductivity of β''-$(ET)_2X$ charge transfer salts*

KAGAWA, Fumitaka [A class; 100 (B), 50 (C)] ()
— *Emergent Electric Field induced by current-driven ferromagnetic domain walls*

KATO, Yasuyuki [A class; 100 (B), 50 (C)] ()
— *Theoretical study of topological phase transition and emergent electromagnetic phenomena in magnetic metals*

1. Hidden topological transitions in emergent magnetic monopole lattices
   Y. Kato and Y. Motome, Phys. Rev. B. **107**, 094437 (2023).
   DOI:10.1103/PhysRevB.107.094437

KIM, Kang [A class; 100 (B), 50 (C)] ()
— *Molecular dynamics simulations for interfacial water in acrylate polymers*

KOBAYASHI, Yoshihiro [A class; 100 (B), 50 (C)] ()
— *Molecular dynamics of nanocarbon heterostructure*

MASAKI, Yusuke [A class; 100 (B), 50 (C)] ()
— *Non-axisymmetric vortices in topological nematic superfluids*

MATSUMOTO, Ryosuke [A class; 100 (B), 50 (C)] ()
— *Pre-study for the dislocation-core structure analyses by DFT and atomistic calculations*

NAKAZAWA, Kazuki [A class; 100 (B), 50 (C)] ()
— *Magnetization angle dependence of transport properties in ferromagnetic Weyl semimetal Co_3Sn_2S*

NODA, Yusuke [A class; 100 (B), 50 (C)] ()
— *Microstructure analysis of polycrystalline silicon using first-principles phase-field method*

OKITSU, Kouhei [A class; 100 (B), 50 (C)] ()
— *Calculation of X-ray diffffraction intensities from protein crystals based on the n-beam dynamical diffraction therory*

SATO, Taku [A class; 100 (B), 50 (C)] ()
— *Quantum pyrochlore magnet*

TADA, Kohei [A class; 100 (B), 50 (C)] ()
— *Theoretical study for diradicals in solids and on surfaces*

TAKAHASHI, Osamu [A class; 100 (B), 50 (C)] ()
— *Electronic structure of aqueous ionic liquids*

TAKEMORI, Nayuta [A class; 100 (B), 50 (C)] ()
— *Band calculation of hypermaterials*

TSUJI, Yuta [A class; 100 (B), 50 (C)] ()
— *Theoretical study of methane conversion catalysts by first-principles calculations*

UCHIDA, Kazuyuki [A class; 100 (B), 50 (C)] ()
— *First-principles Study on Superstructures of Si(111)-r7xr3-In Surface*

UEHARA, Masatomo [A class; 100 (B), 50 (C)] ()
— *Throughput calculations of electron-lattice interactions*

UEMURA, Naoki [A class; 100 (B), 50 (C)] ()
— *A benchmark test using OpenMX for alloy materials*

YAMAMOTO, Go [A class; 100 (B), 50 (C)] ()
— *Machine learning-assisted high-throughput molecular dynamics simulation of high-mechanical performance CNT yarn structure*

YAMAMOTO, Sayoko [A class; 100 (B), 50 (C)] ()
— *Polymer Design by Quantum Chemical Calculation*

YANAGISHIMA, Taiki [A class; 100 (B), 50 (C)] ()
— *Origin and dynamics of devitrification in dense colloidal glasses*

YUKAWA, Ryu [A class; 100 (B), 50 (C)] ()
— *Study of spin structure changes at Sb_2Te_3 surfaces*

□ SCCMS Projects

FUJII, Mikiya [2000 (B), 200 (C)] (368)
— *Data driven analysis for impurity effects on photocatalysts*

FUJITA, Takatoshi [3500 (B), 100 (C)] (359)
— *Exciton Properties in Organic Optoelectronic Devices from Large-Scale Electronic Structure Calculations*
— *Exciton Dynamics in Organic Optoelectronic Devices from Large-Scale Electronic Structure Calculations and Time-Resolved Spectroscopy*

1. Ab Initio Study of Charge Separation Dynamics and PumpProbe Spectroscopy in the P3HT/PCBM Blend
   T. Fujita, T. Hoshi submitted
   DOI:10.26434/chemrxiv-2023-773xs

FUKUSHIMA, Tetsuya [4000 (B), 400 (C)] (364)
— *Development of fundamental simulation code for magnetic materials*
— *Materials design of high performance magnetic materials*

1. A first-principles study on the electrical conductivity of $Ag_2S_{1-x}Se_x$ ($x = 0, 0.25, 0.5$): Electron-phonon coupling
   H. N. Nam, K. Suzuki, A. Masago, T. Q. Nguyen, H. Shinya, T. Fukushima, and K. Sato Appl. Phys. Lett. **120**, 143903 (2022).
   DOI:10.1063/5.0086703

2. Direct and inverse magnetocaloric effects in FeRh alloy: A theoretical study
   H. B. Tran, T. Fukushima, H. Momida, K. Sato, and T. Oguchi, J. Alloys Compd. **926** 166718 (2022).
   DOI:10.1016/j.jallcom.2022.166718

3. Physics-informed machine learning combining experiment and simulation for the design of neodymium-iron-boron permanent magnets with reduced critical-elements content
   A. Kovacs, J. Fischbacher, H. Oezelt, A. Kornell, Q. Ali, M. Gusenbauer, M. Yano, N Sakuma, A. Kinoshita, T. Shoji, A. Kato, Y. Hong, S. Grenier, T. Devillers, N. Dempsey, T. Fukushima, H. Akai, N. Kawashima, T. Miyake, and T. Schrefl, Front. Mater. **9**, 1094055 (2023).
   DOI:https://doi.org/10.3389/fmats.2022.1094055

4. The role of electronphonon scattering on thermoelectric properties of intermetallic compounds XSi (X = Co, Rh)
   H. N. Nam, K. Suzuki, A. Masago, H. Shinya, T. Fukushima, K. Sato Jpn. J. Appl. Phys. **62**, 020904 (2023).
   DOI:10.35848/1347-4065/acb97a

GOHDA, Yoshihiro [2000 (B), 200 (C)] (74)
— *Strain effects at magnetic interfaces*

1. Giant converse magnetoelectric effect in a multiferroic heterostructure with polycrystalline Co_2FeSi
   S. Fujii, T. Usami, Y. Shiratsuchi, A.M. Kerrigan, A.M. Yatmeidhy, S. Yamada, T. Kanashima, R. Nakatani, V.K. Lazarov, T. Oguchi, Y. Gohda, and K. Hamaya, NPG Asia Mater. **14**, 43 (2022).
   DOI:10.1038/s41427-022-00389-1

2. Superconductivity in a two monolayer thick indium film on Si(111)$\sqrt{3} \times \sqrt{3}$-B

T. Ogino, I. Seo, H. Tajiri, M. Nakatake, S. Takakura, Y. Sato, Y. Hasegawa, Y. Gohda, K. Nakatsuji, and H. Hirayama, Phys. Rev. B **106**, 045423 (2022).
DOI:10.1103/PhysRevB.106.045423

3. Origin of anisotropic magnetoresistance tunable with electric field in $Co_2FeSi/BaTiO_3$ multiferroic inetrfaces
S. Tsuna, R. Costa-Amaral, and Y. Gohda, J. Appl. Phys. **132**, 234101 (2022).
DOI:10.1063/5.0128149

4. First-principles phonon calculations of neodymium-magnet compounds
S. Tsuna and Y. Gohda, J. Appl. Phys. **133**, 115103 (2023).
DOI:10.1063/5.0142945

5. Structures of Sm-Cu intermetallics with Fe as subphase candidates in $SmFe_{12}$-based permanent magnets studied by first-principles thermodynamics
S. Nishino and Y. Gohda, Jpn. J. Appl. Phys. **62**, 030902 (2023).
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IMADA, Masatoshi [10000 (B), 1000 (C)] (23)
— *Analysis on Superconducting Mechanism of high-Tc Superconductors*
— *Systematic Analyses on Multi—Layer Copper Oxide Superconductors*

1. Unconventional exciton evolution from the pseudogap to superconducting phases in cuprates
A. Singh, H. Y. Huang, J. D. Xie, J. Okamoto, C. T. Chen, T. Watanabe, A. Fujimori, M. Imada, and D. J. Huang, Nat. Commun. **13**, 7906 (2022).
DOI:10.1038/s41467-022-35210-8

2. *Ab initio*low-energy effective Hamiltonians for the high-temperature superconducting cuprates $Bi_2Sr_2CuO_6$, $Bi_2Sr_2CaCu_2O_8$, $HgBa_2CuO_4$, and $CaCuO_2$
Jean-Baptiste Morée, M. Hirayama, M. T. Schmid, Y. Yamaji, and M. Imada, Phys. Rev. B **106**, 235150 (2022).
DOI:10.1103/PhysRevB.106.235150

3. Unconventional dual 1D-2D quantum spin liquid revealed by *ab initio* studies on organic solids family
K. Ido, K. Yoshimi, T. Misawa, and M. Imada, npj Quantum Mater. **7**, 48 (2022).
DOI:0.1038/s41535-022-00452-8

4. Optimized implementation for calculation and fast-update of Pfaffians installed to the open-source fermionic variational solver mVMC
R.-Q. G. Xu, T. Okubo, S. Todo, and M. Imada, Compt. Phys. Commun., **277**, 108375 (2022).
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MATUBAYASI, Nobuyuki [2000 (B), 500 (C)] (360)
— *Development of an efficient method for calculating miscibility of long-chain polymer blends using molecular dynamics simulations*

MIYAKE, Takashi [1800 (B), 70 (C)] (366)
— *Development of high-performance permanent magnets by large-scale simulation and data-driven approach*

1. A First-principles study on the stability of $(R,Zr)(Fe,Co,Ti)_{12}$ against 2-17 and unary phases (R=Y, Nd, Sm)
T. Fukazawa, Y. Harashima, H. Akai, and T. Miyake, Phys. Rev. Mater. **6**, 054404 (2022).
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2. Explainable active learning in investigating structure-stability of $SmFe_{12-\alpha-\beta}X_\alpha Y_\beta$ structures X, Y= {Mo, Zn, Co, Cu, Ti, Al, Ga}
D.-N. Nguyen, H. Kino, T. Miyake, and H.-C. Dam MRS Bulletin **48**, 1 (2023).
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3. Pareto front analysis and multi-objective Bayesian optimization for $(R,Z)(Fe,Co,Ti)_{12}$ (R=Y, Nd, Sm; Z=Zr, Dy)
T. Fukazawa and T. Miyake, J. Phys. Soc. Jpn. **92**, 014801 (2023).
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4. Evidence-based data mining method to reveal similarities between materials based on physical mechanisms
M.-Q. Ha, D.-N. Nguyen, H. Kino, Y. Ando, T. Miyake, T. Denœux, V.-N. Huynh, and H.-C. Dam J. Appl. Phys. **133**, 053904 (2023).
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OSHIYAMA, Atsushi [10000 (B), 1000 (C)] (48)
— *Quantum-theory-based multiscale simulation for next-generation power devices*

1. An atomistic insight into reactions and free-energy profiles of NH_3 and Ga on GaN surfaces during the epitaxial growth
M. Boero, K. M. Bui, K. Shiraishi, K. Ishisone, Y. Kangawa, and A. Oshiyama, Appl. Surf. Sci. **599**, 153935 (2022).

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