4 PUBLICATION LIST

Example:

LASTNAME, Firstname [project class; # points (B), # points (C)] (Page #)

— *Project title*

1. First paper
   Names of Authors, etc.
2. Second paper
   ...

□ ISSP Joint Research Projects

○ B–E classes

AKASHI, Ryosuke [B class; 400 (B), 80 (C)] (188)

— *Revisiting the conventional superconducting theory: Toward nearly uniform electron systems*

1. Illuminating the Bragg intersections as roots of Dirac nodal lines and high-order van Hove singularities
   Ryosuke Akashi Physical Review Research **6**, 033012 (2024)
   DOI:10.1103/PhysRevResearch.6.033012

AKIBA, Takaki [B class; 300 (B), 70 (C)] (350)

— *Modeling for interaction between gas-phase reaction with pattern formation and solid surface*

AN, MENG [B class; 400 (B), 90 (C)] ()

— *Machine learning-assisted computational design of Ionic thermoelectric materials*

ANDO, Yasunobu [B class; 800 (B), 0 (C)] (167)

— *First-principles calculation for building boron-compounds library*

AOYAMA, Kazushi [B class; 300 (B), 80 (C)] (349)

— *Spin dynamics in J1-J3 antiferromagnets on kagome lattices*

1. Spontaneous chirality selection and nonreciprocal spin wave in breathing-kagome antiferromagnets at zero field
   K. Aoyama and H. Kawamura Phys. Rev. B **111**, 14413 (2025).
   DOI:10.1103/PhysRevB.111.144413

ARAI, Munehito [C,D class; 8520 (B), 0 (C)] (261)

— *Accurate prediction of protein folding mechanisms by statistical mechanical models*

— *Development of a novel protein design method for medical and industrial applications*

1. Product release and substrate entry of aldehyde deformylating oxygenase revealed by molecular dynamics simulations
   M. YOSHIMURA, and M. ARAI Biophys. Physicobiol. **22**, e220003 (2025).
   DOI:10.2142/biophysico.bppb-v22.0003

ARAKI, Takeaki [B,C class; 4100 (B), 430 (C)] (310, 311)
— *The Physical Origin of the Emerging Ferroelectric Nematic Phase*
— *Universaliry of Johari-Goldstein relaxation in supercooled liquids and glasses*

1. Discovery of collective nonjumping motions leading to JohariGoldstein process of stress relaxation in model ionic glass
   M. Saito, T. Araki, Y. Onodera, K. Ohara, M. Seto, Y. Yoda, Y. Wakabayashi Acta Materialia **284**, 120536 (2025).
   DOI:10.1016/j.actamat.2024.120536

2. Formation dynamics of branching structure in the slippery DLCA model
   K. Hirata and T. Araki J. Chem. Phys. **160**, 234901 (2024).
   DOI:10.1063/5.0197122

3. Mechanical properties and cooperative motion of aerogels under isotropic expansion
   K. Hirata and T. Araki Soft Matter (submitted)

4. Impact of charge distribution on the stability of ferroelectric nematic liquid crystals
   M. de Mello, M. R. Wilson, and T. Araki Soft Matter, **21**, 1479 (2025)
   DOI:10.1039/D4SM01292E

ARIMA, Kenta [B class; 300 (B), 0 (C)] (208)
— *Detailed analysis of etching at functional graphene/semiconductor interface*

1. First-principles simulations of scanning tunneling microscopy images exhibiting anomalous dot patterns on armchair-edged graphene nanoribbons
   J. Li, K. Inagaki, and K. Arima Phys. Rev. Res. **6**, 013252 (2024).
   DOI:10.1103/PhysRevResearch.6.013252

ASANO, Yuta [E class; 15000 (B), 1850 (C)] (251)
— *Molecular dynamics analysis on ultrasonic cavitation*
— *Molecular dynamics simulation of ultrasonic cavitation*

BAE, Soungmin [C class; 3400 (B), 350 (C)] (107)
— *Doping strategy design for two-dimensional materials from first principles*

BIN, Xu [C class; 4800 (B), 550 (C)] (72)
— *Modulation of Phonon Heat Transport in Van der Waals Heterostructures Utilizing Machine Learning Potentials*
— *Modulation of the phonon hydrodynamic in 2D materials*

DEKURA, Shun [B class; 400 (B), 0 (C)] ()
— *First-principles prediction of structural changes by vapor sorption in HOFs with dynamic skeleton*

EGAMI, Yoshiyuki [C class; 6400 (B), 700 (C)] (68)
— *First-principles study on electron transport properties in heterostructures made of 2-dimensional materials with honeycomb lattice*
— *First-principles study on strain dependence of carrier transport properties in two-dimensional layered materials*

1. GPU acceleration of overbridging boundary matching method without Green's functions based on real-space finite-difference method
   T. Akamatsu, M. Uemoto, Y. Egami, and T. Ono Computer Physics Communications **312**, 109585 (2025).
   DOI:10.1016/j.cpc.2025.109585

2. Wide regime of Efros-Shklovskii variable-range-hopping in $La_{1-x}Ce_xNiO_2$
M. Kouda, K. Osame, H. Nobukane, S. Shimoda, Y. Egami, and M. Sakoda Journal of Physics: Condensed Matter, submitted.

FUCHIZAKI, Kazuhiro [C class; 1800 (B), 350 (C)] (299)
— *Kinetics of phase transition and polyamorphism*

FUJI, Yohei [B class; 600 (B), 0 (C)] (322)
— *Universality in monitored systems with symmetry*
1. Multifractality in monitored single-particle dynamics
K. Yajima, H. Oshima, K. Mochizuki, and Y. Fuji Phys. Rev. Res. **6**, 043049 (2024).
DOI:10.1103/PhysRevResearch.6.043049

2. Topology and Spectrum in Measurement-Induced Phase Transitions
H. Oshima, K. Mochizuki, R. Hamazaki, and Y. Fuji arXiv:2412.11097 (submitted)

FUJII, Susumu [C class; 3400 (B), 0 (C)] (277)
— *Defect structures and their transport properties in thermoelectric chalcogenides*
1. Lone Pair Induced 1D Character and Weak Cation-Anion Interactions: Two Ingredients for Low Thermal Conductivity in Mixed-Anion Metal Chalcohalide $CuBiSCl_2$
X. Shen, K. Pal, P. Acharyya, B. Reveau, P. Boullay, O.I. Lebedev, C. Prestipino, S. Fujii, C.-C. Yung, I.-Y. Tsao, A. Renaud, P. Lemoine, C. Candolfi, and E. Guilmeau J. Am. Chem. Soc., 146, 42, 29072-29083 (2024).
DOI:10.1021/jacs.4c10520

2. Emerging computational and machine learning methodologies for proton-conducting oxides: materials discovery and fundamental understanding
S. Fujii, J. Hyodo, K. Shitara, A. Kuwabara, S. Kasamatsu, Y. Yamazaki Sci. Technol. Adv. Mater., 25, 1, 2416383 (2024).
DOI:10.1080/14686996.2024.2416383

FUJIMOTO, Yoshitaka [C class; 1800 (B), 0 (C)] (139)
— *Electronic structures of doped carbon nanotubes*
— *First-principles study of Impurity-doped carbon nanotubes*
1. First-Principles Theoretical Design of Graphene-Based Field Effect Transistors
Y. Fujimoto Advanced Nanoscale MOSFET architectures: Current Trends and Future Perspectives, ed. K. Biswass, A. Sarkar (Wiley-IEEE press, USA 2024), Chapter 10, pp.201-220.

2. Electronic transport mechanism for nitrogen doping and detection of harmful molecules in carbon nanotubes
Y. Fujimoto submitted.

FUJINO, Tomoko [C class; 2600 (B), 400 (C)] (285)
— *Elucidation of the Origin of Dimerization Fluctuations in Highly Conductive Oligomeric Charge Transfer Complexes*
1. Orbital hybridization of donor and acceptor to enhance the conductivity of mixed-stack complexes
T. Fujino, R. Kameyama, K. Onozuka, K. Matsuo, S. Dekura, T. Miyamoto, Z. Guo, H. Okamoto, T. Nakamura, K. Yoshimi, S. Kitou, T. Arima, H. Sato, K. Yamamoto, A. Takahashi, H. Sawa, Y. Nakamura, and H. Mori Nature Commun. **15**, 3028 (2024).
DOI:10.1038/s41467-024-47298-1

2. Higher conductivity in doped ethylenedioxythiophene (EDOT) dimers with chalcogen-substituted end groups
K. Onozuka, T. Fujino, T. Miyamoto, T. Yamakawa, H. Okamoto, H. Akiba, O. Yamamuro, E. Kayahara, S. Yamago, H. Oike, and H. Mori J. Mater. Chem. C **12**, 13956-13965 (2024).
DOI:10.1039/D4TC02346C

FUJISAKI, Takaya [C class; 3400 (B), 350 (C)] (105)
— *Exploring the optimal composition of reforming catalysts for improving the efficiency of fuel cells using methane*

FUJISAWA, Shuji [B class; 400 (B), 80 (C)] (187)
— *Structural analysis of a single nanocellulose from wood*

FUJISHIRO, Hiroki [C class; 3000 (B), 0 (C)] ()
— *Strained Band-Structure Engineering for Antimonide-Based Terahertz Transistors*

FUJITA, Takatoshi [C class; 1400 (B), 0 (C)] (149)
— *Computational Investigation of Multi-Exciton Generation Mechanism by Large-Scale Excited-State Method*

FUKAYA, Yuri [B class; 300 (B), 0 (C)] ()
— *Theory of local density of states and transport properties in superconductor junctions*

FUKUDA, Jun-ichi [B class; 750 (B), 160 (C)] (317)
— *Calculation of ordered structures dynamics and optical properties of soft materials*
1. Oscillating edge current in polar active fluid
H. Matsukiyo and J. Fukuda Physical Review E **109**, 054604 (2024).
DOI:10.1103/PhysRevE.109.054604

FUKUDA, Masahiro [B class; 400 (B), 70 (C)] (15)
— *Prediction of AFM images of material surfaces by local density quantities*
1. Atomic Observation on Diamond (001) Surfaces with Near-Contact Atomic Force Microscopy
R. Zhang, Y. Yasui, M. Fukuda, T. Ozaki, M. Ogura, T. Makino, D. Takeuchi, and Y. Sugimoto Nano Letters **25**, 1101 (2025).
DOI:10.1021/acs.nanolett.4c05395
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2. Dimer ribbon structures on diamond (001) surfaces revealed with atomic force microscopy
R. Zhang, Y. Yasui, M. Fukuda, M. Ogura, T. Makino, D. Takeuchi, T. Ozaki, and Y. Sugimoto Phys. Rev. Res. **7**, 023036 (2025).
DOI:10.1103/PhysRevResearch.7.023036

Data Repository
C001_dimer_ribbon_AFM
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C001_dimer_chain_AFM
https://isspns-gitlab.issp.u-tokyo.ac.jp/masahiro.fukuda/C001_dimer_chain_AFM
DOI:10.1021/acs.nanolett.4c05395

FUKUDA, Tuneo [C class; 400 (B), 0 (C)] (198)
— *First-principles Study of In-induced Superstructures on the Si(111) surface*

FUKUI, Ken-ichi [C class; 1800 (B), 100 (C)] (303)
— *Analyses on the Potential-dependent Dynamics of Ionic Liquid Electrolytes Forming Electric Double Layers Facing the Electrodes*

FUKUMOTO, Yoshiyuki [B class; 700 (B), 0 (C)] (320)
— *A series expansion study of magnon dispersion relations in S=1/2 frustrated spin systems*
— *Investigation of efficient methods for introducing long-range interactions in the cluster expansion method*

1. Six magnetization plateau phases in a spin-1/2 distorted kagome antiferromagnet: Application to $Y_3Cu_9(OH)_{19}Cl_8$
   Kazu Bodaiji, Katsuhiro Morita, and Yoshiyuki Fukumoto Phys. Rev. B 110, 104431 (2024).
   DOI:10.1103/PhysRevB.110.104431

GOHDA, Yoshihiro [C class; 4400 (B), 400 (C)] (86)
— *Free-energy evaluation of alloys*

1. Artificial multiferroic heterostructures - electric field effects and their perspectives
   T. Taniyama, Y. Gohda, K. Hamaya, and T. Kimura Sci. Technol. Adv. Mater. **25**, 2412970 (2024).
   DOI:10.1080/14686996.2024.2412970

2. Magnetic-anisotropy modulation in multiferroic heterostructures by ferroelectric domains from first principles
   A.M. Yatmeidhy and Y. Gohda Sci. Technol. Adv. Mater. **25**, 2391268 (2024).
   DOI:10.1080/14686996.2024.2391268

3. Prediction of $NdFe_{16}$-based permanent-magnet compounds with high magnetization
   I. Seo, S. Tanaka, M. Endo, and Y. Gohda Appl. Phys. Express **17**, 075502 (2024).
   DOI:10.35848/1882-0786/ad5fd9

GOHLKE, Matthias [C class; 2000 (B), 300 (C)] (296)
— *Tensor network study of an effective spin model for cuprates*

1. Proximate Tomonaga-Luttinger liquid in an anisotropic Kitaev-Gamma model
   M. Gohlke, J. C. Pelayo, T. Suzuki Phys. Rev. B **109** L220410 (2024).
   DOI:10.1103/PhysRevB.109.L220410

2. Magnon spectra of cuprates beyond spin wave theory
   J. Bao, M. Gohlke, J. G. Rau, N. Shannon Phys. Rev. Research **7** L012053 (2025).
   DOI:10.1103/PhysRevResearch.7.L012053

GONOME, Hiroki [C class; 5800 (B), 650 (C)] (69)
— *Study of the principle of photothermal conversion by ab initio calculations*

HAGITA, Katsumi [C class; 2000 (B), 400 (C)] (294)
— *Physical properties of crosslinked polymer networks through network topology analysis*

1. Coarse-grained molecular dynamics model of AB diblock copolymers composed of blocks with different Lennard-Jones parameters forming lamellar structures
   K. Hagita and T. Murashima Polymer **304**, 127132 (2024).
   DOI:10.1016/j.polymer.2024.127132

2. Coarse-grained molecular dynamics model of conformationally asymmetric AB diblock copolymers forming lamellar structures

K. Hagita and T. Murashima Comput. Mater. Sci. **243**, 113105 (2024).
DOI:10.1016/j.commatsci.2024.113105

3. Critical Importance of Both Bond Breakage and Network Heterogeneity in Hysteresis Loop on StressStrain Curves and Scattering Patterns
K. Hagita and T. Murashima Macromolecules **57**, 1090310911 (2024).
DOI:10.1021/acs.macromol.4c01996

HAGIWARA, Satoshi [B class; 500 (B), 0 (C)] (181)
— *A theoretical study on an oxidation process at a metal surfaces*

1. Bias-dependent surface stress by density functional theory combined with the effective screening medium method
S. Hagiwara, S. Ishibashi, and M. Otani Phys. Rev. B **110**, 155409 (2024).
DOI:10.1103/PhysRevB.110.155409

2. Anion Adsorption-induced Charge Separation at the Alumina/Aluminum Interface
S. Hagiwara, T. Murata, and M. Otani Corr. Sci. under review.

HAMADA, Ikutaro [C,D class; 9400 (B), 1000 (C)] (51)
— *Density functional theory study of adsorption and reaction of molecules on solid surfaces and interfaces*
— *Density functional theory study of adsorption and reaction of molecules on solid surfaces and interfaces: cases of two-dimensional materials*

1. Interplay of hydrogen boride sheets with water: an insight into edge stability
K. I. M. Rojas, Y. Morikawa, and I. Hamada Phys. Rev. Materials **8**, 114004 (2024).
DOI:10.1103/PhysRevMaterials.8.114004

2. Interlayer hydrogen recombination from hydrogen boride nanosheets elucidated by isotope labeling
S-i Ito, K. I. M. Rojas, Y. Yasuda, N. Noguchi, K. Fukuda, M. Hikichi, Z. Kang, M. Yuan, R. Tsuji, O. Oki, S. Roy, Y. Hikita, I. Matsuda, M. Miyauchi, I. Hamada, T. Kondo J. Phys. Chem. Lett. **15**, 10965-10976 (2024).
DOI:10.1021/acs.jpclett.4c01975

3. Isotope-dependent site occupation of hydrogen in epitaxial titanium hydride nanofilms
T. Ozawa, Y. Sugisawa, Y. Komatsu, R. Shimizu, T. Hitosugi, D. Sekiba, K. Yamauchi, I. Hamada, K. Fukutani Nat. Commun. **15**, 9558 (2024).
DOI:10.1038/s41467-024-53838-6

4. Atomic Precision Control of Plasmon-Induced Single-Molecule Switching in a Meta- Semiconductor Nanojunction
Y. Park, I. Hamada, A. Hammud, E. W. Meijer, M. Wolf, T. Kumagai, and A. Shiotari, Nat. Commun. **15**, 6709 (2024).
DOI:10.1038/s41467-024-51000-w

HAMAGUCHI, Satoshi [C class; 7400 (B), 750 (C)] ()
— *Analysis of plasma-material interactions by Machine-Learning-based MD simulation*
— *Dynamical analyses of plasma-surface interactions*

HAMAMOTO, Yuji [C,D class; 3800 (B), 0 (C)] (101, 103)
— *First principles study of the Fano resonance in Copper phthalocyanine adsorbed on Cu(100)*
— *Numerical study of the Fano effect in CuPc adsorbed on the Cu(100) surface using the embedding Green function method*

— *Structure search for germanene on Ag(111) thin films by Gaussian process regression*

HARADA, Kenji [C class; 2000 (B), 400 (C)] (293)
— *Information analysis of complex system with a tensor network formalism*

1. Tensor tree learns hidden relational structures in data to construct generative models
   Kenji Harada, Tsuyoshi Okubo, and Naoki Kawashima Machine Learning: Science and Technology **6**, 025002 (2025).
   DOI:10.1088/2632-2153/adc2c7

HARASHIMA, Yosuke [C class; 1400 (B), 0 (C)] (148)
— *Materials exploration loop with materials informatics.*

1. Data-Driven Approach Considering Imbalance in Data Sets and Experimental Conditions for Exploration of Photocatalysts
   W. Takahara, R. Baba, Y. Harashima, T. Takayama, S. Takasuka, Y. Yamaguchi, A. Kudo, and M. Fujii ACS Omega **10**, 14626-14639 (2025).
   DOI:10.1021/acsomega.4c06997

2. Covariance Linkage Assimilation method for Unobserved Data Exploration
   Y. Harashima, T. Miyake, R. Baba, T. Takayama, S. Takasuka, Y. Shigeta, Y. Yamaguchi, A. Kudo, and M. Fujii submitted to Phys. Rev. Materials.
   DOI:10.48550/arXiv.2408.08539

HARIKI, Atsushi [B class; 550 (B), 0 (C)] (239)
— *Computational study on spin splitting and x-ray spectroscopy responses in altermagnets using DFT+DMFT method*

1. Valence, charge transfer, and orbital-dependent correlation in bilayer nickelates $Nd_3Ni_2O_7$
   Daisuke Takegami, Takaki Okauchi, Edgar Abarca Morales, Koto Fujinuma, Mizuki Furo, Masato Yoshimura, Ku-Ding Tsuei, Grace A Pan, Dan Ferenc Segedin, Qi Song, Hanjong Paik, Charles M Brooks, Julia A Mundy, Takashi Mizokawa, Liu Hao Tjeng, Berit H Goodge, Atsushi Hariki Phys. Rev. B **111**, 165101 (2025).
   DOI:10.1103/PhysRevB.111.165101

2. Magnetic Dichroism in Rutile NiF_2: Separating Altermagnetic and Ferromagnetic Effects
   A Hariki, K Sakurai, T Okauchi, J Kunes npj Quantum Materials in Press

HARUYAMA, Jun [C class; 7000 (B), 850 (C)] (59)
— *Electrochemical reaction analysis using density functional calcula- tion + implicit solvation model 6*
— *Electrochemical reaction analysis using density functional calculation + implicit solvation model 6-2*

1. Effects of chainchain interaction on the configuration of short-chain alkanethiol self-assembled monolayers on a metal surface
   C.-L. Liao, S. M. Faizanuddin, J. Haruyama, W.-S. Liao, and Y.-C. Wen J. Chem. Phys. **160**, 214711 (2024).
   DOI:10.1063/5.0214261

2. Correction to “Effect of Nitrogen Doping and Oxygen Vacancy on the Oxygen Reduction Reaction on the Tetragonal Zirconia(101) Surface ”
   S. Muhammady, J. Haruyama, S. Kasamatsu, and O. Sugino J. Phys. Chem. C **128**, 10248 (2024).
   DOI:10.1021/acs.jpcc.4c03502

3. Elucidation of CO Oxidation and CO2 Desorption Dynamics on Pt(111) by van der Waals DFT Calculations: Hyperthermal Kinetic Energy, Sharp Desorption Angle, and Excited Vibrational

States
H. Li, Y. Kataoka, S. Tanaka, J. Haruyama, O. Sugino, and J. Yoshinobu J. Phys. Chem. C **128**, 15393 (2024).
DOI:10.1021/acs.jpcc.4c03538

HATANO, Naomichi [B class; 500 (B), 0 (C)] (339)
— *Numerical Simulation of Kondo Walk*

HAYAMI, Satoru [C class; 5400 (B), 800 (C)] (218)
— *Efficient search of magnetic skyrmion crystal by using machine learning*
— *Generation of spin model based on machine learning*

1. Classification of Multi-Orbital Superconducting State based on Augmented Multipoles
   A. Kirikoshi and S. Hayami Physical Review B **109**, 174510 (2024).
   DOI:10.1103/PhysRevB.109.174510

2. Field-induced transformation between triangular and square skyrmion crystals in a tetragonal polar magnet
   S. Hayami Physical Review B **109**, 184419 (2024).
   DOI:10.1103/PhysRevB.109.184419

3. Linear and nonlinear spin-current generation in polar collinear antiferromagnets without relativistic spin-orbit coupling
   S. Hayami Physical Review B **109**, 214431 (2024).
   DOI:10.1103/PhysRevB.109.214431

4. Double-Q and quadruple-Q instabilities at low-symmetry ordering wave vectors under tetragonal symmetry
   S. Hayami Physical Review B **110**, 014404 (2024).
   DOI:10.1103/PhysRevB.110.014404

5. Anisotropic skyrmion crystal on a centrosymmetric square lattice under an in-plane magnetic field
   S. Hayami Journal of Magnetism and Magnetic Materials **604**, 172293 (2024).
   DOI:10.1016/j.jmmm.2024.172293

6. XXZ-type interlayer exchange interaction in the bilayer triangular-lattice system as a source of multiple skyrmion phases
   S. Hayami Journal of Magnetism and Magnetic Materials **619**, 172876 (2024).
   DOI:10.1016/j.jmmm.2025.172876

7. Stabilization mechanisms of magnetic skyrmion crystal and multiple-Q states based on momentum-resolved spin interactions
   S. Hayami and R. Yambe Materials Today Quantum **3**, 100010 (2024).
   DOI:10.1016/j.mtquan.2024.100010

HIDA, Kazuo [B class; 700 (B), 140 (C)] (318)
— *Numerical Study of One Dimensional Frustrated Quantum Spin Systems*

1. Ground-State Phase Diagram of (1/2, 1/2, 1) Mixed Diamond Chains
   Kazuo Hida, J. Phys. Soc. Jpn. **93**,044703 (2024).
   DOI:10.7566/JPSJ.93.044703

HIGUCHI, Yuji [C class; 8200 (B), 800 (C)] (259)
— *Crystal structure and mechanical properties of polymers with helical structure*
— *Fracture process of semicrystalline polymers using large-scale simulation*

1. Rotational Dynamics of Water near Osmolytes by Molecular Dynamics Simulations
   Yuji Higuchi, Md. Abu Saleh, Takahisa Anada, Masaru Tanaka, and Mafumi Hishida J. Phys. Chem. B **128**, 5008 (2024).
   DOI:10.1021/acs.jpcb.3c08470

2. Reversibility of Semicrystalline Polymers in Creep Testing by Coarse-Grained Molecular Dynamics Simulations
   Yuji Higuchi and Go Matsuba Macromol. Chem. Phys. **225**, 2400076 (2024).
   DOI:10.1002/macp.202400076

3. Hydration Water Dynamics in Zwitterionic Phospholipid Membranes Mixed with Charged Phospholipids
   Md. Khalidur Rahman, Takeshi Yamada, Norifumi L. Yamada, Yuji Higuchi, and Hideki Seto J. Phys. Chem. B **129**, 3998 (2025).
   DOI:10.1021/acs.jpcb.4c07371

HIRATA, Kenji [C class; 1000 (B), 0 (C)] (158)
— *First-principles calculation of dielectric constant in oxide-based phosphor*

HIRATSUKA, Masaki [B class; 400 (B), 70 (C)] ()
— *Calculation of vibrational spectra using graph neural network force field*

HIYAMA, Miyabi [B class; 650 (B), 0 (C)] (321)
— *Analysis for absorption- and fluorescence-spectra of seMpai by quantum chemical calculations*
— *Analysis for in situ absorption spectra in firefly bioluminescence by quantum chemical calculations*

HO, Ngoc [C class; 1800 (B), 300 (C)] ()
— *Pt-based high entropy alloys for fuel cell applications from multiscale simulations and machine learning method*

HOSHI, Takeo [C class; 4600 (B), 400 (C)] (37)
— *HPC-based fusion of simulation experiment analysis and data-driven science*

HOSONO, Nobuhiko [C class; 3000 (B), 300 (C)] (279)
— *Molecular Dynamics Simulation of Polymer Extraction Process from Nanopores*

1. Detecting Single-Point Isomeric Differences in Polymer Chains by MOF Column Chromatography
   N. HOSONO, Y. KONO, N. MIZUTANI, D. KOGA and T. UEMURA Chem. Commun. **60**, 13690 (2024).
   DOI:10.1039/D4CC04902K

HOTTA, Chisa [B,C class; 4200 (B), 400 (C)] ()
— *Analysis on the critical phases using quantum Glauber dynamics*
— *Disorder and dynamics of strongly correlated elecron in a multi-orbital systems*

HOTTA, Takashi [C class; 3400 (B), 0 (C)] (227)
— *Research of quantum critical points in the vicinity of three-channel Kondo phase*

HUKUSHIMA, Koji [C class; 4200 (B), 0 (C)] (270)
— *Large scale computation for spin glasses using extended ensemble methods*

IDO, Kota [C class; 8600 (B), 850 (C)] (258)
— *Ground-state phase diagram of extended Kondo lattice models*
— *Ground-state phase diagram of frustrated itinerant magnets*

1. Many-body Chern insulator in the Kondo lattice model on a triangular lattice
   Kota Ido, Takahiro Misawa Phys. Rev. B **109**, 245114 (2024).
   DOI:10.1103/PhysRevB.109.245114

IITAKA, Toshiaki [C class; 1600 (B), 250 (C)] (304)
— *Calculation of high dimensional systems at finite temperature using random quantum sates of general variational wave functions*

IKEMOTO, Hiroyuki [B class; 300 (B), 60 (C)] (352)
— *Structures of Sulphur Confined in Carbon Nanotubes*

IMADA, Masatoshi [E class; 12000 (B), 1100 (C)] (216)
— *Studies on Quantum Many-Body Problem by Machine Learning*

1. Dome structure in pressure dependence of superconducting transition temperature for HgBa2Ca2Cu3O8: Studies by ab initio low-energy effective Hamiltonian
   Jean-Baptiste Morée, Youhei Yamaji, and Masatoshi Imada Phys. Rev. Res. , **6** (2024) 023163
   DOI:10.1103/PhysRevResearch.6.023163

2. Fermi Machine — Quantum Many-Body Solver Derived from Correspondence between Noninteracting and Strongly Correlated Fermions
   Masatoshi Imada J. Phys. Soc. Jpn., **93** (2024) 104002
   DOI:10.7566/JPSJ.93.104002

3. Variational Benchmarks for Quantum Many-Body Problems
   Dian Wu, Masatoshi Imada, Yusuke Nomura, Rico Pohle, Michael Schmid, iuseppe Carleo *et al.*
   Science, **386**, (2024) 6719
   DOI:10.1126/science.adg9774

4. Forecasting long-time dynamics in quantum many-body systems by dynamic mode decomposition
   Ryui Kaneko, Masatoshi Imada,Yoshiyuki Kabashima, and Tomi Ohtsuki Phys. Rev. Res. , **7** (2025) 013085
   DOI:10.1103/PhysRevResearch.7.013085

INAGAKI, Kouji [B class; 300 (B), 60 (C)] (204)
— *Analyses of semiconductor surface processes by machine-learning based potentials*

INAOKA, Takeshi [B class; 300 (B), 70 (C)] (200)
— *Search and realization of novel electronic properties of surfaces and interfaces and of nanostructures*

1. First principles study of electronic structure of x-form phthalocyanine crystals doped with one-dimensional iodine atomic chains
   T. Inaoka AIP Advances **14**, 085016 (9 pages) (2024).
   DOI:10.1063/5.0216635

INOUE, Kazutoshi [C class; 4000 (B), 200 (C)] (95)
— *Theoretical exploring of the functionalities in ceramics interfaces*

1. Grain Boundary Structural Transformation and the Effect of Impurities in MgO
   Q. Chen, M. Saito, K. Kawahara, A. Nakamura, K. Inoue, Y. Ikuhara under review (2025).

2. Modeling and Epitaxial Matching of Incoherent and Heterointerfaces

K. Inoue, M. Saito, K. Kawahara, Q. Chen, M. Kotani, Y. Ikuhara under review (2025).

ISHIBASHI, Shoji [C class; 1800 (B), 0 (C)] (138)
— *Prediction of properties of organic ferroelectrics and piezoelectrics by first-principles calculations*

1. Unveiling high electro-optic performance in a proton-π-electron-coupled ferroelectric crystal
   K. SUNAMI, S. HORIUCHI, S. ISHIBASHI, and J. TSUTSUMI Adv. Electron. Mater. **11**, 2400346 (2025).
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ISHIDA, Kunio [B class; 1100 (B), 190 (C)] ()
— *Coherent dynamics of strongly coupled electron-phonon-photon systems*

ISHIDA, Takato [B class; 400 (B), 0 (C)] (348)
— *Long-term Reliability Assessment of Reinforced Concrete Structures with Polymer Barrier Layers on the Surface*

1. Coarse-grained Molecular Dynamics Simulation of Oxidative Aging of Polymers - Effect of free radical diffusivity -
   T. Ishida, Y. Doi, T. Uneyama, and Y. Masubuchi Polymer Journal, 56, 10691078 (2024).
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2. Analysis of non-Gaussian diffusion of Hydrogen and Oxygen in Cement Paste Using a Two-State Fluctuating Diffusivity Model
   F. Nakai, and T. Ishida Nihon Reoroji Gakkaishi (J Soc Rheol Jpn) , 52(2), 83-89 (2024).
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ISHII, Fumiyuki [C class; 10400 (B), 900 (C)] (47)
— *Development and application of computational programs for spin conversion physical properties using first-principles methods*
— *Development of a first-principles computational method for thermoelectric effects in thin film systems and application to van der Waals systems*

ISHIKAWA, Takahiro [C class; 1200 (B), 100 (C)] (150)
— *Search for high temperature superconductivity in hydrides*

ISOBE, Masaharu [B class; 400 (B), 70 (C)] (342)
— *Local structure analysis and non-equilibrium phase transition in self-propelled hard polygon systems*

1. Simple and efficient methods for local structural analysis in polydisperse hard disk systems
   D. Mugita, K. Souno, H. Koyama, T. Nakamura, and M. Isobe, J. Chem. Phys. **160**, 174104 (2024).
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2. Microscopic mechanisms of diffusion dynamics : a comparative efficiency study of event-chain Monte Carlo variants in dense hard disk systems
   D. Mugita and M. Isobe, J. Chem. Phys. **161**, 154508 (2024).
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3. Recursive algorithm to the centroid of free area for inherent structure and hopping motion in deeply supercooled binary hard disk systems
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IZUMI, Yasuo [B class; 450 (B), 90 (C)] (177)

— *Clarification of the Activation Principle of Photocatalyts by Doping Metal Atom*

1. Exchange of CO2 with CO as Reactant Switches Selectivity in Photoreduction on CoZrO2 from C13 Paraffin to Small Olefins
   T. Loumissi, R. Ishii, K. Hara, T. Oyumi, I. Abe, C. Li, H. Zhang, R. Hirayama, K. Niki, T. Itoi, and Y. Izumi Angew. Chem. Int. Ed. **63**, e202412090 (2024).
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   T. Oyumi, I. Abe, M. Sasaki, and Y. Izumi Chem. Commun. **61**, submitted on March 3 2025 and under review (2025).

3. The Role of Oxygen Vacancy on the Carbon Dioxide Photoreduction Using Monoclinic and Tetragonal-phase Zirconium Oxide
   Ayana Omata, Keisuke Hara, Tomoki Oyumi, Rento Ishii, Yasuo Izumi, and Kaori Niki e-J. Surf. Sci. Nanotechnol. **22**, 327-333 (2024).
   DOI:10.1380/ejssnt.2024-032

JESCHKE, Harald [C class; 2600 (B), 0 (C)] (292)

— *Superconducting critical temperature and gap structure of kappa-type BEDT-TTF superconductors*

1. Pressure tuning of intrinsic and extrinsic sources to the anomalous Hall effect in $CrGeTe_3$
   G. Scharf, D. Guterding, B. Hen, P. M. Sarte, B. R. Ortiz, G. Kh. Rozenberg, T. Holder, S. D. Wilson, H. O. Jeschke, and A. Ron Phys. Rev. Res. **7**, 013127 (2025).
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2. Near room-temperature ferromagnetism from double exchange in the van der Waals material $CrGeTe_3$: Evidence from optical conductivity under pressure
   J. Ebad-Allah, D. Guterding, M. Varma, M. Diware, S. Ganorkar, H. O. Jeschke, and C. A. Kuntscher Phys. Rev. B **111**, L140402 (2025).
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3. $CuAg(SO_4)_2$: A doubly strongly correlated altermagnetic three-dimensional analog of the parent compounds of high-Tc cuprates
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JIA, Xue [C class; 2200 (B), 0 (C)] (127)

— *Designing low-cost Metal Oxide Heterostructure catalysts for oxygen evolution reaction through High-Throughput Calculations*

1. Divergent Activity Shifts of Tin - Based Catalysts for Electrochemical CO2 Reduction: pH - Dependent Behavior of Single - Atom Versus Polyatomic Structures
   Y. Wang, D. Zhang, B. Sun, X. Jia, L. Zhang, H. Cheng, J. Fan, and H. Li Angew. Chem. Int. Ed. **64**, e202418228 (2025).
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   J. Jiang, Z Guo, S. Deng, X. Jia, H. Liu, J. Xu, H. Li, L. Cheng ChemSusChem **17**, e202400827

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JIE, Sun [C class; 3800 (B), 400 (C)] (93)
— *High-order phonon database and high-performance thermal switch of two-dimensional materials*

KADARISMAN, Hana [B class; 300 (B), 60 (C)] (203)
— *Spin-splitting calculation of Si Ge and Diamond materials*

KAGESHIMA, Hiroyuki [C class; 1800 (B), 300 (C)] (129)
— *Study on physical properties of structural elementary excitations at solid surfaces and interfaces*

1. First-principles Study of Intrinsic hBN Island Nucleated During CVD Initial Growth on Cu(111)
   R. Imamura, I. Seo, and H. Kageshima, e-J. Surf. Sci. Nanotechnol. 23 (2025) *advanced online publication* (13 pages).
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KAIJU, Hideo [B class; 1450 (B), 270 (C)] (141)
— *Electronic structure analysis of Heusler-alloy-based magnetic tunnel junctions using first-principles calculation*
— *Electronic structure analysis of half-metal based magnetic tunnel junctions using first-principles calculation*
— *Electronic structure analysis of organic spin valve devices using first-principles calculation*

KANEKO, Ryui [B class; 900 (B), 170 (C)] (312, 314)
— *Calculating entanglement dynamics in free boson systems by random sampling*
— *Dynamic mode decomposition of time-series data in quantum many-body systems*

1. Entanglement entropy dynamics of non-Gaussian states in free boson systems: Random sampling approach
   R. Kaneko, D. Kagamihara, and I. Danshita Phys. Rev. A **111**, 032412 (2025).
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2. Forecasting long-time dynamics in quantum many-body systems by dynamic mode decomposition
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3. Ground-state phase diagram of the SU(4) Heisenberg model on a plaquette lattice
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   DOI:10.1103/PhysRevA.110.023326

KARIYADO, Toshikaze [B class; 400 (B), 50 (C)] (346)
— *Theoretical study of magnetic properties in atomically thin materials*

1. Strongly hybridized phonons in one-dimensional van der Waals crystals
   S. Sun, Q. Lin, Y. Li, D. Kozawa, H. Wu, S. Maruyama, P. Moon, T. Kariyado, R. Kitaura, and S. Zhao Phys. Rev. Lett, accepted (2025).

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   T. Kariyado Materials Today Quantum, accepted (2025).

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— *Understanding Fast Ion Conduction in Inhomogeneous Materials*

1. Comparison of intermediate-range order in GeO2 glass: Molecular dynamics using machine-learning interatomic potential vs reverse Monte Carlo fitting to experimental data
   Kenta Matsutani, Shusuke Kasamatsu, and Takeshi Usuki, J. Chem. Phys. **161**, 204103 (2024).
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2. Emerging computational and machine learning methodologies for proton conducting oxides: materials discovery and fundamental understanding
   Susumu Fujii, Junji Hyodo, Kazuki Shitara, Akihide Kuwabara, Shusuke Kasamatsu, and Yoshihiro Yamazaki, Sci. Technol. Adv. Mater., 25, 1, 2416383 (2024).
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— *Numerical Simulation of Anyons in Fractional Quantum Hall Systems*

KATOW, Hiroki [B class; 400 (B), 0 (C)] ()
— *Development of Numerical methods for Light-Matter Interaction*

KAWAKATSU, Toshihiro [C class; 4000 (B), 0 (C)] (271)
— *Multiscale simulations for complex flows*

KAWAMURA, Hikaru [C class; 600 (B), 0 (C)] ()
— *Novel order in frustrated magnets*

KAWAMURA, Taira [B class; 450 (B), 90 (C)] (333)
— *A study of the dynamics of thermal equilibrium and nonequilibrium FFLO states using the nonequilibrium Green's function technique*

1. Engineering nonequilibrium superconducting phases in a voltage-driven superconductor under an external magnetic field
   T. Kawamura, and Y. Ohashi arXiv:2503.04179
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2. Nonequilibrium electron distribution function in a voltage-biased metal wire: A nonequilibrium Green ' s function approach
   T. Kawamura, and Y. Kato arXiv:2503.05141
   DOI:10.48550/arXiv.2503.05141

KAWANO, Shoya [B class; 400 (B), 0 (C)] (196)
— *first-principles calculation of tungsten alloy*

KAWASHIMA, Naoki [E class; 29500 (B), 0 (C)] (249)
— *New low-rank approximation by tensor ring decomposition and its application to critical phenomena*

1. Generating Function for Projected Entangled-Pair States
   Wei-Lin Tu, Laurens Vanderstraeten, Norbert Schuch, Hyun-Yong Lee, Naoki Kawashima, and Ji-Yao Chen Physical Review X Quantum 5, 010335 (2024).
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2. Programmable Order by Disorder Effect through Quantum Simulator
Huan-Kuang Wu, Takafumi Suzuki, Naoki Kawashima, Wei-Lin Tu Physical Review Research 6, 023297 (2024).
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3. Faithfulness of Real-Space Renormalization Group Maps
Katsuya O. Akamatsu and Naoki Kawashima Journal of Statistical Physics 191, 109 (2024).
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4. Nuclear norm regularized loop optimization for tensor network
Kenji Homma, Tsuyoshi Okubo, Naoki Kawashima Physical Review Research 6, 043102 (2024).
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5. Emergent intermediate phase in the J 1-J 2 XY model from tensor network approaches
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6. Multi-impurity method for the bond-weighted tensor renormalization group
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https://isspns-gitlab.issp.u-tokyo.ac.jp/kawashima/monte-carlo-database-on-quantum-spin-models

KEIJI, Yashiro [B class; 500 (B), 100 (C)] ()
— *Study of hydrogen sulfide adsorbent for high efficiency of fuel cells with direct biogas supply*

KITAO, Akio [C class; 3400 (B), 350 (C)] (273)
— *Efficient sampling simulation of the soft modes significantly contribute to protein properties*

KOBAYASHI, Akito [B class; 400 (B), 80 (C)] (240)
— *Elucidation of novel order induced by electronic correlation in organic conductors and related anomalous properties*

1. Compensated Ferrimagnets with Colossal Spin Splitting in Organic Compounds
Taiki Kawamura, Kazuyoshi Yoshimi, Kenichiro Hashimoto, Akito Kobayashi, and Takahiro Misawa Phys. Rev. Lett. 132, 15, 156502 (2024).
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2. H-wave - A Python package for the Hartree-Fock approximation and the random phase approximation
Tatsumi Aoyama, Kazuyoshi Yoshimi, Kota Ido, Yuichi Motoyama, Taiki Kawamura, Takahiro Misawa, Takeo Kato, Akito Kobayashi Computer Physics Communications 298, 109087 (2024).
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KOBAYASHI, Katsuyoshi [B class; 500 (B), 80 (C)] (175)
— *Theoretical study on electronic properties of new nanoscale surfaces and interfaces*

KOBAYASHI, Nobuhiko [C class; 3800 (B), 350 (C)] (96)
— *Quantum transport theory by large scale first-principles electron transport calculations*

1. The efficient method for searching stable structures in herringbone-phase organic semiconductors using density functional theory
S. Hakata, H. Ishii, H. Takaki, T. Okamoto, J. Takeya, N. Kobayashi Appl. Phys. Express 17

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2. Order-N calculations for thermoelectric power factor based on linear response theory
H. Ishii, N. Kobayashi, K. Hirose J. Phys.: Condens. Matter 36 335903 (2024).
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KOBAYASHI, Yoshihiro [B class; 250 (B), 70 (C)] (355)
— *Molecular dynamics simulation of graphene-nanosapcer stacking structure*

1. Experimental and Theoretical Investigation of Nanodiamond Insertion on the Interlayer Interaction in Multilayer Stacking Graphene
M. Ding, T. Inoue, J. I. Enriquez, H. H. Handoko, Y. Ogawa, Y. Taniyasu, Y. Hamamoto, Y. Morikawa, Y. Kobayashi Carbon **229**, 119464 (2024).
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KOGA, Akihisa [C,D class; 4600 (B), 600 (C)] (220)
— *Analyzing Ferromagnetic Order in Multi-Component Fermionic Systems using DMFT*
— *Numerical analysis of the dissipation-induced superfluidity in non-Hermitian SU(N) Hubbard model*

KOSHOJI, Ryotaro [C class; 1400 (B), 350 (C)] (301)
— *Mathematical Crystal Chemistry*

1. Mathematical crystal chemistry: A mathematical programming approach to crystal structures of inorganic compounds
R. Koshoji and T. Ozaki Phys. Rev. Materials **8**, 113801 (2024).
DOI:10.1103/PhysRevMaterials.8.113801

2. Mathematical crystal chemistry II: Random search for ionic crystals and analysis on oxide crystals registered in ICSD
R. Koshoji arXiv:2503.20273
DOI:10.48550/arXiv.2503.20273

KOURA, Akihide [C class; 2600 (B), 0 (C)] (122)
— *Ab Initio Study on Static Structure of White Light Generating Amorphous Molecular Materials*

1. Intermolecular Correlations in Liquid Lactic Acid Based on ab initio Molecular Dynamics Simulations Combined with High-Energy X-ray Diffraction Measurements
Kai Ito, Hironori Shimakura, Shuta Tahara, Koji Ohara, Akihide Koura, Kohei Shimamura, and Fuyuki Shimojo Journal of Physical Society of Japan **93**, 054601 (2024).
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2. Thermal Conductivity Calculation using Homogeneous Non-equilibrium Molecular Dynamics Simulation with Allegro
K. Shimamura, S. Hattori, K. Nomura, A. Koura, and F. Shimojo International Journal of Heat and Mass Transfer **234**, 126106 (2024).
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3. Phase Behavior and Atomic Dynamics in Rb_xNa_{1-x}: Insights from Machine Learning Interatomic Potentials based on Ab Initio Molecular Dynamics
A. Irie, Akihide Koura, Kohei Shimamura, and Fuyuki Shimojo Journal of Physics: Condensed Matter **37**, 065401 (2025).
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4. Intermolecular Correlations in Liquid Racemic Lactic Acid: A Comparison with Liquid L-Lactic

Acid
Kai Ito, Hironori Shimakura, Shuta Tahara, Koji Ohara, Akihide Koura, Kohei Shimamura, Fuyuki Shimojo Journal of the Physical Society of Japan, accepted for publication, (2025).

KUNISADA, Yuji [C class; 7400 (B), 0 (C)] (67)
— *Development of Ceramic Protective Coating for High Corrosion Resistance of Metallic Materials*
— *Development of Ceramic Protective Coating to suppress hydrogen embrittlement of metallic materials*

1. Unveiling the origin of diffusion suppression of hydrogen isotopes at the α-$Al_2O_3(0001)/\alpha$-$Cr_2O_3(0001)$ interfaces
   Y. Kunisada, R. Sano, and N. Sakaguchi, International Journal of Hydrogen Energy **97**, 1327 (2025).
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KUROKI, Kazuhiko [C class; 4800 (B), 0 (C)] (221)
— *Theoretical search for new high T_c nickelate superconductors based on structural and phonon DFT analysis*

KUSAKABE, Koichi [C class; 3200 (B), 0 (C)] (112)
— *Theoretical evaluation of mechanical properties of nano-carbon device structures*

1. Surface terminations control charge transfer from bulk to surface states in topological insulators
   K. Fukumoto, S. Lee, S. Adachi, Y. Suzuki, K. Kusakabe, R. Yamamoto, M. Kitatani, K. Ishida, Y. Nakagawa, M. Merkel, D. Shiga, and H. Kumigashira Sci. Rep. **14**, 10537 (2024).
   DOI:10.1038/s41598-024-61172-6

2. Giant Rashba spin-orbit coupling on light-element polar superlattices
   Y. Wicaksono, J.-Y. You, B. Gu, A. Evseev, I. Piyanzina, K. Kusakabe, S. Yunoki, and S. Maekawa Phys. Rev. B **110**, L220408 (2024).
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3. Designing a Polymerized Phenalenyl Tessellation Molecule to Realize a Super-honeycomb Antiferromagnetic S = 3/2 Spin System
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4. Synthesis, crystal and electronic structures, and second harmonic generation of La4Ge3S12
   H. Ohtsuki, S. Nakata, Y. Yamane, R. Takahashi, K. Kusakabe, and H. Wadati Z. anorg. allg. Chem. e202500029, (2025).
   DOI:10.1002/zaac.202500029

LEE, Minhyeok [C class; 800 (B), 250 (C)] (156)
— *Modeling of the Ammonia Decomposition Reaction and Nitriding on Metal Surfaces*

LI, Hao [C class; 4800 (B), 0 (C)] (84)
— *Understanding Hydrogen Energy Materials by Ab Initio Calculations and Multiscale Modeling and Simulations*

LUONG, HuuDuc [C,D class; 7800 (B), 600 (C)] ()
— *Investigation of promising cathode material for Na-ion battery.*
— *Investigation on positive electrodes applicable for Na-ion batteries*

MAEHIRA, Takahiro [B class; 200 (B), 50 (C)] (209)
— *Electronic Structure of WO_3*

MAKINO, Takayuki [B class; 400 (B), 70 (C)] (192)
— *Excitonic properties of delafossite-type cuprates*

MASAKI, Yusuke [B class; 300 (B), 70 (C)] (351)
— *Solitons and phase transitions in quantum chiral spin model in tilted magnetic field*

MATSUKAWA, Hiroshi [C class; 2800 (B), 300 (C)] ()
— *Physics of Friction*

MATSUSHITA, Katsuyoshi [C class; 600 (B), 0 (C)] ()
— *Stability Analysis of Collective Cell Movement due to Different Polarity Symmetry*
— *The Investigation of Effects of Cell Polarity Symmetries on Motion Order of Cells*

MATSUSHITA, Yu-ichiro [E class; 16000 (B), 1950 (C)] (43)
— *Emergence of new functions by controlling atomic structures in wide-gap semiconductors based on first-principles calculations*
— *Identification of Killer Defects in SiC-MOS Devices by First-Principles Calculations*

1. Optimized synthesis of circuits for diagonal unitary matrices with reflection symmetry
   Xinchi Huang ,Taichi Kosugi ,Hirofumi Nishi ,and Yu-ichiro Matsushita J. Phys. Soc. Jpn. **93**, 054002 (2024).
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2. Channel attention for quantum convolutional neural networks
   Gekko Budiutama, Shunsuke Daimon, Hirofumi Nishi, Ryui Kaneko, Tomi Ohtsuki, Yu-ichiro Matsushita Phys. Rev. A **110**, 012447(2024).
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3. Orbital-free density functional theory with first-quantized quantum subroutines
   Yusuke Nishiya, Hirofumi Nishi, Taichi Kosugi, Yu-ichiro Matsushita arXiv:2407.16191(2024).
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4. A probabilistic imaginary-time evolution quantum algorithm for advection-diffusion equation: Explicit gate-level implementation and comparisons to quantum linear system algorithms
   Xinchi Huang, Hirofumi Nishi, Taichi Kosugi, Yoshifumi Kawada, Yu-ichiro Matsushita arXiv:2409.18559v2(2024).
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5. Qubit encoding for a mixture of localized functions
   Taichi Kosugi, Shunsuke Daimon, Hirofumi Nishi, Yu-ichiro Matsushita Phys. Rev. A **110**, 062407(2024).
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6. Tensor decomposition technique for qubit encoding of maximal-fidelity Lorentzian orbitals in real-space quantum chemistry
   Taichi Kosugi, Xinchi Huang, Hirofumi Nishi, Yu-ichiro Matsushita arXiv:2501.07211(2024).
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7. Encoded probabilistic imaginary-time evolution on a trapped-ion quantum computer for ground and excited states of spin qubits
   Hirofumi Nishi, Yuki Takei, Taichi Kosugi, Shunsuke Mieda, Yutaka Natsume, Takeshi Aoyagi, Yu-ichiro Matsushita Phys. Rev. Applied **23**, 034016(2025).
   DOI:10.1103/PhysRevApplied.23.034016

8. Approximate real-time evolution operator for potential with one ancillary qubit and application to first-quantized Hamiltonian simulation

Xinchi Huang, Taichi Kosugi, Hirofumi Nishi, Yu-ichiro Matsushita Quant. Inf. Proc. **24**, 85(2025).
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9. Machine Learning Supported Annealing for Prediction of Grand Canonical Crystal Structures
Yannick Couzinie, Yuya Seki, Yusuke Nishiya, Hirofumi Nishi, Taichi Kosugi, Shu Tanaka, Yu-ichiro Matsushita J. Phys. Soc. Jpn. **94**, 044802(2025).
DOI:10.7566/JPSJ.94.044802

MINAMI, Susumu [B class; 400 (B), 80 (C)] (186)
— *First-principles study for anomalous Nernst effect in topological magnets*

MISAWA, Masaaki [B class; 400 (B), 0 (C)] (195)
— *Computational study of surface and interface phenomena and mechanical properties of functional materials based on atomic-scale structures*

MISAWA, Takahiro [E class; 13500 (B), 1150 (C)] (366)
— *Study of correlated topological insulators using the ab initio method for correlated electron systems*

MITARAI, Yoko [B class; 850 (B), 90 (C)] (159)
— *Phase transformation and electric state of high entropy alloys*

1. Effect of reactive elements in MCrAlX bond coat for durability improvement of thermal barrier coatings
M. Negami, R. Morihashi, T. Yoshino, R. Sahara, Y. Yamabe-Mitarai Corrosion Science 237, 112329 (2024).
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2. Deformation mechanisms of hexagonal close-packed-multi-principal element alloys (HCP-MPEAs) with equiaxed structures
S. J. Liang, T. Yoshino, R. Matsumoto, R. Sahara, Y. Toda, S. Matsunaga, G. Miyamoto, Y. Yamabe-Mitarai Materials Science and Engineering A 929, 148143 (2025).
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MIZUKAMI, Wataru [C class; 7600 (B), 400 (C)] (263)
— *Creating a quantum computing database for sensor materials*

1. Comparative study on compact quantum circuits of hybrid quantum-classical algorithms for quantum impurity models
Rihito Sakurai, Oliver J. Backhouse, George H. Booth, Wataru Mizukami, Hiroshi Shinaoka, Phys. Rev. Research 6, 023110 (2024).
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2. Universal neural network potentials as descriptors: Towards scalable chemical property prediction using quantum and classical computers
Tomoya Shiota, Kenji Ishihara, Wataru Mizukami, Digital Discovery 3, 1714 (2024).
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3. Ab initio extended Hubbard model of short polyenes for efficient quantum computing
Yuichiro Yoshida, Nayuta Takemori, Wataru Mizukami, J. Chem. Phys. 161, 084303 (2024).
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4. Hunting for quantum-classical crossover in condensed matter problems
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5. Lowering the exponential wall: accelerating high-entropy alloy catalysts screening using local surface energy descriptors from neural network potentials
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6. Taming Multi-Domain, -Fidelity Data: Towards Foundation Models for Atomistic Scale Simulations
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7. Enhancing quantum computations with the synergy of auxiliary field quantum Monte Carlo and computational basis tomography
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MOCHIZUKI, Masahito [B class; 400 (B), 40 (C)] (241)
— *Theoretical study on the correlation effects of magnon-band topology and their optical detections*

MOCHIZUKI, Yasuhide [C class; 4000 (B), 400 (C)] (91)
— *Elucidation of negative thermal expansion behavior based on the first-principles molecular-dynamics calculations using machine-learning potential*

MOID, Mohammad [E class; 800 (B), 0 (C)] ()
— *Heterogeneous nucleation of water droplet*

MORIKAWA, Yoshitada [E class; 24000 (B), 2300 (C)] (41)
— *Theoretical study on chemical reaction processes at surfaces and interfaces using density functional theory and machine learning methods*

1. Stabilization of oxygen vacancy ordering and electrochemical-proton-insertion-and-extraction-induced large resistance modulation in strontium iron cobalt oxides $Sr(Fe,Co)O_y$
Y. Isoda, T. N. Pham, R. Aso, S. Nakamizo, T. Majima, S. Hosokawa, K. Nitta, Y. Morikawa, Y. Shimakawa, and D. Kan, Nature Communications **16**, 56 (2025).
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2. Origin of the Surface Facet Dependence in the Thermal Degradation of the Diamond (111) and (100) Surfaces in Vacuum Investigated by Machine Learning Molecular Dynamics Simulations
J. I. G. Enriquez, H. H. Halim, T. Yamasaki, M. Michiuchi, K. Inagaki, M. Geshi, I. Hamada, Y. Morikawa Carbon **226**, 119223 (2024).
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3. Identification of Chemical Species on Plasma-treated Polytetrafluoroethylene Surface by Ab-initio Calculations of Core-energy-level Shift in X-ray Photoelectron Spectra
M. Nishino, K. Inagaki, Y. Morikawa, K. Yamamura, and Y. Ohkubo Appl. Surf. Sci. **655**, 159369 (2024).
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5. Stability of Pd_xO_y Particles Supported on Strontium Titanate Perovskite under Three-Way Catalyst Operating Conditions: Implications for Sintering Resistance
T. N. Pham, B. A. Choi Tan, Y. Hamamoto, K. Inagaki, I. Hamada, and Y. Morikawa ACS Catal. **14**, 1443-1458 (2024).
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MORITA, Satoshi [B class; 500 (B), 80 (C)] (331)
— *Bond-weight optimization in tensor network renormalization groups*

1. Optimization of conveyance of quantum particles by moving potential-well
S. Morita, Y. Teranishi, and S. Miyashita Phys. Rev. Research **6**, 043329 (2024).
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2. Multi-impurity method for the bond-weighted tensor renormalization group
S. Morita and N. Kawashima Phys. Rev. B **111**, 054433 (2025).
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Multi-impurity method for the bond-weighted tensor renormalization group
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MOTOME, Yukitoshi [C,D class; 20000 (B), 1400 (C)] (212)
— *Numerical study of extended Kitaev models in three dimensions by the pseudo-fermion functional renormalization group method*
— *Theoretical study of strongly correlated electron systems using quantum many-body simulation and information science*

1. SP-STM study of the multi-Q phases in $GdRu_2Si_2$
J. Spethmann, N. D. Khanh, H. Yoshimochi, R. Takagi, S. Hayami, Y. Motome, R. Wiesendanger, S. Seki, and K. von Bergmann Phys. Rev. Materials **8**, 064404 (2024).
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2. Inverse Hamiltonian design of highly-entangled quantum systems
K. Inui and Y. Motome Phys. Rev. Research **6**, 033080 (2024).
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3. Eight-color chiral spin liquid in the $S = 1$ bilinear-biquadratic model with Kitaev interactions
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4. Magnetic field effects on the Kitaev model coupled to environment
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5. Topological transitions by magnetization rotation in kagome monolayers of the ferromagnetic Weyl semimetal Co-based shandite
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6. Exploring rare-earth Kitaev magnets by massive-scale computational analysis
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7. Exchange interactions in rare-earth magnets A_2PrO_3 (A= alkali metals)
S.-H. Jang and Y. Motome Phys. Rev. B **110**, 155124 (2024).

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8. Topological phase diagram of the Haldane model on a Bishamon-kikko–honeycomb lattice
S. Ikegami, K. Fukui, S. Okumura, Y. Kato, and Y. Motome Phys. Rev. B **110**, 245107 (2024).
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9. Pressure-induced quantum melting of chiral spin order and subsequent transition to a degenerate semiconductor state in FeGe
Y. Fujishiro, C. Terakura, A. Miyake, N. Kanazawa, K. Nakazawa, N. Ogawa, H. Kadobayashi, S. Kawaguchi, T. Kagayama, M. Tokunaga, Y. Kato, Y. Motome, K. Shimizu, and Y. Tokura Phys. Rev. B **110**, L220401 (2024).
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10. Possible realization of Kitaev spin liquids in van der Waals heterostructures of α-$RuCl_3$ and CrX_3 (X=Cl and I)
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11. Altermagnetic perovskites
M. Naka, Y. Motome, and H Seo npj Spintronics **3**, 1 (2025).
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12. Soliton penetration from edges in a monoaxial chiral magnet
K. Shimizu, S. Okumura, Y. Kato, and Y. Motome Phys. Rev. B **111**, 024411 (2025).
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13. Current-induced motion of nanoscale magnetic torons over the wide range of the Hall angle
K. Shimizu, S. Okumura, Y. Kato, and Y. Motome Commun. Phys. **8**, 69 (2025).
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14. Spin Seebeck Effect as a Probe for Majorana Fermions in Kitaev Spin Liquids
Y. Kato, J. Nasu, M. Sato, T. Okubo, T. Misawa, and Y. Motome Phys. Rev. X **15**, 011050 (2025).
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15. Quantum reservoir probing: an inverse paradigm of quantum reservoir computing for exploring quantum many-body physics
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Y.-F. Zhao, S.-H. Jang, and Y. Motome submitted to Phys. Rev. B

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19. Gapping the spin-nodal planes of an anisotropic p-wave magnet to induce a large anomalous Hall effect
R. Yamada, M. T. Birch, P. R. Baral, S. Okumura, R. Nakano, S. Gao, Y. Ishihara, K. K. Kolincio, I. Belopolski, H. Sagayama, H. Nakao, K. Ohishi, T. Nakajima, Y. Tokura, T. Arima, Y. Motome, M. M. Hirschmann, and M. Hirschberger submitted to Nature

MOTOTAKE, Yoh-ichi [B class; 300 (B), 60 (C)] (202)
— *Ab initio molecular dynamics study of inorganic polymer*

MURASHIMA, Takahiro [C class; 4000 (B), 400 (C)] (365)
— *Elongational Flow Simulation of Polymers*

NADA, Hiroki [B,C class; 4500 (B), 0 (C)] (338)
— *A Large-Scale Metadynamics Simulation Study on the Mechanism of Habit Change of NaCl Crystal by Additives*
— *A Large-scale Molecular Dynamics Simulation Study on the Melt Growth Mechanism of High-Pressure Ice III*

1. Unknown crystal-like phases formed in an imidazolium ionic liquid: A metadynamics simulation study
   H. Nada J. Chem. Phys. **160**, 204501 (2024).
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2. Multiple freezing-melting pathways of high-density ice at room temperature
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NAKAGAWA, Naoko [C class; 3000 (B), 200 (C)] (281)
— *Free energy and phase coexistence in various boundary conditions*

1. Heat-Induced Liquid Hovering in Liquid-Gas Coexistence under Gravity
   A. Yoshida, N. Nakagawa, and S.-i. Sasa Phys. Rev. Lett. 133, 117101 (2024).
   DOI:10.1103/PhysRevLett.133.117101

NAKAGAWA, TAKESHI [B class; 350 (B), 80 (C)] (194)
— *Structural analysis of single layer borophene and boride on Ni surfaces*

NAKAI, Fumiaki [B class; 500 (B), 0 (C)] (336)
— *Mechanism of Size Segregation in Granular Media under Vibration: Analysis Based on Effective Interparticle Forces*

NAKAMURA, Kazuma [C class; 1600 (B), 0 (C)] (143)
— *Ab initio Material Design for Solar Absorption Films*
— *Ab initio calculation of the rotation effect of oxygen octahedron in Ca2MnO4 on electronic properties*

1. Reflectance spectral studies of spark plasma sintered tungsten carbide pellet
   T. Chono, H. Tokutomi, K. Nakamura, K. Miyazaki Jpn. J. Appl. Phys. **64**, 010905 (2025).
   DOI:10.35848/1347-4065/ad9a43

2. Tc and resistivity variation induced by external bending strain in flexible film of strain-sensitive (La,Sr)2CuO4
   T. Horide, T. Maekawa, T. Aikawa, T. Kitamura, K. Nakamura Phys. Rev. Materials **8**, 094802 (2024).
   DOI:10.1103/PhysRevMaterials.8.094802

NAKAMURA, Kohji [C class; 1800 (B), 0 (C)] (137)
— *Material search and spin-orbit coupling induced properties at artificial interfaces and multilayers*

1. Magnon dispersion and terahertz antiferromagnetic resonance frequencies in 3d transition-metal monoxides
   A. Gumarilang, K. Nawa, K. Nakamura Journal of Magnetism and Magnetic Materials **610**, 172499 (2024).
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2. Effect of change in number of electrons to optical properties and surface plasmon resonance of noble metals
   M. Riswan, M. Arifin, I. Santoso, K. Nawa, K. Nakamura, E. Suharyadi Computational Materials Science **247**, 113519 (2024).
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3. Spin direction, quantum size effects, layer stacking, and microstructure of ultrathin Co films on W(110)
   M. Suzuki, K. Nakamura, T. Yasue, T. Koshikawa, E. Bauer Physical Review B **111**, 054405 (2025).
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4. Band engineering for large perpendicular magnetocrystalline anisotropy and low magnetic Gilbert damping constant by anion substitution at Fe/MgO interface
   Y. N. Apriati, K. Nawa, K. Nakamura Applied Physics Letters **126**, 082403 (2025).
   DOI:10.1063/5.0248379

NAKANO, Hiroki [C class; 1200 (B), 200 (C)] (308)
— *Numerical study on low-energy states of quantum spin systems*

1. The spin-S Heisenberg antiferromagnet on the orthogonal-dimer lattice
   H. Nakano and T. Sakai, J. Phys.: Condens. Matter 36 455805 (2024).
   DOI:10.1088/1361-648X/ad6522

NAKANO, Hiroyoshi [C,E class; 11600 (B), 1500 (C)] (253)
— *A comprehensive numerical investigation of suppression of fluctuations near solid wall*
— *Development of a numerical solver for fluctuating hydrodynamics and its applications*

1. Power-law correlation in the homogeneous disordered state of anisotropically self-propelled systems
   K. Adachi, H. Nakano Phys. Rev. Research **6**, 033234 (2024).
   DOI:10.1103/PhysRevResearch.6.033234

2. Long-Range Correlations under Temperature Gradients: A Molecular Dynamics Study of Simple Fluids
   H. Nakano, K. Yokota Phys. Rev. E (accepted)
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3. Looking at bare transport coefficients in fluctuating hydrodynamics
   H. Nakano, Y. Minami, K. Saito arXiv.2502.15241
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4. Energy diffusion in the long-range interacting spin systems
   H. Nishikawa, K. Saito arXiv.2502.10139
   DOI:10.48550/arXiv.2502.10139

NAKAYAMA, Akira [C class; 4000 (B), 400 (C)] (90)
— *Multiscale simulation for liquid/oxide interface based on first-principle calculations*

NASU, Joji [C class; 3400 (B), 400 (C)] (23)
— *Creation mechanism of non-Abelian anyons in quantum spin liquids*
— *Driving non-Abelian anyons by external fields in quantum spin liquids*

1. Effects of Magnetic Fields and Orbital Angular Momentum on Excitonic Condensation in Two-Orbital Hubbard Model
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2. Thermal Hall effect incorporating magnon damping in localized spin systems
   S. Koyama and J. Nasu Phys. Rev. B 109, 174442 (2024).
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3. Real-time control of non-Abelian anyons in Kitaev spin liquid under energy dissipation
   C. Harada, A. Ono, and J. Nasu Phys. Rev. B 110, 214426 (2024).
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4. Spin Seebeck Effect as a Probe for Majorana Fermions in Kitaev Spin Liquids
   Y. Kato, J. Nasu, M. Sato, T. Okubo, T. Misawa, Y. Motome Phys. Rev. X 15, 011050 (2025).
   DOI:10.1103/PhysRevX.15.011050

NGUYEN, Thi [C class; 2600 (B), 300 (C)] ()
— *Quantum anomalous Hall effect in 2D transition metal halides*

NIKI, Kaori [C class; 1600 (B), 400 (C)] (134)
— *Development of photoelectron intensity calculation method for organic molecular thin films*

1. The Role of Oxygen Vacancy on the Carbon Dioxide Photoreduction Using Monoclinic and Tetragonal-phase Zirconium Oxide
   A. Omata, K. Hara, T. Oyumi, R. Ishii, Y. Izumi, and K. Niki e-J. Surf. Sci. Nanotech. **22**(4), 327-333 (2024).
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2. Establishment of a Calculation Method for Investigating Surface Characteristics Using Light
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   T. Loumissi, R. Ishii, K. Hara, T. Oyumi, I. Abe, C. L. H. Zhang, R. Hirayama, K. Niki, T. Itoi, and Y. Izumi Angew. Chem Int. Ed., **63**(51), e202412090 (2024).
   DOI:10.1002/anie.202412090

NISHIDATE, Kazume [C class; 600 (B), 0 (C)] (173)
— *Theoretical study of work function and band gap of double-perovskite*
Data Repository
Computer Simulation with C
http://web.cc.iwate-u.ac.jp/ nisidate/main.pdf

NISHIGUCHI, Kazutaka [B class; 300 (B), 70 (C)] (242)
— *Theoretical study of enhancement mechanism of thermoelectric properties with spin fluctuations: A weak-coupling approach*

NISHIKAWA, Yoshihiko [C class; 3600 (B), 0 (C)] (275)
— *Numerical study of the dynamical transition near the glass transition in the s ensemble*

NOGUCHI, Hiroshi [C class; 5800 (B), 500 (C)] (265)
— *structure formation of biomembrane*

NOGUCHI, Yoshifumi [C class; 7200 (B), 750 (C)] (58)
— *Beyond GW: Development of second-order exchange term*
— *Development of first-principles GW*
Gamma method

1. All-electron first-principles GWΓ simulations for accurately predicting core-electron binding energies considering first-order three-point vertex corrections
   K. Yoneyama, Y. Noguchi, and K. Ohno J. Chem. Phys., **161**, 154102 (2024).
   DOI:10.1063/5.0227580

NOMURA, Yusuke [E class; 12000 (B), 1100 (C)] (214)
— *Variational Ansatz based on Vision Transformers*

1. Ab initio study on heavy-fermion behavior in LiV_2O_4: Role of Hund ' s coupling and stability
   Steffen Backes, Yusuke Nomura, Ryotaro Arita, and Hiroshi Shinaoka Phys. Rev. B **111**, L041102 (2025).
   DOI:10.1103/PhysRevB.111.L041102

NOZAWA, Kazuki [C class; 1400 (B), 550 (C)] (135)
— *First-principles study of surface atomic structure and chemical properties of intermetallic compounds*

1. First-principles Study of Adsorption of Atomic Oxygen on PdZn(111) Surface
   K. Iwamura, Y. Otani, Y. Takahashi, Y. Ishii, and K. Nozawa Materials Transactions, ¥bf 65, 1126 (2024).
   DOI:10.2320/matertrans.MT-M2024060

NUNOURA, Teppei [B class; 300 (B), 0 (C)] (207)
— *Study on catalytic hydrothermal liquefaction of kraft lignin with carbon-nanofiber-supported Ni/CeO2*

OBATA, Masao [B class; 500 (B), 90 (C)] (174)
— *First-principles investigation on magnetic shape memory*

1. Comparative Study of Electronic Structure in Ferromagnetic Heusler Alloys Ni_2MnX (X = Al, Ga, In) Using the Quasi-Particle Self-Consistent GW Method
   J. Lutinec, M. Obata, R. Majumder, K. Hyodo, T. Kotani, L. Kalvoda, and T. Oda J. Magn. Soc. Jpn. 48(6), 94107 (2024).
   DOI:10.3379/msjmag.2411r001

2. Effect of excess Mn on the electronic structure of magnetic shape memory Ni-Mn-Ga alloy via GGA+U and quasiparticle self-consistent GW approaches
   M. Obata, L. Straka, O. Heczko, T. Kotani, T.Oda Proceedings of CCP2023-34th IUPAP Conference on Computational Physics, in press

OCHI, Masayuki [C class; 4600 (B), 0 (C)] (87)
— *Accuracy verification of structural optimizaiton using first-principles wave function theory*

1. Efficient electron doping into $KTaO_3$ by hydrogen ion beam
   S. Hirata, G. Lim, T. Ozawa, M. Wilde, K. Fukutani, M. Ochi, Y. Takagi, H. Kitagawa, and M. Maesato Phys. Rev. Mater. **9**, 025002 (2025).
   DOI:10.1103/PhysRevMaterials.9.025002

2. Theoretical study of the crystal structure of the bilayer nickel oxychloride $Sr_3Ni_2O_5Cl_2$ and analysis of possible unconventional superconductivity
M. Ochi, H. Sakakibara, H. Usui, and K. Kuroki Phys. Rev. B **111**, 064511 (2025).
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3. First-principles Study of Metallic-atom Diffusion in Thermoelectric Material Mg_3Sb_2
M. Ochi, K. Nishiguchi, C. H. Lee, and K. Kuroki J. Phys. Soc. Jpn. **94**, 024704 (2025).
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4. Nonreciprocal charge transport in polar Dirac metals with tunable spin-valley coupling
M. Kondo, M. Kimata, M. Ochi, T. Kaneko, K. Kuroki, K. Sudo, S. Sakaguchi, H. Murakawa, N. Hanasaki, and H. Sakai Phys. Rev. Res. **7**, 013041 (2024).
DOI:10.1103/PhysRevResearch.7.013041

5. Theoretical study of spin-fluctuation-mediated superconductivity in two-dimensional Hubbard models with an incipient flat band
T. Aida, K. Matsumoto, D. Ogura, M. Ochi, and K. Kuroki Phys. Rev. B **110**, 054516 (2024).
DOI:10.1103/PhysRevB.110.054516

6. Pair correlations of the hybridized orbitals in a ladder model for the bilayer nickelate $La_3Ni_2O_7$
M. Kakoi, T. Kaneko, H. Sakakibara, M. Ochi, and K. Kuroki Phys. Rev. B **109**, L201124 (2024).
DOI:10.1103/PhysRevB.109.L201124

7. Theoretical analysis on the possibility of superconductivity in the trilayer Ruddlesden-Popper nickelate $La_4Ni_3O_{10}$ under pressure and its experimental examination: Comparison with $La_3Ni_2O_7$
H. Sakakibara, M. Ochi, H. Nagata, Y. Ueki, H. Sakurai, R. Matsumoto, K. Terashima, K. Hirose, H. Ohta, M. Kato, Y. Takano, and K. Kuroki Phys. Rev. B **109**, 144511 (2024).
DOI:10.1103/PhysRevB.109.144511

ODA, Masato [B class; 150 (B), 0 (C)] ()
— *Vibrational mode analysis of GaN crystals containing a large size of defects*

ODA, Tatsuki [C class; 6800 (B), 600 (C)] (65)
— *Analyses on electronic structure and magnetic anisotropy in high-performance spintronics magnetic materials and parallelization development/application in quasi-particle self-consistent GW*
— *Analyses on electronic structure and magnetic anisotropy in high-performance spintronics magnetic materials and parallelization development/application in quasi-particle self-consistent GW code*

1. Comparative study of electronic structure in ferromagnetic Heusler alloys Ni2MnX (X = Al, Ga, In) using the quasi-particle self-consistent GW method
J. Lutinec, M. Obata, R. Majumder, K. Hyodo, T. Kotani, L. Kalvoda, T. Oda J. Magn. Soc. Jpn.**48**, 94 (2024).
DOI:10.3379/msjmag.2411R001

2. Electronic structures in magnetic shape memory alloys Fe_3X (X=Pd, Pt) by quasi-particle self-consistent GW approach
A. Akatov, M, OBATA, T. Oda Sci. Rep. Kanazawa Univ. **68**, 83 (2025).

OHKOSHI, Shin-ichi [C class; 3400 (B), 0 (C)] ()
— *Theoretical studies on the physical properties of novel functional phase transition materials*

OHKUBO, Yuji [B class; 650 (B), 60 (C)] (169)
— *Clarification of adhesion mechanism at interface between plasma-treated fluoropolymer and CuO using*

DFT+U method -Influence of oxygen vacancy diffusion in CuO layer-
— Clarification of adhesion mechanism at interface between plasma-treated fluoropolymer and copper oxide using first-principles calculations

OHMURA, Satoshi [C class; 4000 (B), 0 (C)] (98)
— Ab initio molecular-dynamics study of CO_2 adsorption mechanisms in cement hydration process
1. 第一原理分子動力学法による 1.1-nm トバモライトが有する層状構造の力学特性
I. Kanemasu, S. Ohmura, N. Takeda, F. Shimojo セメント・コンクリート論文集、**78**, 18-25, (2025).
DOI:10.14250/cement.78.18

OHNISHI, Masato [E class; 8500 (B), 1550 (C)] (53)
— Development of anharmonic phonon property database using first-principles calculations
— Development of database of anharmonic phonon properties using first-principles calculation
1. Enhancing thermoelectric performance of Si-based clathrates via carrier optimization considering finite temperature effects
M. Ohnishi, T. Yamamoto, K. Fujimura, H. Shimizu, K. Yamamoto, and J. Shiomi ACS Chemistry of Materials 36, 10595 (2024).
DOI:10.1021/acs.chemmater.4c02098

2. Optimally Suppressed Phonon Tunneling in van der Waals GrapheneWS2 Heterostructure with Ultralow Thermal Conductivity
W. Ding, Z-Y Ong, M. An, B. Davier, S. Hu, M. Ohnishi, and J. Shiomi Nano Letters 24, 13754 (2024).
DOI:10.1021/acs.nanolett.4c03930

3. Database and deep-learning scalability of anharmonic phonon properties by automated brute-force first-principles calculations
Masato Ohnishi, Tianqi Deng, Pol Torres, Zhihao Xu, Terumasa Tadano, Haoming Zhang, Wei Nong, Masatoshi Hanai, Zhiting Tian, Ming Hu, Xiulin Ruan, Ryo Yoshida, Toyotaro Suzumura, Lucas Lindsay, Alan J. H. McGaughey, Tengfei Luo, Kedar Hippalgaonkar, and Junichiro Shiomi arXiv:2504.21245

OHNO, Kaoru [C class; 4600 (B), 400 (C)] (79)
— Improvement and application of all-electron mixed basis program
1. Optical properties of rutile TiO_2 with Zr, Mo, Zn, Cd impurities
K. Ohno, R. Sahara, T. Nanri, and Y. Kawazoe Comput. Cond. Matter **41**, e00977 (2024).
DOI:10.1016/j.cocom.2024.e00977

2. Non-adiabatic excited-state time-dependent $\boldsymbol{GW}$ (TD$\boldsymbol{GW}$) molecular dynamics simulation of nickel-atom aided photolysis of methane to produce hydrogen molecule
A. Manjanath, R. Sahara, Y. Kawazoe, and K. Ohno Nanomaterials **14**, 1775 (2024).
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OHSAWA, Kazuhito [C class; 800 (B), 0 (C)] (165)
— Study of interaction between radiation damage and lattice defect

OHTO, Tatsuhiko [C class; 1800 (B), 0 (C)] (136)
— First-principles molecular dynamics simulations for confined water

OHTSUKI, Tomi [C class; 4800 (B), 100 (C)] (268)
— Level statistics and critical phenomena in non-Hermitian systems
1. Negative longitudinal resistance of monolayer graphene in the quantum Hall regime

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— *Finite temperature property of frustrated spin systems*
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OKUMURA, Hisashi [C class; 3400 (B), 350 (C)] (272)
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ONO, Shota [B,C class; 1050 (B), 190 (C)] (151, 152)
— *Freestanding cubic crystals in the monolayer limit*
— *Nonequilibrium electron dynamics based on Boltzmann equation: Application to carbon nanotubes*

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— *Friction law for macroscopic objects driven at high speed*

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— *High-precision evaluation of critical universality by relaxation analysis of fluctuations using Gaussian process regression*

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PHUNG, Manh [C class; 1400 (B), 0 (C)] (147)
— *Studying C-H bond activation in zeolite using DFT and highly accurate multi-reference theory*

1. Selective Design of Mesoporous Bi2Se3 Films with Orthorhombic and Rhombohedral Crystals
M. Han, T. Nagaura, H. N. Nam, Z. Yang, A. Alowasheeir, Q. M. Phung, T. Yanai, J. Kim, S. M. Alshehri, T. Ahamad, Y. Bando, and Y. Yamauchi Small, Accepted (2025).

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1. Gravitational wave analogs in spin nematics and cold atoms
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— *Reduction of Rare Metals in Fuel Cell and Formic Acid Decomposition Catalysts*

1. Stability and Oxygen Reduction Reaction Activity of Pt Single-Atom Catalysts on Heteroatom-Doped Graphene
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SAKAKIBARA, Hirofumi [B class; 500 (B), 0 (C)] (179)
— *First-principles study of multi-orbital and multi-layer compounds*

1. Pair correlations of the hybridized orbitals in a ladder model for the bilayer nickelate $La_3\ Ni_2\ O_7$

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SAKASHITA, Tatsuya [B class; 150 (B), 160 (C)] (357)
— *Development of integrated interface of eigensolvers Rokko and application to quantum spin systems*

SASAKI, Ryoma [B class; 550 (B), 100 (C)] ()
— *Microscopic investigation of Li-ion conduction mechanism on grain boundary of organic solid electrolyte*

SASAKI, Takehiko [C class; 2000 (B), 350 (C)] (126)
— *Study on poisoning states of platinum nanoparticles*

SATO, Ryuhei [C class; 2400 (B), 0 (C)] (124)
— *Interfacial Reaction Study Driven by Mathematical Science MI and Molecular Dynamics*
1. Hydrogen Absorption Promoted by Surface Melting: Thermodynamic Criteria for High-Pressure Polyhydride Synthesis
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SATO, Shunsuke [B,C class; 5300 (B), 0 (C)] (74)
— *First-principles analysis on optical-control of current in solids*
— *First-principles calculation of optical control on semiconductor transport properties*
1. Core-level signature of long-range charge-density-wave order and short-range excitonic correlations probed by attosecond broadband spectroscopy
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— *A molecular dynamics simulation study for immiscible polymer blends*

SAU, Kartik [C class; 800 (B), 0 (C)] ()
— *Developing Advanced Hydride Materials using Theoretical Simulation Toward Next-Generation All-Solid-State-Battery Heat/cooling Management Systems and Hydrogen Storage application.*

SEINO, Kaori [C class; 3000 (B), 400 (C)] (111)
— *First-principles study of surface and defect systems for power-electronics materials*

SEKI, Yuya [B class; 500 (B), 80 (C)] (330)
— *Analysis of Ising model in statistical-mechanical infomatics*

1. Black-box optimization for integer-variable problems using Ising machines and factorization machines
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— *Deep learning glassy dynamics by graph neural networks*

SHIMADA, Takahiro [B class; 400 (B), 80 (C)] (184)
— *First-principles lattice defects engineering for atomic-scale multiferroics*

SHIMADA, Toshihiro [B class; 600 (B), 100 (C)] ()
— *Analysis of reaction mechanism and physical properties of molecular crystals that undergoes polymerization under high pressure*

SHIMAMURA, Kohei [C class; 2800 (B), 300 (C)] (113)
— *Improving Stability of Molecular Dynamics Simulation using Machine-Learning Interatomic Potentials*

1. Thermal conductivity calculation using homogeneous non-equilibrium molecular dynamics simulation with Allegro
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— *Analysis of defect structures and ion migration using first-principles calculations and machine learning*

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SHIMOJO, Fuyuki [C class; 4800 (B), 400 (C)] (78)
— *First-Principles Molecular-Dynamics Study of Structural and Electronic Properties of Disordered Materials under Extreme Conditions*

1. Intermolecular Correlations in Liquid Lactic Acid Based on ab initio Molecular Dynamics Simulations Combined with High-Energy X-ray Diffraction Measurements
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— *Multipartite entanglement in quantum frustrated magnets*
— *Thermal effects on quantum frustrated magnets*

SHINAOKA, Hiroshi [B class; 500 (B), 80 (C)] (328)
— *Tensor learning approaches to computational physics*

1. Physics-informed neural network model for quantum impurity problems based on Lehmann rep-

resentation
F. Kakizawa, S. Terasaki, and H. Shinaoka arXiv:2411.18835.
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SHINODA, Wataru [E class; 30500 (B), 2550 (C)] (247)
— *Large-scale Molecular Simulation of Soft Materials using All-Atom and Coarse-Grained Model*

1. Proteinlipid acyl chain interactions: Depth-dependent changes of segmental mobility of phospholipid in contact with bacteriorhodopsin
Yuichi Umegawa, Sho Kato, Sangjae Seo, Wataru Shinoda, Satoshi Kawatake, Shigeru Matsuoka, Michio Murata Biophys. Chem. **308**, 107204 (2024).
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8. Fully atomistic molecular dynamics modeling of photoswitchable azo-PC lipid bilayers: structure, mechanical properties, and drug permeation
Kevin A Alberto, MN Hasna Begam, Hejian Xiong, Wataru Shinoda, Paul A Slesinger, Zhenpeng Qin, Steven O Nielsen Nanoscale **17**, 2032-2042 (2025).
DOI:10.1039/D4NR02509A

9. NMR and molecular simulation studies on the structure elucidation of the amphotericin B ion channel using 13 C and 19 F labelling
Yuichi Umegawa, Hiroshi Tsuchikawa, Wataru Shinoda, Michio Murata Org. Biomol. Chem. **23**, 1233-1252 (2025).
DOI:10.1039/D4OB01468E

10. Selective adsorption of unmethylated DNA on ZnO nanowires for separation of methylated DNA
Marina Musa, Zetao Zhu, Hiromi Takahashi, Wataru Shinoda, Yoshinobu Baba, Takao Yasui Lab Chip **25**, 1637-1646 (2025).
DOI:10.1039/D4LC00893F

SHINOHARA, Yasushi [C class; 1200 (B), 0 (C)] (153)
— *First-principles simulations for photoelectron spectra via extremely nonlinear processes*

SHIOMI, Junichiro [E class; 8000 (B), 900 (C)] (55)
— *Analysis of phonon transport properties in disordered systems*

1. The efficient method of lattice dynamics calculation: Monte Carlo integration with importance sampling
Michimasa Morita, Junichiro Shiomi J. Phys.: Condens. Matter 37, 135902 (2025).
DOI:10.1088/1361-648X/adb231

SHIRAI, Tatsuhiko [B class; 400 (B), 0 (C)] (347)
— *Dissipation effects on quantum algorithm*

1. Accelerated decay due to operator spreading in bulk-dissipated quantum systems
T. Shirai, and T. Mori Phys. Rev. Lett. **133**, 040201 (2024).
DOI:10.1103/PhysRevLett.133.040201

SHIRAISHI, Kenji [C class; 7800 (B), 0 (C)] (61, 62)
— *Clarification of Hole Trap at GaN/SiO2 Interfaces and Fabrication of GaN-MOSFET*
— *Theoretical Studies on New Types of Electron Trap Defects Origninated from Localized Floating States in a-SiN towards Flash Memories Application*

1. Theoretical investigation of NH3 nitridation on Cl-terminated Si(100)-2x1 surfaces
T. Nagahashi, H. Karasawa, R. Horiike, and K. Shiraishi Surface Science **753**, 1222655 (2025).
DOI:10.1016/j.susc.2024.122655

2. Theoretical study of the influence of GaOx interfacial layer on the GaN/SiO_2 interface property
S. Hattori, A. Oshiyama, K. Shiraishi J. Appl. Phys. **135**, 175303 (2024).
DOI:10.1063/5.0204285

3. Passivation mechanisms of oxygen-vacancy-induced hole traps by Mg acceptor atoms at GaN/SiO_2 interface
S. Hattori, A. Oshiyama, K. Shiraishi Appl. Phys. Lett. **125**, 161601 (2024).
DOI:10.1063/5.0223569

SHUDO, Ken-ichi [B class; 400 (B), 80 (C)] (183)
— *Impurity control of chalcogenides by surface-modification*

SUGIHARA, Kaori [B class; 400 (B), 90 (C)] ()
— *Investigating the Molecular Mechanisms Behind the Synergistic Antibacterial Actions of LL-37 and HNP1 Peptides Through Molecular Dynamics Simulations*

SUGINO, Osamu [E class; 6000 (B), 650 (C)] ()
— *Computational study of the material property of metals and oxides*

SUMITA, Shuntaro [B class; 200 (B), 0 (C)] (361)
— *Proposal of novel superconducting states coexisting/competing with higher-order magnetic multipole order or helical magnetism*

SUMIYA, Yosuke [B class; 450 (B), 90 (C)] ()
— *Elucidation of adhesion mechanism of adhesive polymer materials based on first-principle calculations*

SUWA, Hidemaro [C class; 3200 (B), 350 (C)] (223)
— *Magnetic field-induced phases emerging from frustrated spin systems coupled to multiple degrees of freedom*

1. Electronic Raman scattering of antiferromagnetic excitonic insulators
   Hidemaro Suwa, Shang-Shun Zhang, and Cristian D. Batista arXiv:2410.13715
   DOI:10.48550/arXiv.2410.13715

SUZUKI, Takafumi [B,C class; 4800 (B), 520 (C)] (267)
— *Ground state phase diagram of an extended Kitaev model on a honeycomb lattice*
— *Supersolid in Bose-Hubbard model with tilted dipole interactions*

1. Programmable order by disorder effect and underlying phases through dipolar quantum simulators
   Huan-Kuang Wu, Takafumi Suzuki, Naoki Kawashima, Wei-Lin Tu Phys. Rev. Research **6**, 023297 (2024).
   DOI:10.1103/physrevresearch.6.023297

2. Proximate Tomonaga-Luttinger liquid in an anisotropic Kitaev-Gamma model
   Matthias Gohlke, Jose Carlos Pelayo, Takafumi Suzuki Phys. Rev. B **109**, L220410 (2024).
   DOI:10.1103/physrevb.109.l220410

SUZUKI, Takehito [B class; 150 (B), 40 (C)] (363)
— *Analysis of phase transition generated by context-sensitive grammar*
— *Analysis of phase transition in languages based on Combinatory Categorial Grammar*

SUZUKI, Yuji [C class; 2800 (B), 0 (C)] (116)
— *Development of Stretchable Electret Materials for Energy Harvesting with the Aid of Machine Learning*

TADA, Kohei [B class; 700 (B), 160 (C)] (160, 162)
— *Theoretical design of bistable functional materials based on calculations for diradical-solid interaction*
— *Theoretical investigation to design of novel Na-ion battery materials with low environmental impact and high durability*

1. Systematic Investigation on Surface Diradicals Using Theoretical Models: 2M/MgO and 2M/BaO (M = Cu, Ag, and Au)
   K. Tada, K. Masuda, R. Kishi, Y. Kitagawa Chemistry **6**, 1572 (2024).
   DOI:10.3390/chemistry6060095

2. Difference in spin structure of magnetic metal-organic frameworks between cluster model and periodic system
   N. Amamizu, K. Tada, R. Kishi, W. Kosaka, H. Miyasaka, Y. Kitagawa Chemistry Letters **53**, upae230 (2024).
   DOI:10.1093/chemle/upae230

TAHARA, Shuta [B class; 400 (B), 70 (C)] (191)
— *Study on Ag conducting mechanism by comparison between $RbAg_4I_5$ and Rb_2AgI_3*

TAKAHASHI, Osamu [B class; 300 (B), 0 (C)] (205)
— *Electronic structure of aqueous polymers*

TAKAYAMA, Akari [B class; 300 (B), 0 (C)] (358)
— *Structure analysis of atomic layer alloy with Rashba effect studied by TRHEPD*

TAKEMORI, Nayuta [C class; 600 (B), 200 (C)] (164)
— *Exploration of photonic hypermaterials with complete-gap*

TAKETSUGU, Tetsuya [C class; 3600 (B), 350 (C)] (99)
— *Ab initio study on the structure and functions of nanomaterials*

1. Electrocatalytic Ammonia Oxidation to Nitrite and Nitrate with NiOOH-Ni
   H. Liu, C.-J. Yang, C.-L. Dong, J. Wang, X. Zhang, A. Lyalin, T. Taketsugu, Z. Chen, D. Guan, X. Xu, Z. Shao, and Z. Huang Adv. Energy Mater. **14**, 2401675 (2024)
   DOI:10.1002/aenm.202401675

2. Boron-induced transformation of ultrathin Au films into two-dimensional metallic nanostructures
   A. Preobrajenski, N. Vinogradov, D. A. Duncan, T.-L. Lee, M. Tsitsvero, T. Taketsugu, and A. Lyalin Nat. Commun. **15**, 10518 (2024)
   DOI:10.1038/s41467-024-54464-y

3. Theoretical design of nanocatalysts based on $(Fe_2O_3)_n$ clusters for hydrogen production from ammonia
   S. Ibragimov, A. Lyalin, S. Kumar, Y. Ono, T. Taketsugu, and M. Bobrowski J. Chem. Phys. **162**, 054305 (2025).
   DOI:10.1063/5.0242310

TAMAYA, TOMOHIRO [D class; 1000 (B), 500 (C)] (306)
— *Research on quantum spin currents induced by high-intensity terahertz light*

TAMURA, Ryo [B class; 500 (B), 0 (C)] (335)
— *Development of black-box optimization method for materials exploration*

1. Performance of uncertainty-based active learning for efficient approximation of black-box functions in materials science
   Ai Koizumi, Guillaume Deffrennes, Kei Terayama, and Ryo Tamura Sci. Rep. **14, 27019 (2024). DOI:10.1038/s41598-024-76800-4**

TANAKA, Katsuhiro [B,C class; 1850 (B), 190 (C)] (132)
— *First-principles exploration of physical properties of antiferromagnets and its application to magnetic tunnel junction*
— *First-principles study on tunnel magnetoresistance effect using antiferromagnetic metals*

TANAKA, Shu [B class; 500 (B), 90 (C)] (324)
— *Study on hybrid algorithms for Ising machines*

1. Machine Learning Supported Annealing for Prediction of Grand Canonical Crystal Structures
   Yannick Couzinie, Yuya Seki, Yusuke Nishiya, Hirofumi Nishi, Taichi Kosugi, Shu Tanaka, Yuichiro Matsushita J. Phys. Soc. Jpn. **94**, 044802 (2025).
   DOI:10.7566/JPSJ.94.044802

TANAKA, Tomonori [C class; 3400 (B), 350 (C)] (104)
— *Non-perturbative calculation of exchange coupling tensor*

1. Nonperturbative calculation of exchange coupling parameters
   T. Tanaka and Y. Gohda arXiv:2410.11256
   DOI:10.48550/arXiv:2410.11256

2. Efficient first-principles approach to Gibbs free energy with thermal expansion
   K. Hashimoto, T. Tanaka, and Y. Gohda arXiv:2410.11256
   DOI:10.48550/arXiv.2410.11256

TATETSU, Yasutomi [C class; 1800 (B), 300 (C)] (128)
— *First-principles study on stability of nano particles and permanent magnets*

TEN-NO, Seiichiro [C,D class; 9000 (B), 500 (C)] (88)
— *First-principles analysis of perovskite semiconductors toward improving photocatalytic performance*
— *First-principles materials design of perovskite semiconductors toward improving photocatalytic performance*

1. Divalent Cation Doping into $SrTiO_3$ for Enhancing the Photocatalytic Performance of Water Splitting
   K. Nishiguchi, T. Takayama, S. Takasuka, Y. Harashima, M. Fujii, and S. L. Ten-no J. Phys. Chem. Lett. **16**, 11, 2823 (2025).
   DOI:10.1021/acs.jpclett.5c00070

TERAO, Takamichi [B class; 800 (B), 150 (C)] (316)
— *Screening in concentrated electrolytes*

1. Order-Parameter-Free Analysis of Soft Matter: Applications of Machine Learning via Image Recognition
   Terao, and M. Kondo Ann. Phys. (Berlin) **537**, 2400197 (2024).
   DOI:10.1002/andp.202400197

TEZUKA, Masaki [C class; 3800 (B), 400 (C)] (269)
— *Understanding scrambling dynamics in quantum many-body systems and realizing the dynamics in quantum computers*

1. A model of randomly-coupled Pauli spins
   Masanori Hanada, Antal Jevicki, Xianlong Liu, Enrico Rinaldi, and Masaki Tezuka, J. High Energy Phys. **2405**, 280 (2024).
   DOI:10.1007/JHEP05(2024)280

2. Hayden-Preskill Recovery in Hamiltonian Systems
   Yoshifumi Nakata and Masaki Tezuka, Phys. Rev. Research **6**, L022021 (2024).
   DOI:10.1103/PhysRevResearch.6.L022021

TODO, Synge [C class; 4600 (B), 400 (C)] ()
— *Development of tensor-network Markov-chain Monte Carlo and application to quantum many-body systems*

TOH, Daisetsu [C class; 2600 (B), 0 (C)] (120)
— *Study on the etching mechanism of Si in catalyst-referred etching*

TOHYAMA, Takami [C class; 3400 (B), 0 (C)] (226)
— *Novel quantum phases with current and spin current textures due to electron correlation*

1. Keldysh crossover in one-dimensional Mott insulators
   K. Shinjo and T. Tohyama APL Mater. **12**, 041109 (2024).
   DOI:10.1063/5.0198384

TONEGAWA, Takashi [B class; 300 (B), 0 (C)] ()
— *Numerical Study of the One-Dimensional Quantum Spin Systems*

TRAN, Ba [E class; 3000 (B), 700 (C)] ()
— *Computational material design for hydrogen liquefaction*

TSUJI, Yuta [C class; 3000 (B), 550 (C)] (110)
— *Theoretical study of carbon dioxide reduction catalysts using first-principles calculations*
— *Theoretical study of ceria-based composite catalysts using first-principles calculations*

1. Electronic Interaction of Epoxy Resin with Copper at the AdheredInterface
   S. Saeki, D. Kawaguchi, Y. Tsuji, S. Yamamoto, K. Yoshizawa, and K. Tanaka Langmuir **40**, 9725 (2024).
   DOI:10.1021/acs.langmuir.4c00711

2. Mechanistic and Electronic Insights into Efficient Carbon DioxideReduction Driven by Visible Light Using a Coordination Polymer
   Y. Tsuji, S. Yamamoto, Y. Kamakura, C. Suppaso, D.Tanaka, and K. Maeda ACS Appl. Energy Mater. **7**, 4472 (2024).
   DOI:10.1021/acsaem.4c00408

3. Effect of Condensed Water at an Alumina/Epoxy Resin Interface onCuring Reaction
   S. Yamamoto, Y. Tsuji, R. Kuwahara, K. Yoshizawa, and K. Tanaka Langmuir **40**, 12613 (2024).
   DOI:10.1021/acs.langmuir.4c01081

4. Giant anisotropic thermal expansion of copper-cyanido flat layers with flexible copper nodes
   Y. Iwai, M. Nakaya, Y. Tsuji, B.L. Ouay, M.Ohba, and R. Ohtani Chem. Commun. **60**, 6512 (2024).
   DOI:10.1039/d4cc01232a

5. Effects of Curing Agents on the Adhesion of Epoxy Resin to Copper:A Density Functional Theory Study
   Y. Kawashima, and Y. Tsuji Langmuir **40**, 12622 (2024).
   DOI:10.1021/acs.langmuir.4c01093

6. Density Functional Theory Study of Adhesion Mechanism betweenEpoxy Resins Cured with 4,4′-Diaminodiphenyl Sulfone and 4,4′-Diaminodiphenylmethane and Carboxyl Functionalized CarbonFiber
   A. Shrestha, Y. Sumiya, K. Okazawa, Y. Tsuji, and K. Yoshizawa Langmuir **40**, 21573 (2024).
   DOI:10.1021/acs.langmuir.4c02473

7. σ Interference: Through-Space and Through-Bond Dichotomy
   Y. Tsuji, K. Okazawa, T. Tatsumi, and K. Yoshizawa J. Am. Chem. Soc. **146**, 32506 (2024).
   DOI:10.1021/jacs.4c09771

8. Investigating Ni nanoparticles on CeO2 for methane dissociation: a comparative study of theoretical calculations and experimental insights
   T. Fujisaki, Y. Tsuji, P.H. Tu, T.C.D. Doan, D.S.R. Rocabado, A.T. Staykov, K. Yashiro, and Y. Shiratori Phys. Chem. Chem. Phys. **27**, 5024 (2025).

DOI:10.1039/d4cp01324g

9. Van der Waals interactions between nonpolar alkyl chains and polar oxide surfaces prevent catalyst deactivation in aldehyde gas sensing
K. Nakamura, T. Takahashi, T. Hosomi, W. Tanaka, Y. Yamaguchi, J. Liu, M. Kanai, Y. Tsuji, and T. Yanagida Nat. Commun. **15**, 9211 (2024).
DOI:10.1038/s41467-024-53577-8

10. Experimental and Theoretical Investigation of Anisotropic ProtonConduction in Two-Dimensional Metal − Organic Frameworks
Y. Shi, S. Kimura, Y. Iwai, Y. Tsuji, B.L. Ouay, M. Ohba, and R. Ohtani Inorg. Chem. **63**, 22194 (2024).
DOI:10.1021/acs.inorgchem.4c03816

11. Rectified Water Migration Behavior in the NoncentrosymmetricChannels of a Ferroelectric Proton Conductor
Y. Tsuji, and R. Ohtani Inorg. Chem. **64**, 3868 (2025).
DOI:10.1021/acs.inorgchem.4c05053

12. Solvato/Vapochromism-Based Alcohol Sensing throughMetalOrganic Framework Thin Films with CoordinativelyUnsaturated Metal Sites
Y. Toki, K. Okada, A. Fukatsu, Y. Tuji, and M. Takahashi Small Sci. **8**, 2400634 (2025).
DOI:10.1002/smsc.202400634

TSUKAHARA, Noriyuki [B class; 300 (B), 70 (C)] (199)
— *DFT calculations of adsorbed molecules captured by metal-organic films on Cu(111)*

1. Element-specific cluster growth on the two-dimensional metalorganic network
N. Tsukahara, R. Arafune, and J. Yoshinobu Jpn. J. Appl. Phys. 63, 065504 (2024).
DOI:10.35848/1347-4065/ad50b3

TSUMURAYA, Takao [C class; 1200 (B), 200 (C)] ()
— *First-Principles Study on the Origin of Mechanical Properties on Magnesium based Alloys*

TSUNEYUKI, Shinji [C class; 4800 (B), 0 (C)] (82)
— *Advancement of methods for predicting dielectric properties and structure exploration of materials*

1. Nuclear quantum effect on the elasticity of ice VII under pressure: A path-integral molecular dynamics study
J. Tsuchiya, M. Shiga, S. Tsuneyuki, and E.C. Thompson Phys. Rev.. Research ¥bf 6, 02330 (2024).
DOI:10.1103/PhysRevResearch.6.023302

2. Chemical bond based machine learning model for dipole moment: Application to dielectric properties of liquid methanol and ethanol
T. Amano, T. Yamazaki, and S. Tsuneyuki Phys. Rev. B ¥bf 110, 165159 (2024).
DOI:10.1103/PhysRevB.110.165159

3. Data-assimilated crystal growth simulation for multiple crystalline phases
Y. Kubo, R. Sato, Y. Zhao, T. Ishikawa, and S. Tsuneyuki J. Chem. Phys. ¥bf 161, 214113 (2024).
DOI:10.1063/5.0223390

4. Assessing the possible superconductivity in the doped perovskite hydride $KMgH_3$: Effects of lattice anharmonicity and spin fluctuations

S. Lu, R. Akashi, M. Kawamura, and S. Tsuneyuki accepted to Phys. Rev. B

5. Transferability of the chemical-bond-based machine learning model for dipole moment: The GHz to THz dielectric properties of liquid propylene glycol and polypropylene glycol
T. Amano, T. Yamazaki, N. Matsumura, Y. Yoshimoto, and S. Tsuneyuki accepted to Phys. Rev. B

6. Superconducting $LaPtH_6$ with triatomic hydrogen units
T. Ishikawa, Y. Tanaka, and S. Tsuneyuki submitted

TSURUTA, Kenji [B class; 550 (B), 100 (C)] (171)
— *Ab-initio and classical molecular-dynamics simulation on electron/phonon localization and transport in multilayer 2D materials*

UCHIDA, Takashi [B class; 200 (B), 60 (C)] (360)
— *Molecular spin dynamics study on the multiple-Q orders in Hubbard models*

UEMURA, Naoki [C class; 5400 (B), 650 (C)] (70)
— *First-principles study of mechanical properties on alloys*
1. First-Principles Study of Generalized Stacking Fault Energy in MgZnY Alloy with Long-Period Stacking-Ordered Structures
N. Uemura, S. Singhaneka, and R. Matsumoto Mater. Trans. **65**, 1080 (2024).
DOI:10.2320/matertrans.MT-M2024056

USUI, Hidetomo [B class; 400 (B), 90 (C)] (182)
— *First principles study on the thermoelectric properties of goniopolar compounds*

VENGAYIL, Krishnan [B class; 500 (B), 0 (C)] (334)
— *Criticality mediated interactions in supercooled liquids*
— *Yielding and aging of colloidal gels*

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

WANG, Tianyi [C class; 1200 (B), 0 (C)] ()
— *Explore magnetic properties of transition metal carbide catalysts for nitrogen reduction reaction*

WANG, Yinqiao [C class; 800 (B), 200 (C)] ()
— *Mechanical and thermal properties of hyperuniform glasses*

WATANABE, Hiroshi [E class; 11000 (B), 1050 (C)] (255)
— *Analysis of the many-body effect of red blood cells in flow*
1. Fluctuation of a Bilayer Composed by Amphipathic Molecules
S. Kikuchi and H. Watanabe, J. Phys. Soc. Jpn. **93**, 114601 (2024).
DOI:10.7566/JPSJ.93.114601

2. Structural Changes and Percolation Transition in Networks after Aging Processes
R. Sekikawa and H. Watanabe, J. Phys. Soc. Jpn. **94**, 044004 (2025).
DOI:10.7566/JPSJ.94.044004

Data Repository
Simulation data of the aging process in a network

https://isspns-gitlab.issp.u-tokyo.ac.jp/kaityo256/aging_network_data

WATANABE, Hiroshi [B class; 400 (B), 70 (C)] (244)
— *Theoretical study of BCS-BEC crossover in strongly-correlated electron systems*

WATANABE, Satoshi [C class; 10400 (B), 900 (C)] (45)
— *Analyses on correlation between material properties and atomic structures in complex structures via ab-initio-based methods*
— *Analyses on local properties at complex structures via ab-initio-based methods*

1. The tendency of V segregation in Pd/V(110) and Pd/V(100) surfaces induced by H adsorption
   M. A. Palmero, K. Shimizu, H. Nakanishi, S. Watanabe, and A. A. B. Padama Phys. Scripta **99**, 065933 (2024).
   DOI:10.1088/1402-4896/ad3f88

2. Enhanced ionic conductivity through crystallization of glass-Li_3PS_4 by machine learning molecular dynamics simulations
   K. Shimizu, P. Bahuguna, S. Mori, A. Hayashi, and S. Watanabe J. Phys. Chem. C **128**, 10139-10145 (2024).
   DOI:10.1021/acs.jpcc.4c01076

3. Enthralling anodic protection by molybdate on high-entropy alloy based electrocatalyst for sustainable seawater oxidation
   S. Khatun, K. Shimizu, S. Pal, S. Nandi, S. Watanabe, and P. Roy Small **20**, 2402720 (2024).
   DOI:10.1002/smll.202402720

4. Two-Stage Feature Selection for Machine Learning-aided DFT-based Surface Reactivity Study on Single-Atom Alloys
   V. Z. Ordillo, K. Shimizu, D. B. Putungan, A. B. Santos-Putungan, S. Watanabe, R. L. de Leon, J. D. Ocon, K. E. S. Pilario, and A. A. B. Padama Model. Simul. Mater. Sci. Eng. **32**, 065003 (2024).
   DOI:10.1088/1361-651X/ad53ee

5. First-principles study of charge states effects of nitrogen vacancies on phonon properties in III-nitride semiconductors
   Y. Dou, K. Shimizu, H. Fujioka, and S. Watanabe Comput. Mater. Sci. **244**, 113264 (2024).
   DOI:10.1016/j.commatsci.2024.113264

6. Uncovering the Dynamics of Li–Au Alloying and Li Nucleation at the Au/LiPON Interface with In Situ Z Contrast and Surface Roughness Contrast Imaging via Scanning Electron Microscopy
   M. Motoyama, K. Shimizu, T. Kimura, T. Yamamoto, S. Watanabe, and Y. Iriyama JACS Au **4**, 4700-4714 (2024).
   DOI:10.1021/jacsau.4c00530

7. Investigating electronic properties of defective WS_2 thin films via neural network potential-aided first-principles study
   R. Otsuka, K. Shimizu, H. Wakabayashi and S. Watanabe Appl. Phys. Express **17**, 115501 (2024).
   DOI:10.35848/1882-0786/ad8b0c

8. Machine learning and density functional theory-based analysis of the surface reactivity of high entropy alloys: The case of H atom adsorption on CoCuFeMnNi
   A. A. B. Padama, M. A. Palmero, K. Shimizu, T. Chookajorn, and S. Watanabe Comput. Mater. Sci. **247**, 113480 (2025).
   DOI:10.1016/j.commatsci.2024.113480

9. Machine-learning potential for phonon transport in AlN with defects in multiple charge states
Y. Dou, K. Shimizu, J. Carrete, H. Fujioka, and S. Watanabe Phys. Rev. Mater. **9**, 034601 (2025).
DOI:10.1103/PhysRevMaterials.9.034601

10. Dimensionality-Induced Transition from Degenerate to Nondegenerate States in Nb-Doped WSe_2
K. Kanahashi, I. Tanaka, T. Nishimura, K. Aso, A. K. A. Lu, S. Morito, L. Chen, T. Kakeya, S. Watanabe, Y. Oshima, Y. Yamada-Takamura, K. Ueno, A. Azizi, and K. Nagashio ACS Nano **19**, 10244-10254 (2025).
DOI:10.1021/acsnano.4c17660

11. Construction of machine learning potentials toward the exploration of alloy cluster catalysts
K. Miyamoto, K. Shimizu, A. K. A. Lu, and S. Watanabe e-J. Surf. Sci. Nanotechnol., in press

12. Representing Born effective charges with equivariant graph convolutional neural networks
A. Kutana, K. Shimizu, S. Watanabe, and R, Asahi Sci. Rep., submitted.

13. Charge States of Ions around Σ5(310)/[001] Grain Boundary in Cubic-ZrO_2 Revealed by First-Principles Calculations
S. Arai, K. Shimizu, A. K. A. Lu, H. Masuda, H. Yoshida, and S. Watanabe e-J. Surf. Sci. Nanotechnol., submitted.

YAMADA, Atsuo [C class; 2600 (B), 400 (C)] (114)
— Exploration of novel rechargeable battery materials using first-principles and molecular dynamics calculations

1. Electrochemical Proton Intercalation Properties of Bronze-Type Vanadium Dioxide in Nonaqueous Protic Electrolyte
S. Park, S. Nishimura, A. Kitada, A. Yamada ACS Applied Energy Materials **7**, 4347 (2024).
DOI:10.1021/acsaem.4c00139

2. Sequential Structural Evolution Triggered by O — O Dimerization in Oxygen-Redox Reactions
X. Shi, K. Kawai, M. Okubo, A. Yamada, Advanced Energy Materials **15**, 2405714 (2025).
DOI:10.1002/aenm.202405714

YAMADA, Atsushi [C class; 1000 (B), 300 (C)] (234)
— A study of superconductivity and magnetism of strongly correrated electron systems using Hubbard model.

YAMADA, Masahiko [C class; 1400 (B), 350 (C)] (366)
— Large-scale calculation with a flux insertion for SU(N)-symmetric DMRG

YAMAGUCHI, Naoya [C class; 1600 (B), 450 (C)] (131)
— Development of Fast Calculation Codes of Berry Phases in First-principles Calculations and its Application to Energy Conversion Materials

1. First-Principles study on proton transfer in triazole molecules
K. Yakin, N. Yamaguchi, T. Nakajima, M. Mizuno, and F. Ishii Chem. Phys. Lett. **856**, 141582
DOI:10.1016/j.cplett.2024.141582

2. Effect of poly(acrylic acid) on proton transfer in triazole molecules: a first-principles study
K. Yakin, N. Yamaguchi, M. Mizuno, and F. Ishii Sci. Rep. Kanazawa Univ. **67**, 69

3. Dirac Electrons in Graphene Flakes
W. Amalia, N. Yamaguchi, S. Yunitasari, and F. Ishii J. Phys. Soc. Jpn. **93**, 104707

DOI:10.7566/jpsj.93.104707

YAMAJI, Youhei [E class; 6000 (B), 800 (C)] (217)
— *Massively parallel variational Monte Carlo method augmented by non-Markovian Monte Carlo and artificial neural networks*

1. Moiré superlattices of antimonene on a Bi(111) substrate with van Hove singularity and Rashba-type spin polarization
   T. Nakamura, Y. Chen, R. Nemoto, W. Qian, Y. Fukushima, K. Kawaguchi, R. Mori, T. Kondo, Y. Yamaji, S. Tsuda, K. Yaji, and T. Uchihashi Communications Materials **5**, 167 (2024).
   DOI:10.1038/s43246-024-00615-z

2. Self-Energy Spectroscopy and Artificial Neural Network
   Y. Yamaji J. Phys. Soc. Jpn. **94**, 031005 (2025).
   DOI:10.7566/JPSJ.94.031005

YAMAMOTO, Go [C class; 7600 (B), 800 (C)] (260)
— *Designing MWCNT Fiber Structures for High Mechanical Performance Composites*
— *Machine learning-assisted high-throughput MD simulation on structure-mechanical property relationships in carbon nanotube yarns*

YAMAMOTO, Tsuyoshi [D class; 450 (B), 0 (C)] (344)
— *Quantum heat flow in a dissipative qubit under continuous quantum measurement*

1. Energy exchange and fluctuations between a dissipative qubit and a monitor under continuous measurement and feedback
   T. Yamamoto, and Y. Tokura SciPost Phys. Core **8**, 016 (2025).
   DOI:10.21468/SciPostPhysCore.8.1.016

Data Repository
Numerical dataset for quantum trajectory simulations of a dissipative qubit under continuous measurement and feedback
https://zenodo.org/records/14252485
DOI:10.5281/zenodo.14252485

YAMASHITA, Tomoki [C class; 2400 (B), 350 (C)] (118)
— *Materials Development by Crystal Structure Prediction and First-principles Calculations*

1. Crystal structure prediction of $Li_{4x}Mg_{2(1-x)}P_2O_7$ by first-principles calculations
   T. Sato, T. Otani, S. Namamori, F. Utsuno, T. Honma, and T. Yamashita Jpn. J. Appl. Phys. **63**, 075503 (2024).
   DOI:10.35848/1347-4065/ad531d

YAMAUCHI, Kunihiko [C class; 3200 (B), 350 (C)] (109)
— *Understanding of spin-splitting phenomena in altermagnets*

1. Wide-range thermal conductivity modulation based on protonated nickelate perovskite oxides
   Hao-Bo Li, Zhiping Bian, Mitsuki Yoshimura, Kohei Shimoyama, Chengchao Zhong, Keiji Shimoda, Azusa N. Hattori, Kunihiko Yamauchi, Ikutaro Hamada, Hiromichi Ohta, and Hidekazu Tanaka, Applied Physic Letter **124**, 191901 (2024).
   DOI:10.1063/5.0201268

2. Observation of edge states derived from topological helix chains
   K. Nakayama, A. Tokuyama, K. Yamauchi, A. Moriya, T. Kato, K. Sugawara, S. Souma, M. Kitamura, K. Horiba, H. Kumigashira, T. Oguchi, T. Takahashi, K. Segawa, and T. Sato Nature

631, 54 (2024).
DOI:doi.org/10.1038/s41586-024-07484-z

3. Indication of exchange interaction induced spin splitting in unoccupied electronic states of the high-TC ferromagnet (Cr0.35Sb0.65)2Te3
C. W. Chuang, Y. Nakata, K. Hori, S. Gupta, F. M. F. de Groot, A. Fujimori, T. P. T. Nguyen, K. Yamauchi, I. Rajput, A. Lakhani, F.-H. Chang, H.-J. Lin, C.-T. Chen, F. Matsukura, S. Souma, T. Takahashi, T. Sato, and A. Chainani Phys. Rev. B 109, 195134 (2024).
DOI:10.1103/PhysRevB.109.195134

4. Isotope-dependent site occupation of hydrogen in epitaxial titanium hydride nanofilms
T. Ozawa, Y. Sugisawa, Y. Komatsu, R. Shimizu, T. Hitosugi, D. Sekiba, K. Yamauchi, I. Hamada, and K. Fukutani Nat. Commun. 15, 9558 (2024).
DOI:10.1038/s41467-024-53838-6

Data Repository
Isotope-dependent site occupation of hydrogen in epitaxial titanium hydride nanofilms
https://archive.materialscloud.org/record/2024.168
DOI:10.24435/materialscloud:je-ev

YANAGISAWA, Susumu [C class; 6800 (B), 0 (C)] ()
— *First-principles bandstructure calculation with the electron-phonon interaction of organic semiconductor crystals*
— *First-principles study on the electron-phonon coupling in organic semiconductors*

YANAGISAWA, Takashi [B class; 800 (B), 150 (C)] (235)
— *Optimized variational Monte Carlo study of high-temperature superconductivity of strongly correlated electrons*
— *Study of strongly correlated many-body problem based on the optimization quantum variational Monte Carlo method*

1. Strongly Correlated Electrons and High Temperature Superconductivity
T. Yanagisawa High-Temperature Materials 1, 10004 (2024).
DOI:10.35534/htm.2024.10004

2. Superconductivity and Inhomogeneous charge-ordered state in the two-dimensional Hubbard model
T. Yanagisawa preprint

YASUDA, Chitoshi [B,C class; 2600 (B), 70 (C)] (290, 291)
— *Effects of deficit on quantum spin systems*
— *Magnetism in the multiple-spin exchange model on a honeycomb lattice*

1. Classical Ground-State Phase Diagram of the Multiple-Spin Exchange Model on a Honeycomb Lattice
C. Yasuda and Y. Chibana submitted to J. Phys. Soc. Jpn.

YASUHARA, Sou [C class; 5200 (B), 0 (C)] (76, 77)
— *Exploration of Stable Structure in K2NdTa5O15 using First-Principles Phonon Calculations*
— *Investigation of atomic displacement mechanism during a polarization switching in LiGaO2*

YOKO, Akira [C class; 2600 (B), 350 (C)] (115)
— *Distortion of ultrasmall metal oxides and their electronic state*

1. Nonequilibrium Process for Doping Under Continuous-Flow Hydrothermal Synthesis of Cerium Oxide-Based Nanoparticles

Yoko, A., Han, C., Sakonaka, A., Seong, G., Tomai, T., Ohara, S., Adschiri, T. Precision Chemistry, (2025).
DOI:10.1021/prechem.5c00004

YOKOI, Tatsuya [C class; 2800 (B), 0 (C)] ()
— *Hierarchical machine-learning model for accurately predicting thermal and electronic properties of grain boundaries in compound semiconductors*

YOSHIMI, Kazuyoshi [C class; 2000 (B), 200 (C)] (232)
— *Ab-initio analysis of pressure-induced quantum phase transitions in molecular materials*

1. Combined x-ray diffraction, electrical resistivity, and ab initio study of $(TMTTF)_2PF_6$ under pressure
   Miho Itoi, Kazuyoshi Yoshimi, Hanming Ma, Takahiro Misawa, Takao Tsumuraya, Dilip Bhoi, Tokutaro Komatsu, Hatsumi Mori, Yoshiya Uwatoko, Hitoshi Seo Phys. Rev. Research **6**, 043308.
   DOI:10.1103/PhysRevResearch.6.043308

2. Pressure-induced topological changes in Fermi surface of two-dimensional molecular conductor
   T. Kobayashi, K. Yoshimi, H. Ma, S. Sekine, H. Taniguchi, N. Matsunaga, A. Kawamoto, Y. Uwatoko Phys. Rev. Materials **9**, L021801 (2025).
   DOI:10.1103/PhysRevMaterials.9.L021801

Data Repository
Dataset for Ab initio study of TMTTF2PF6 under pressure: implications to the unified phase diagram
https://isspns-gitlab.issp.u-tokyo.ac.jp/k-yoshimi/tmttfpf6-pdep
Dataset for Pressure-Induced Topological Changes in the Fermi Surface of the Two-Dimensional Molecular Conductor
https://isspns-gitlab.issp.u-tokyo.ac.jp/k-yoshimi/betap-ET2ICl2

YOSHIOKA, Hironori [C class; 1000 (B), 50 (C)] (154)
— *Calculation of electronic states for improving characteristics at the channel interface of power MOSFETs*

YUAN, Jiaxing [C class; 600 (B), 350 (C)] ()
— *Key roles of hydrodynamic interactions on coil-globule transition of polyelectrolytes*

YUHARA, Junji [B class; 400 (B), 90 (C)] (172)
— *Structural analysis of oxide quasicrystal thin films*

1. Schematic structural analysis of honeycomb structure ultrathin Ce-Ti-O films on Pt(111) using photoelectron holography and ab initio calculation
   X. Li, S. Yamada, Y. Yamada, M. Yoshida, Y. Hashimoto, T. Matsushita, W. Ma, E. Gaudry, and J. Yuhara J. Phys. Chem. C 128, 20238 (2024).
   DOI:10.1021/acs.jpcc.4c05269

ZHANG, Di [C class; 1400 (B), 0 (C)] (145)
— *Spin Promotion Effect in Magnetic Catalysis: Exploring High-Performance Metal-Nitrogen-Carbon Catalysts under External Magnetic Fields*

1. The potential of zero charge and solvation effects on single-atom MNC catalysts for oxygen electrocatalysis
   Di Zhang, Hao Li, Journal of Materials Chemistry A, 12, 23, 13742-13750 (2024).
   DOI:10.1039/D4TA02285H

2. Chromium Promotes Phase Transformation to Active Oxyhydroxide for Efficient Oxygen Evolu-

tion
Yong Wang, Sijia Liu, Yunpu Qin, Yongzhi Zhao, Luan Liu, Di Zhang, Jianfang Liu, Yadong Liu, Aimin Chu, Haoyang Wu, Baorui Jia, Xuanhui Qu, Hao Li, Mingli Qin, ACS Catalysis 14, 18, 13759-13767 (2024).
DOI:10.1021/acscatal.4c03974

3. Mapping degradation of ironnitrogencarbon heterogeneous molecular catalysts with electron-donating/withdrawing substituents
Fangzhou Liu, Di Zhang, Fangxin She, Zixun Yu, Leo Lai, Hao Li, Li Wei, Yuan Chen, ACS Catalysis, 14, 12, 9176-9187 (2024).
DOI:10.1021/acscatal.4c01752

4. Spin Manipulation of Heterogeneous Molecular Electrocatalysts by an Integrated Magnetic Field for Efficient Oxygen Redox Reactions
Zixun Yu, Di Zhang, Yangyang Wang, Fangzhou Liu, Fangxin She, Jiaxiang Chen, Yuefeng Zhang, Ruijie Wang, Zhiyuan Zeng, Li Song, Yuan Chen, Hao Li, Li Wei, Advanced Materials, 36, 45, 2408461 (2024).
DOI:10.1002/adma.202408461

5. Carbon-anchoring synthesis of Pt1Ni1@Pt/C core-shell catalysts for stable oxygen reduction reaction
Jialin Cui, Di Zhang, Zhongliang Liu, Congcong Li, Tingting Zhang, Shixin Yin, Yiting Song, Hao Li, Huihui Li, Chunzhong Li, Nature Communications, 15, 1, 9458 (2024).
DOI:10.1038/s41467-024-53808-y

6. Unraveling the Complexity of Divalent Hydride Electrolytes in Solid - State Batteries via a Data - Driven Framework with Large Language Model
Qian Wang, Fangling Yang, Yuhang Wang, Di Zhang, Ryuhei Sato, Linda Zhang, Eric Jianfeng Cheng, Yigang Yan, Yungui Chen, Kazuaki Kisu, Shin-ichi Orimo, Hao Li, Angewandte Chemie International Edition, e202506573 (2025).
DOI:10.1002/anie.202506573

7. Data - Driven Accelerated Discovery Coupled with Precise Synthesis of Single - Atom Catalysts for Robust and Efficient Water Purification
Keng-Qiang Zhong, Fu-Yun Yu, Di Zhang, Zheng-Hao Li, Dong-Hua Xie, Ting-Ting Li, Yun Zhang, Li Yuan, Hao Li, Zhen-Yu Wu, Guo-Ping Sheng, Angewandte Chemie International Edition, e202500004 (2025).
DOI:10.1002/anie.202500004

8. Why Do Weak-Binding MNC Single-Atom Catalysts Possess Anomalously High Oxygen Reduction Activity?
Di Zhang, Fangxin She, Jiaxiang Chen, Li Wei, Hao Li, Journal of the American Chemical Society, 147, 7, 60766086 (2025).
DOI:10.1021/jacs.4c16733

9. Divergent Activity Shifts of Tin - Based Catalysts for Electrochemical CO2 Reduction: pH - Dependent Behavior of Single - Atom Versus Polyatomic Structures
Yuhang Wang, Di Zhang, Bin Sun, Xue Jia, Linda Zhang, Hefeng Cheng, Jun Fan, Hao Li, Angewandte Chemie International Edition, 64, 8, e202418228 (2025).
DOI:10.1002/anie.202418228

10. Surface Charge Transfer Enhanced Cobalt - Phthalocyanine Crystals for Efficient CO2 - to - CO Electroreduction with Large Current Density Exceeding 1000 mA cm − 2
Tengyi Liu, Di Zhang, Yutaro Hirai, Koju Ito, Kosuke Ishibashi, Naoto Todoroki, Yasutaka Matsuo, Junya Yoshida, Shimpei Ono, Hao Li, Hiroshi Yabu, Advanced Science, 2501459 (2025).

DOI:10.1002/advs.202501459

ZHOU, Zizhen [D class; 10000 (B), 500 (C)] ()
— *Research on Improving Solid-State Battery Performance through Doped LiNbO3 Modification*

○ 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 ( ).

AKUTSU, Hiroki [A class; 100 (B), 50 (C)] ()
— *Band structural calculations of organic conductors*

HAN, Jihae [A class; 100 (B), 50 (C)] ()
— *Reductive decomposition mechanism of fluorine-containing solvent at the electrode/electrolyte interface of lithium sulfur batteries by first-principles calculations*

KANEKO, Masashi [A class; 100 (B), 50 (C)] ()
— *Correlation between nuclear decay and electronic orbitals in actinide compounds using density functional theory calculations*

KAWAMURA, Taira [A class; 100 (B), 50 (C)] (333, 397)
— *Spatiotemporal dynamics of a superconducting order parameter in a nonequilibrium superconducting wire*

KIKUCHI, Shuta [A class; 100 (B), 50 (C)] ()
— *Analysis of the methods for improving the performance of Ising machines*

KINEFUCHI, Ikuya [A class; 100 (B), 50 (C)] ()
— *Preliminary study on gas separation mechanisms in facilitated transport membranes*

KITOH, Hirotaka [A class; 100 (B), 50 (C)] ()
— *Electronic Structure Calculations of Organic Solar Cell Materials*

1. Carrier Mobility and Luminescence Properties of a One-Step Synthesized π-Extended Diketopyrrolopyrrole Derivative
   T. Nishiyama, T. Yamaoka, K. Nakajima, S. Nakajima, Z. L. Goo, R. Akiyoshi, H. Kitoh-Nishioka, S. Tanaka, K. Sugimoto, D. Tanaka, and T. Okubo ACS Omega **10**, 11334 (2025).
   DOI:10.1021/acsomega.4c11150

KITOU, Shunsuke [A class; 100 (B), 50 (C)] ()
— *Analysis of short-range order in pyrochlore-type compounds using X-ray diffuse scattering data*

KOSHOJI, Ryotaro [A class; 100 (B), 50 (C)] (301, 397)
— *Mathematical Crystal Chemistry*

KUDO, Koji [A class; 100 (B), 50 (C)] ()
— *Topological phases in quantum Hall superconductor hybrids*

KUSANO, Akane [A class; 100 (B), 50 (C)] ()
— *Theoretical study on the structure and stability of new carbon allotropes*
— *Fundamental Materials Informatics Research on Binary Systems of Materials*

MIWA, Kazutoshi [A class; 100 (B), 50 (C)] ()
— *Theoretical prediction of thermal conductivity of hydrogen storage materials*

MURAMATSU, Mayu [A class; 100 (B), 50 (C)] ()
— *Development of a MD-FEM Coupling Analysis Method*

MURAOKA, Azusa [A class; 100 (B), 50 (C)] ()
— *Theoretical Study on Defect Structure of Sn/Ge Double Perovskite Solar Cells Using First-Principles Calculations*

ODA, Masato [A class; 100 (B), 50 (C)] (410)
— *Vibrational mode analysis of GaN crystals containing a large size of defects*

OSADA, Wataru [A class; 100 (B), 50 (C)] ()
— *The surface electronic state and adsorption property of the Be-Cu alloy*

SATO, Takeshi [A class; 100 (B), 50 (C)] (332, 418)
— *A molecular simulation study for dynamics of polyelectrolyte solutions*

SATO, Yusuke [A class; 100 (B), 50 (C)] ()
— *Development of the analysis programs for investigating the photoemission angular distribution*

SUMIYA, Yosuke [A class; 100 (B), 50 (C)] (422)
— *Elucidation of adhesion mechanism based on first principle calculations*

TADA, Yasuhiro [A class; 100 (B), 50 (C)] ()
— *Study of spin liquids under external fields*

TATSUMI, Toshinobu [A class; 100 (B), 50 (C)] ()
— *Theoretical study on molecular adsorption on metal catalyst surface*

UMEBAYASHI, Yasuhiro [A class; 100 (B), 50 (C)] ()
— *All-atom molecular dynamics simulation of the interaction between the cathode and the lithium metal anode and electrolytes for lithium sulfur batteries*

WANG, Jinxin [A class; 100 (B), 50 (C)] ()
— *Development of an MP-PIC-based solver for 3D circulating fluidized bed full-loop analyses*

YING, Chen [A class; 100 (B), 50 (C)] ()
— *Exploring new materials with noval properties using first-principles approaches combing machine learning*

YUHARA, Junji [A class; 100 (B), 50 (C)] (172, 432)
— *Structural analysis of oxide quasicrystal thin films*

□ SCCMS Projects

FUKUSHIMA, Tetsuya [2000 (B), 200 (C)] (371)
— *High-throughput calculations for magnetic materials with configurational and structural disorders*

1. Optimizing the composition of (Ce,La)(Co,Fe)5 for permanent magnet applications using density functional theory
   H. Okumura, T. Fukushima, T. Fukazawa, T. Miyake, H. Akai, and M. Ogura Journal of Physics: Condensed Matter **37**, 015802 (2024).
   DOI:10.1088/1361-648X/ad80f0

MATUBAYASI, Nobuyuki [2000 (B), 200 (C)] (373)
— *All-atom model calculations of the solubility of artificial polypeptides in solvents and factors important for their dissolution*

1. Solvent-Environment Dependence of the Excess Chemical Potential and Its Computation Scheme Formulated through Error Minimization
   Stefan Herv-Hansen, Kazuya Okita, Kento Kasahara, and Nobuyuki Matubayasi J. Chem. Theory Comput. **21**, 1064-1077 (2025).
   DOI:10.1021/acs.jctc.4c01000

2. Development of a force field for ATP how charge scaling controls self-association
   Tuan Minh Do, Nobuyuki Matubayasi, and Dominik Horinek Phys. Chem. Chem. Phys. **27**, 6325-6333 (2025).
   DOI:10.1039/d4cp04270k

MISAWA, Takahiro [4000 (B), 400 (C)] (368)
— *Estimation of Hamiltonians of quantum magnets using Bayes optimization*

SHIMAZAKI, Tomomi [4000 (B), 100 (C)] (370)
— *Theoretical study on proton behavior in fuel cell material based on first-principles method*Theoretical study on proton transfer in fuel cell material based on first-principles method with nuclear quantum effect

1. A theoretical study of the molecular passivation of p-/n-type defects on tin- and germanium-mixed perovskite surfaces using Lewis base/acid
   Emi Kino, Makito Takagi, Takumi Naito, Masanori Tachikawa, Koichi Yamashita, Tomomi Shimazaki Phys. Chem. Chem. Phys. **27**, 7429 (2025).
   DOI:10.1039/d4cp03817g

2. One-dimensional C60 arrays in noncovalent benzidine networks
   Takatsugu Wakahara, Chika Hirata, Dorra Mahdaoui, Kazuko Fujii, Yoshitaka Matsushita, Osamu Ito, Makito Takagi, Tomomi Shimazaki, Masanori Tachikawa, Shinjiro Yagyu, Yubin Liu, Yoshiyuki Nakajima, Takuro Nagai, Kazuhito Tsukagoshi Carbon **233**, 119838 (2025).
   DOI:10.1016/j.carbon.2024.119838

3. Theoretical study of short-range exchange interaction based on semiconductor dielectric function model toward time-dependent dielectric density functional theory
   Tomomi Shimazaki, Masanori Tachikawa J. Chem. Phys. **829**, 140744 (2024).
   DOI:10.1039/d4cp04656k

4. Theoretical and machine learning models for reaction-barrier predictions: acrylate and methacrylate radical reactions
   Makito Takagi, Tomomi Shimazaki, Osamu Kobayashi, Takayoshi Ishimoto, Masanori Tachikawa

Phys. Chem. Chem. Phys **27**, 1777 (2024).
DOI:10.1021/acs.jpcc.4c01525

5. Theoretical Study on Rate-Determining Reactions for Constructing Self-Assembling Molecular Cages Controlled by Distorted Ditopic Ligands
Yu Ichinose, Osamu Kobayashi, Tomomi Shimazaki, Shuichi Hiraoka, Masanori Tachikawa J. Phys. Chem. C **128**, 10643 (2024).
DOI:10.1021/acs.jpcc.4c01525

TADANO, Terumasa [2000 (B), 200 (C)] (375)
— *Development of functional Heusler alloys by first-principles calculations and data-driven approaches*

Data Repository
DXMag Heusler database
https://www.nims.go.jp/group/spintheory/database/