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), 70 (C)] (195)

— *Reexamination of the electron renormalization in conventional superconducting theory*

1. Uniform electron benchmark for the first-principles GW0-Eliashberg theory
   R. Akashi, and H. Shinaoka Phys. Rev. B **113**, 014507 (2026).
   DOI:10.1103/fkvr-t2n8

2. Electronic Structure Theory of H3S: Plane-Wave-Like Valence States, Density-of-States Peak and Its Guaranteed Proximity to the Fermi Level
   R. Akashi Annalen der Physik **538**, e00003 (2026).
   DOI:10.1002/andp.202600003

AKIBA, Takaki [BC class; 2850 (B), 400 (C)] (315)

— *Development of reactive system for interactions of gas phase kinetics and solid surface*

— *Transformation technology of non-linear dynamics to Hamiltonian system*

1. GPU Benchmark through QPE Emulator with cuQuantum for Practical Quantum Applications
   Takaki Akiba and Youhi Morii arXiv:2507.17175 (2025).
   DOI:10.48550/arXiv.2507.17175

ANDO, Yasunobu [B class; 400 (B), 70 (C)] ()

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

AOYAMA, Kazushi [B class; 250 (B), 70 (C)] ()

— *Ordering of localized spins in a charge-density-wave (CDW) state*

ARAI, Munehito [C class; 7800 (B), 450 (C)] (270)

— *Accurate prediction of protein dynamics by statistical mechanical models*

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

ARAKI, Takeaki [BC class; 2650 (B), 330 (C)] (320, 321)

— *Stress propagation in colloidal gels*

— *The physical picture of Johari-Goldstein relaxation in metallic glasses*

1. Mechanical properties and cooperative motion of aerogels under isotropic expansion

K. Hirata and T. Araki Soft Matter (submitted)

2. Topological-Defect-Mediated Glass-Like Viscoelasticity in a Quasi-Two-Dimensional Crystal
Ryoga Moroboshi, Masashi Kobayashi, Tetsuya Abe, Nobumoto Nagasawa, Yoshitaka Yoda, Yusuke Wakabayashi, Takeaki Araki, Makina Saito Communications Physics (submitted)

3. Hydrodynamics substantially affects induced structure formation in magnetic fluids
Henning Reinken, Markus Heiber, Takeaki Araki and Andreas M. Menzel Physical Review Letters (submitted)

ASANO, Yuta [E class; 14500 (B), 1500 (C)] (260)
— *Molecular dynamics simulation of bubble-ring cavitation*
— *Molecular dynamics simulations of cavitation erosion in hydrodynamic lubrication*
1. 100-Billion-Atom Molecular Dynamics Simulation of Acoustic Cavitation in a Simple Liquid
Y. Asano J. Phys. Soc. Jpn., in press.

BAE, Soungmin [C class; 5000 (B), 400 (C)] (72)
— *First-Principles Design of Chemical Doping of Two-Dimensional Transition Metal Dichalcogenides*

BIN, Xu [C class; 6000 (B), 650 (C)] (273)
— *Machine-Learning-Assisted Thermal Transport Analysis in Twisted van der Waals Interfaces*
— *Numerical evaluation of the effect of twist angle on phonon hydrodynamics in twisted 2D materials*

COSTA-AMARAL, Rafael [C class; 2200 (B), 250 (C)] (122)
— *Investigating the role of oxidation in amorphous TeO2 properties from first principles*
1. Oxygen-deficiency-driven phase segregation enables enhanced hole transport in amorphous tellurium oxides
R. Costa-Amaral and Y. Kumagai submitted to Chemistry of Materials; arXiv:2510.00473.

EGAMI, Yoshiyuki [C class; 6800 (B), 0 (C)] (64)
— *First-principles study of molecular adsorption properties on low-dimensional material surfaces and their electronic properties*
— *First-principles study on the control of valley transport properties in two-dimensional honeycomb structured materials*
1. Wide regime of Efros-Shklovskii variable-range-hopping in $La_{1-x}Ce_xNiO_2$
M. Kouda, K. Osame, S. Koura, H. Nobukane, S. Shimoda, K. Takahama, Y. Egami, and M. Sakoda Journal of Physics: Condensed Matter, resubmitted.

FUCHIZAKI, Kazuhiro [C class; 1600 (B), 0 (C)] (336)
— *Kinetics of phase transition and polyamorphism*

FUJI, Yohei [B class; 450 (B), 0 (C)] (357)
— *Symmetry and universality in measurement-induced phase transitions*

FUJII, Susumu [C class; 3000 (B), 400 (C)] (311)
— *Effect of PbTe grain boundary structures on thermoelectric properties*
1. Proton Conduction Mechanisms in Spinel Compounds: A First-Principles Study of Structural and Elemental Effects
S. Yoshida, S. Fujii, M. Yoshiya J. Phys. Chem. C, 129, 17, 8030-8037 (2025).
DOI:10.1021/acs.jpcc.5c01341

2. Lattice Dynamics and Ionic Transport in Antiperovskites M3XCh (M = Li, Na; X = H, F; Ch = S, Se, Te): A First-Principles Study Incorporating Anharmonicity and Vacancy Effects
Y. Kim, S. Fujii, W. Sekimoto, C. Kim, T. Tran, M. Yoshiya, H. Kageyama J. Phys. Chem. C, 129, 20, 9282-9290 (2025).
DOI:10.1021/acs.jpcc.5c01371

3. Origin of reduced thermal conduction by native point defects in PbTe: Perturbed molecular dynamics with neural network potential
T. Yokoi, S. Fujii, Y. Ogura, K. Matsunaga Phys. Rev. B, 112, 2, 024111 (2025).
DOI:10.1103/1175-sd2m

4. Nanoscale thermal transport at PbTe grain boundaries: a neural-network-potential molecular dynamics study
S. Fujii, T. Yokoi, K. Matsunaga J. Mater. Chem. A, published online (2026).
DOI:10.1039/D5TA09725H

FUJIMOTO, Yoshitaka [C class; 1000 (B), 0 (C)] (166)
— *Study on electronic devices using doped carbon nanotubes*
— *Theoretical study on electronic devices using nitrogen-doped carbon nanotubes*

1. Theoretical study on detection of harmful molecules for designing carbon-nanotube-based sensors
Y. Fujimoto Chemical Physics **601**, 112933 (2026).

2. Enhanced Hydrogen Release from Hydrogen Boride Nanosheets via Carbon Doping
R. Kawamura, R. Kawamura, A. Varadwaj, K. Kisu, R. Tanaka, A. Yamamoto, R. Ishibiki, S. Ito, T. Fujita, T. Tokunaga, O. Oki, Y. Fujimoto et al. Small Structures, e202500578 (2025).

FUJINO, Tomoko [C class; 2800 (B), 350 (C)] (316)
— *Investigation of Unique Charge Density Gradient Variations in Electron Correlation-Controlled Oligomer Conductors*

1. Distinct Hole and Electron Transport Anisotropy in Ambipolar Nickel Dithiolene-based Semiconductor
M. Ito, T. Fujino, T. Higashino, M. Hishida, H. Mori Angew. Chem. Int. Ed. **64**, e202512609 (2025).
DOI:10.1002/anie.202512609

FUJISAKI, Takaya [C class; 4400 (B), 450 (C)] (214)
— *Design of hetero-doped CeO2 catalysts for high efficiency fuel cells with direct biogas supply*

FUJISHIRO, Hiroki [C class; 3800 (B), 0 (C)] ()
— *Strained Band-Structure Engineering for Antimonide-Based Terahertz Transistors and Diodes*

FUJITA, Takatoshi [C class; 1400 (B), 0 (C)] (148)
— *Exciton Properties of Functional Supramolecules Using First-Principles Calculations*

1. Exciton dissociation pathways in donor/acceptor blends studied by the wave packet dynamics approach
T. Fujita, M. Nozaki Phys. Chem. Chem. Phys. **38**, 20765 (2025).
DOI:10.1002/adom.202503396

2. Dipole-Driven Polymorphism in Azobenzene: A Supramolecular Strategy for Photoresponsive Microresonators
M. Yamauchi, E. Machida, M. Nozaki, T. Fujita, H. Sotome, K. Yamamoto, Y. Mizuhata, N. Aratani, H. Yamada, S. Masuo Adv. Opt. Mater. **14**, e03396 (2026).

DOI:10.1039/D5CP01637A

FUKUDA, Jun-Ichi [B class; 750 (B), 150 (C)] ()
— *Calculation of ordered structures, dynamics and optical properties of soft materials*

FUKUDA, Masahiro [B class; 400 (B), 70 (C)] (194)
— *Analysis of electronic chirality density in material surfaces*

1. Regional chemical potential analysis for material surfaces
M. Fukuda, M. Senami, Y. Sugimoto, and T. Ozaki J. Chem. Phys. **164**, 084123 (2026).
DOI:10.1063/5.0288934

Data Repository
Regional Chemical Potential Analysis for Material Surfaces
https://isspns-gitlab.issp.u-tokyo.ac.jp/masahiro.fukuda/RCP_Analysis_for_Material_Surfaces
DOI:10.1063/5.0288934

FUKUDA, Tuneo [B class; 400 (B), 0 (C)] (200)
— *First-principles study of thin Ag films formed on Ni(110) surfaces*

1. Initial stage of silver overlayer formation on the Ni(110) surface
A. Mizuhara, T. Fukuda, and K. Umezawa Surf. Sci. 761, 122807 (2025).
DOI:10.1016/j.susc.2025.122807

2. First-principles study of Ag stripe formation on the Ni(110) surface
Aoi Mizuhara, DaeGwi Kim, and Tsuneo Fukuda e-J. Surf. Sci. Nanotechnol. 24, 13 (2026).
DOI:10.1380/ejssnt.2026-003

FUKUI, Ken-Ichi [C class; 1800 (B), 100 (C)] (341)
— *Analyses on the dynamics of metal ion solutes in ionic liquid based electrolyte at the interfaces*

FUKUMOTO, Yoshiyuki [B class; 400 (B), 20 (C)] (360, 361)
— *Numerical study of magnon crystal states in a spin-1/2 distorted kagome antiferromagnet*
— *Numerical study of the dynamical structure factor on the triangular-lattice Heisenberg antiferromagnet*

1. Numerical Calculation of the Quantum Phase Transition due to the DzyaloshinskiiMoriya Interaction in the Kagome Lattice Antiferromagnet Using the Linked-Cluster Expansion Method
Tomoki Kobayashi, and Yoshiyuki Fukumoto: J. Phys. Soc. Jpn. 95, 025003 (2026).

GOHDA, Yoshihiro [C class; 3800 (B), 350 (C)] (92)
— *First-principles electron theory of strain-induced magnetic switching*

1. Orbital magnetic moment controlled converse magnetoelectric eect in bcc-Co3Mn/Fe/V/PMN-PT multiferroic heterostructures
T. Usami, Y. Murakami, R. Watarai , Y. Shiratsuchi, Y. Gohda, and K. Hamaya Adv. Sci. **2026**, e22581 (2026).
DOI:10.1002/advs.202522581

2. Electric Field Modulation of Interlayer Coupling via Piezostrain in a Synthetic Antiferromagnet
Y. Hisada, S. Komori, K. Imura, C. Shen, Y. Gohda, C.C.I. Ang, W.S. Lew, and T. Taniyama Adv. Sci. **13**, e17798 (2026).
DOI:10.1002/advs.202517798

3. Strain-induced magnetocrystalline anisotropy in L21 Co2FeSi: first-principles study
R. Watarai and Y. Gohda npj Spintronics **3**, 50 (2025).
DOI:10.1038/s44306-025-00116-w

4. Tunable Magnetic Coupling of Monolayer CrI2 by Strain Engineering
H. Y. Widyandaru and Y. Gohda npj Spintronics **3**, 34 (2025).
DOI:10.1038/s44306-025-00100-4

5. Efficient first-principles approach to Gibbs free energy with thermal expansion
K. Hashimoto, T. Tanaka, and Y. Gohda Phys. Rev. B **111**, 224309 (2025).
DOI:10.1103/6qsr-xzgb

6. First-Principles Exploration of NdFe Magnetic Compounds Assisted by Transfer Learning and Genetic Algorithm
S. Ito, I. Seo, S. Tanaka, M. Endo, Y. Tsutsui, T. Tanaka, and Y. Gohda J. Phys. Soc. Jpn., in press.

7. Physically Interpretable Force Constants Based on Spherical Tensor Expansion: Ecient Parameter Reduction for Low-Symmetry Systems
D. Ito, K. Hashimoto, T. Tanaka, and Y. Gohda J. Phys. Soc. Jpn., in press.

GOHLKE, Matthias [C class; 2600 (B), 350 (C)] (322)
— *Tensor network study of an effective spin model for square-lattice antiferromagnets*

GONOME, Hiroki [C class; 1600 (B), 250 (C)] (138)
— *Study of the principle of photothermal conversion by ab initio calculations*

HAGITA, Katsumi [C class; 1600 (B), 300 (C)] (332)
— *Physical properties of crosslinked polymer networks through network topology analysis*

1. Butterfly Patterns for Stretched Inhomogeneous Gel Networks Using Large-Scale Molecular Dynamics Simulations
K. Hagita and T. Murashima Macromolecules **58**, 53685376 (2025).
DOI:10.1021/acs.macromol.5c00207

2. Nano-structuring for strengthening semi-crystalline polymers
K. Hagita and T. Murashima NPG Asia Materials **17**, 44 (2025).
DOI:10.1038/s41427-025-00625-4

HAGIWARA, Satoshi [C class; 2000 (B), 0 (C)] (135)
— *Adsorption reactions at the solid electrode/aqueous solution interfaces*

1. Anion Adsorption-induced Charge Separation at the Alumina/Aluminum Interface
S. Hagiwara, T. Murata, and M. Otani Corrosion Sci. **256**, 113150 (2025).
DOI:10.1016/j.corsci.2025.113150

2. An Efficient Implementation of the ESM-RISM Method for Simulating Electrode/Electrolyte Interfaces
S. Hagiwara, and M. Otani J. Chem. Theory Comput. **22**, 3633 (2026).
DOI:10.1021/acs.jctc.5c01920

HALIM, Harry Handoko [C class; 2000 (B), 250 (C)] (127)
— *Machine Learning Accelerated Path Sampling for Exploration of Rate and Mechanisms of Rare Events on Heterogenous Catalysis*

1. Bridging the Pressure Gap in Hydrogenation of CO_2 to Formate on Cu(100) by Machine Learning Molecular Dynamics and First-Principles Microkinetic Modeling
W. O. N. F. Rajaelo, H. H. Halim, M. F. Anshor, Y. Yamada, S. Ramadhani, F. A. Mubarok, S.

E. M. Putra, A. L. Ivansyah, T. D. K. Wungu, Suprijadi, Y. Morikawa, and F. Muttaqien ACS Catalysis **16**, 5068–5079 (2026).
DOI:10.1021/acscatal.5c09279

2. CO Coadsorption Effects on Water–Gas Shift Reaction over Cu Clusters on Cu(111): Insights from Machine Learning Force Field and Microkinetic Modeling
M. F. Anshor, H. H. Halim, and Y. Morikawa Phys. Chem. Chem. Phys. (2026), in press.
DOI:10.1039/D5CP05031F

HAMADA, Ikutaro [C class; 9600 (B), 850 (C)] (48)

— *Density functional theory study of adsorption and reaction of molecules on solid surfaces*

1. Interlayer Hydrogen–Hydrogen Spacing Regulates the Formation of Molecular Hydrogen from Hydrogen Boride Nanosheets
Y. Yasuda, O. Ok, K. Goto, N. Noguchi, S. Ito, M. Hikichi, R. Tsuji, Y. Nakahira, R. Utsumi, H. Saitoh, S. Nakano, S. Naka, I. Hamada, S. Orimo, and T. Kondo ACS Nano **20**, 9951 (2026).
DOI:10.1021/acsnano.5c20691

2. Interlayer Hydrogen–Hydrogen Spacing Regulates the Formation of Molecular Hydrogen from Hydrogen Boride Nanosheets
Y. Yasuda, O. Ok, K. Goto, N. Noguchi, S. Ito, M. Hikichi, R. Tsuji, Y. Nakahira, R. Utsumi, H. Saitoh, S. Nakano, S. Naka, I. Hamada, S. Orimo, and T. Kondo ACS Nano **20**, 9951 (2026).
DOI:10.1021/acsnano.5c20691

3. Predicting Reactive Graphene Edge-Adsorbed Pt Single-Atom Catalyst Structures for Oxygen Reduction via Machine Learning-Enhanced Calculations
B. A. C. Tan, N. A. Sofi, T. N. Pham, K. I. M. Rojas, S. E. P. Masan, Y. Hamamoto, I. Hamada, and Y. Morikawa Philos. Trans. R. Soc. A **384**, 20240555 (2026).
DOI:10.1098/rsta.2024.0555

4. Assessing the Accuracy of Exchange–Correlation Functionals in Density Functional Theory for Hydrogen–Benzene and Hydrogen–Hydrogen Interactions
Y. Kataoka and I. Hamada Phys. Rev. B **113**, 085143 (2026).
DOI:10.1103/PhysRevB.113.085143

5. Electronic States of Ag and Au Atoms on Graphene/Rh(111)
H. Okuyama, H. Ogawa, K. Kusumoto, S. Hatta, K. Hirashima, and I. Hamada J. Phys. Chem. C **129**, 19396 (2025).
DOI:10.1021/acs.jpcc.5c05109

6. Density Functional Theory Study on the Structure and Hydrogen Storage Performance of Hydrogen Boride Sheet
S. Naka, K. I. M. Rojas, and I. Hamada e-J. Surf. Sci. Nanotechnol. **23**, 339 (2025).
DOI:10.1380/ejssnt.2025-048

7. Submolecular-Resolution Probing of Vibrational Anharmonicity Using Tip-Enhanced Raman Spectroscopy
Y. Park, I. Hamada, M. Wolf, and A. Shiotari Angew. Chem. Int. Ed. e202514215 (2025).
DOI:10.1002/anie.202514215

8. Vibrational Recognition of Local Structures in Hydrogen Boride Sheets
K. I. M. Rojas, L. T. Ta, S. Naka, Y. Morikawa, and I. Hamada J. Chem. Phys. **163**, 124702 (2025).
DOI:10.1063/5.0280856

HAMAGUCHI, Satoshi [C class; 6600 (B), 700 (C)] (272)
— *Development of machine-learning force fields to analyze atomic layer processing II*
— *Development of machine-learning force fields to analyze atomic layer processing*

HAMAMOTO, Yuji [CD class; 2600 (B), 0 (C)] (120, 121)
— *First principles study of germanene superstructures on Ag(111)*
— *Structure search for planar silicene on Au(111) thin films based on Gaussian regression*
— *Band structure calculation of germanene superstructures on Ag(111)*

HAN, Jihae [AB class; 500 (B), 130 (C)] (187)
— *First-principles investigation of reaction mechanisms at the electrode/electrolyte interface in Li-S batteries*
— *Reductive decomposition mechanism of electrolyte at electrode/electrolyte interface by first-principles calculations*

HARADA, Kenji [C class; 1800 (B), 300 (C)] (329)
— *Development of tensor network algorithms*
1. Plastic tensor networks for interpretable generative modeling
   Katsuya O Akamatsu, Kenji Harada, Tsuyoshi Okubo, Naoki Kawashima Machine Learning: Science and Technology **7**, (2026) 015014.
   DOI:10.1088/2632-2153/ae3048

HARASHIMA, Yosuke [C class; 1800 (B), 0 (C)] (141)
— *Prediction of materials properties and exploration of materials 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, 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 Phys. Rev. Materials **9**, 093803 (2025).
   DOI:10.1103/8tjv-wtx5

3. Materials Dual-Source Knowledge Retrieval-Augmented Generation for Local Large Language Models in Photocatalysts
   W. Takahara, Y. Yamaguchi, M. Ogano, F. Kakami, Y. Harashima, T. Takayama, S. Takasuka, A. Kudo, and M. Fujii J. Chem. Inf. Model. **65**, 13098 (2025).
   DOI:10.1021/acs.jcim.5c01941

HARIKI, Atsushi [B class; 1100 (B), 0 (C)] (243, 244)
— *Computational Study of Magnetic Circular Dichroism in Resonant Inelastic X-ray Scattering Spectra of Strongly Correlated Materials*
— *Computational study on two-particle responses in correlated altermagnets using DFT+DMFT method*
1. Circular Dichroism in Resonant Inelastic X-Ray Scattering: Probing Altermagnetic Domains in MnTe
   D Takegami, Takuya Aoyama, T Okauchi, T Yamaguchi, S Tippireddy, S Agrestini, M Garca-Fernndez, T Mizokawa, K Ohgushi, Ke-Jin Zhou, J Chaloupka, J Kune, A Hariki, Hakuto Suzuki Phys. Rev. Lett. **135**, 196502 (2025).
   DOI:10.1103/512v-n5f9

2. Fingerprints of Mott and Slater gaps in the core-level photoemission spectra of antiferromagnetic iridates
K Nakagawa, A Hariki, T Okauchi, H Fujiwara, K-H Ahn, Y Murakami, S Hamamoto, Y Kanai-Nakata, T Kadono, A Higashiya, K Tamasaku, M Yabashi, T Ishikawa, A Sekiyama, S Imada, J Kune, K Takase, A Yamasaki Phys. Rev. B **111**, 195114 (2025).
DOI:10.1103/PhysRevB.111.195114

3. Theory of circular dichroism in resonant inelastic x-ray scattering
M. Furo, A. Hariki, J. Kunes Phys. Rev. B **112**, 214429 (2025).
DOI:10.1103/x96x-znr8

4. UTe2: A narrow-band superconductor
Martin Sundermann, Takaki Okauchi, Naoki Ito, Denise S Christovam, Andrea Marino, Daisuke Takegami, Andrei Gloskovskii, Priscila FS Rosa, Jan Kune, Shin-ichi Fujimori, Liu Hao Tjeng, Andrea Severing, Atsushi Hariki Phys. Rev. Research **7**, 043195 (2025).
DOI:10.1103/t6hm-q647

HARUYAMA, Jun [C class; 3600 (B), 400 (C)] (93)
— *Electrochemical reaction analysis using density functional calculation + implicit solvation model 7*

1. Benchmarking of Oxygen Adsorption Using TPD Spectroscopy for Accurate DFT Prediction of ORR on Anatase Titanium Dioxide(101)
S. Muhammady, J. Haruyama, S. Kasamatsu, and O. Sugino J. Phys. Chem. C **129**, 20079 (2025).
DOI:10.1021/acs.jpcc.5c04600

2. Elucidation of superionic conduction in K2NiF4-type BaLi oxyhydrides from a first-principles molecular dynamics study
J. Haruyama, F. Takeiri, G. Kobayashi, and O. Sugino J. Mater. Chem. A **14**, 8332 (2026).
DOI:10.1039/d5ta08063k

Data Repository
BLHO_DFT-MD
https://isspns-gitlab.issp.u-tokyo.ac.jp/j-haruyama/BLHO_DFT-MD
DOI:10.1039/d5ta08063k

HAYAMI, Satoru [C class; 3600 (B), 350 (C)] (301)
— *Generation of spin model with higher-order spin interactions based on machine learning*

1. Square skyrmion lattice in multi-orbital f -electron systems
Y. Zha and S. Hayami Physical Review B **111**, 165155 (2025).
DOI:10.1103/PhysRevB.111.165155

2. Bimeron Crystals by a Linearly Polarized AC Electric Field in Frustrated Magnets
T. Shirato, R. Yambe, and S. Hayami J. Phys. Soc. Jpn. **94**, 063601 (2025).
DOI:10.7566/JPSJ.94.063601

3. Finite-q antiferrotoroidal and ferritoroidal order in a distorted kagome structure
A. Kirikoshi and S. Hayami Physical Review B **111**, L201112 (2025).
DOI:10.1103/PhysRevB.111.L201112

4. Symmetry Rules on Multipole Interactions under Crystallographic Point Groups and Application to Multiple-Q Multipole States
R. Yambe and S. Hayami J. Phys. Soc. Jpn. **94**, 074704 (2025).
DOI:10.7566/JPSJ.94.074704

5. Multiple-Q spin textures induced by spiralstaggered interference in one-dimensional itinerant magnets
S. Hayami and K. Okigami J. Phys. Soc. Jpn. **95**, 034706 (2026).
DOI:10.7566/JPSJ.95.034706

6. Four-spin interactions as a route to multiple-Q topological magnetic order
K. Okigami and S. Hayami Phys. Rev. B **113**, 064442 (2025).
DOI:10.1103/3njw-f1jt

7. Finite-Temperature Stability of Skyrmion Crystals in Frustrated Magnets: Role of Sixfold Anisotropy and Uniform Spin Mode in Momentum Space
K. Okigami and S. Hayami J. Phys. Soc. Jpn. **95**, 044702 (2026).
DOI:10.7566/JPSJ.95.044702

HIDA, Kazuo [B class; 300 (B), 60 (C)] (369)
— *Numerical Study of One Dimensional Frustrated Quantum Spin Systems*

1. Ground-State Phase Diagram of (1/2,1/2,1) Mixed Diamond Chains with Single-Site Anisotropy
Kazuo Hida to be published in J. Phys. Soc. Jpn.; arXiv:2601.20328
DOI:10.48550/arXiv.2601.20328

HIGUCHI, Yuji [C class; 9200 (B), 850 (C)] (32)
— *Deformation Process of Crystalline Polymer and Filler*
— *Interfacial Delamination between Crystalline Polymer and Filler*

1. Influences of secondary and tertiary amines in epoxy resins on water dynamics by all-atomic molecular dynamics simulations
Yuji Higuchi, Yasuyuki Nakamura, Masanobu Naito, and Yoshihisa Fujii Chem. Phys. **597**, 112766 (2025).
DOI:10.1016/j.chemphys.2025.1

2. Interfacial delamination between semicrystalline polymers and filler materials by coarse-grained molecular dynamics simulations
Yuji Higuchi, Yuta Hikima, Naoto Kamiuchi, Erica Uehara, Yutaka Oya, Go Yamamoto, and Keita Sakakibara Polymer **333**, 128539 (2025).
DOI:10.1016/j.polymer.2025.128

3. Effect of zwitterionic monomer polymerization on water dynamics: a molecular dynamics simulation study supported by differential scanning calorimetry and terahertz spectroscopy
Md Abu Saleh, Yuji Higuchi, Shohei Shiomoto, Takahisa Anada, Mafumi Hishida, and Masaru Tanaka Polym. J. **57**, 1127 (2025).
DOI:10.1038/s41428-025-01066-0

4. Ion distribution in the vicinity of phase-separated membrane
Yuji Higuchi, Hiroaki Ito, Naofumi Shimokawa, Jurij Reščič, Stefano Maset, Klemen Bohinc J. Mol. Liq. **444**, 129168 (2025).
DOI:10.1016/j.molliq.2025.1291

HIRAMATSU, Ryoya [C class; 4600 (B), 0 (C)] (79)
— *Ab Initio Study of Finite-Temperature Magnetic Properties in Transition Metal Systems*

1. First-Principles Calculations of Magnetization Curves and Spin Susceptibility in the High-Anisotropy Alloy $L1_0$-FePt
R. Hiramatsu, A. Sakuma, T. Miyake, and T. Fukushima submitted to Phys. Rev. B.

HIYAMA, Miyabi [B class; 350 (B), 0 (C)] (372)
— *Theoretical study for excited states of firefly bioluminescence emitters*

1. Absorption and fluorescence properties and assignments of firefly bioluminescence substrate analog: seMpai
   M. Harada, T. Nakano, R. Ono, T. Uchiyama, Y. Noguchi, R. Saito-Moriya, N. Kitada, S. A. Maki, T. Hirano, H.i Aoyama, M. Kobayashi, H. Akiyama, K. Kanno, H. Itabashi, and M. Hiyama Photochem. Photobiol. **102**, 237-247 (2026).
   DOI:10.1111/php.14121

HO, Ngoc Nam [C class; 1200 (B), 250 (C)] ()
— *Computational design of high-entropy alloy catalysts for direct methanol fuel cells*

HOSHI, Takeo [C class; 3200 (B), 300 (C)] (102)
— *HPC-based fusion of simulation, experiment analysis and datadriven science*

1. Monte Carlo simulation method for incoherent Thomson scattering spectra from arbitrary electron distribution functions
   Kentaro Sakai, Kentaro Tomita, Takeo Hoshi, Ryo Yasuhara Journal of Instrumentation 21, C01002 (2025).
   DOI:10.1088/1748-0221/21/01/c01002

Data Repository
2DMAT Gallery
https://isspns-gitlab.issp.u-tokyo.ac.jp/2dmat-dev/2dmat-gallery

ODAT-SE Gallery
https://isspns-gitlab.issp.utokyo.ac.jp/takeohoshi/odat-se-gallery

HOSHINO, Shintaro [B class; 450 (B), 80 (C)] (179)
— *First principles calculation for electron chirality*

HOTTA, Chisa [C class; 1400 (B), 0 (C)] (338)
— *Disorder and glassy dynamics of strongly correlated multi-orbital electric systems*
— *Effect of quenched disorder in the triangular lattice Heisenberg magnet*

1. Specific heat and susceptibility of S=1/2 antiferromagnets on square, triangular, and kagome lattices
   C. Hotta Zeitschrift für Naturforschung A ,in press (arXiv:2605.17420).
   DOI:10.1515/ZNA-2025-0392

HOTTA, Takashi [C class; 1800 (B), 0 (C)] (333)
— *Research of superconductivity induced by multipole fluctuations in the bi-layer orbital degenerate Hubbard model*

1. Effect of Γ_7 and Γ_8 Hybridizations on Three-Channel Kondo Phase Emerging from Ho Ions
   T. Hotta J. Phys. Soc. Jpn. **94**, 114702 (2025).
   DOI:10.7566/JPSJ.94.114702

HUKUSHIMA, Koji [C class; 4000 (B), 0 (C)] (300)
— *Development of Tensor-Network-based Monte Carlo Methods*

1. High-dimensional asymptotics of VAEs: threshold of posterior collapse and dataset-size dependence of rate-distortion curve

Yuma Ichikawa, and Koji Hukushima J. Stat. Mech. 073402 (2025).
DOI:10.1088/1742-5468/adde3e

2. Ratio divergence learning using target energy in restricted Boltzmann machines: Beyond Kullback-Leibler divergence learning
Yuichi Ishida, Yuma Ichikawa, Aki Dote, Toshiyuki Miyazawa, and Koji Hukushima Phys. Rev. E 112, 045306 (2025).
DOI:10.1103/fxnm-y5pd

IDO, Kota [E class; 6000 (B), 600 (C)] (23)
— *Stability of many-body topological states in strongly correlated quantum systems*

IIMURA, Soshi [D class; 7000 (B), 500 (C)] (63)
— *Hydrogen Ion Doping on Solid Acid and Base Sites and the Exploration of New Functions*

IITAKA, Toshiaki [C class; 1800 (B), 250 (C)] (330)
— *Calculation of quantum spin systems at finite temperature using random quantum states of Plaquette variational wave functions*

IKEDA, Hiroaki [B class; 450 (B), 90 (C)] ()
— *Electron chirality and spin current in chiral materials*

IMADA, Masatoshi [DE class; 35000 (B), 2550 (C)] (217)
— *Development and application of Fermi machine*
— *Development and application of quantum many-body solver*
— *Development of Fermi Machine for Quantum Many-Body Solver*

1. Unified description of cuprate superconductors by fractionalized electrons emerging from integrated analyses of photoemission spectra and quasiparticle interference
Sakai, Shiro and Yamaji, Youhei and Imoto, Fumihiro and Tamegai, Tsuyoshi and Kaminski, Adam and Kondo, Takeshi and Kohsaka, Yuhki and Hanaguri, Tetsuo and Imada, Masatoshi Phys. Rev. X **16** (2026) 011018
DOI:10.1103/mww7-32gn

2. Quantum Many-Body Solver Using Artificial Neural Networks and its Applications to Strongly Correlated Electron Systems
Yusuke Nomura, asatoshi Imada J. Phys. Soc. Jpn., **94** (2025) 031001
DOI:10.7566/JPSJ.94.031001

INAGAKI, Kouji [B class; 300 (B), 60 (C)] (209)
— *Analyses of semiconductor surface processes by machine-learning based potentials*

INAOKA, Takeshi [B class; 400 (B), 70 (C)] (192)
— *Search and realization of novel electronic properties of surfaces and interfaces and of nanostructures*

INAYOSHI, Ken [B class; 350 (B), 0 (C)] (255)
— *Development of computational methods for quantum field theories of nonequilibrium systems utilizing information compression techniques and its applications*

1. A causality-based divide-and-conquer algorithm for nonequilibrium Green's function calculations with quantics tensor trains
Ken Inayoshi, Maksymilian Sroda, Anna Kauch, Philipp Werner, and Hiroshi Shinaoka SciPost Phys.
DOI:10.21468/SciPostPhys.20.3.077

INOUE, Kazutoshi [C class; 4000 (B), 200 (C)] (90)
— *Exploring stable atomic structures and segregation behavior at ceramics interfaces*
— *Investigation of stable atomic structure in twist grain boundaries and their segregation behavior by theoretical calculations*

1. Structural transition and the effect of Ca impurities in MgO Σ5(210) grain boundary
   Q. Chen, M. Saito, K. Kawahara, A. Nakamura, K. Inoue, Y. Ikuhara J. Euro. Ceram. Soc. **46**, 118068 (2026)
   DOI:10.1016/j.jeurceramsoc.2025.118068

ISHIBASHI, Shoji [C class; 2200 (B), 0 (C)] (131)
— *Prediction of properties of organic ferroelectrics and piezoelectrics by first-principles calculations*

1. Field-Effect Crystal Engineering in Proton-π-Electron Correlated Systems
   S. Horiuchi, H. Minemawari, J. Tsutsumi, and S. Ishibashi Crystals **15**, 736 (2025).
   DOI:10.3390/cryst15080736

ISHIDA, Kunio [B class; 300 (B), 60 (C)] (367)
— *Coherent dynamics of strongly coupled electron-phonon-photon systems*

1. Phonon-mediated Chirality Control in Molecular Triangles by Photoirradiation
   Noriyuki Aoyagi, Hiroaki Matsueda, and Kunio Ishida Journal of the Physical Society of Japan 95, 014702 (2026).
   DOI:10.7566/JPSJ.95.014702

ISHII, Fumiyuki [C class; 8400 (B), 800 (C)] (52)
— *Development and Application of First-Principles Methods for Spin Conversion Materials*
— *Development and application of first-principles computational methods for real-space analysis of transport coefficients*

1. First-principles study of interface states in diamond(111)/Al2O3 with different terminations
   Y. Zhang, N. Yamaguchi, X. Zhang, M. Saito, N. Tokuda, and F. Ishii Surfaces and Interfaces **72**, 107147 (2025).
   DOI:10.1016/j.surfin.2025.107147

2. First-principles study of electric-dipole-induced Rashba spin-splitting in Janus WSSe
   S. A. Putri, M. A. U. Absor, N. Yamaguchi, and F. Ishii Japanese Journal of Applied Physics **64**, 10SP21 (2025).
   DOI:10.35848/1347-4065/ae00cf

3. Direct determination of layer anomalous Hall conductivity using uniaxial Wannier functions
   Y. Morishima, F. Ishii, and N. Yamaguchi arXiv:2506.01160 (2025).

4. Real-Space Imaging and Topological Indices of Finite Skyrmion Systems
   J. Yang, N. Yamaguchi, and F. Ishii submitted.

5. Capacitance profile of graphene via effective screening medium method: first-principles study
   A. Sohib, N. Yamaguchi, and F. Ishii Japanese Journal of Applied Physics **64**, 11SP11 (2025).
   DOI:10.35848/1347-4065/ae0cd3

6. First-principles study of thickness-dependent vertical polarization in multilayer hexagonal boron nitride
   N. M. Chadiza, H. P. Kadarisman, N. Yamaguchi, and F. Ishii Japanese Journal of Applied Physics **64**, 11SP09 (2025).
   DOI:10.35848/1347-4065/ae0e2b

7. The effect of interlayer coupling on thermoelectricity in atomically thin CaGe2: a first-principles study
A. A. Ghiffari, R. Syariati, Y. Morishima, N. Yamaguchi, and F. Ishii Japanese Journal of Applied Physics **64**, 11SP31 (2025).
DOI:10.35848/1347-4065/ae11bf

8. Tunable visible-light shift current in strain-engineered ferroelectric perovskite CsPbI3
Y. Y. S. Teweng, N. Yamaguchi, and F. Ishii Applied Physics Express **18**, 121001 (2025).
DOI:10.35848/1882-0786/ae241f

9. Band Unfolding in Finite Nanostructures: Visualizing Dirac, Spin-Valley, and Rashba Features
N. Yamaguchi, S. Yunitasari, W. Amalia, C.-C. Lee, T. Ozaki, and F. Ishii Nano Letters **25**, 17725–17732 (2025).
DOI:10.1021/acs.nanolett.5c04721

10. First-principles calculations of the effect of X-site halogen composition ratio on the stability of vacuum deposited CsPbIxBr3-x-based perovskite films
S. Miura, N. Yamaguchi, Md. Shahiduzzaman, Md. Akhtaruzzaman, M. Nakano, M. Karakawa, J. M. Nunzi, F. Ishii, and T. Taima Japanese Journal of Applied Physics **65**, 04SP02 (2026).
DOI:10.35848/1347-4065/ae37b5

11. Ab initio prediction of large thermoelectric effect in distorted Heusler alloy Ti-Fe-Sb compound
R. Syariati, A. Vora-ud, F. Ishii, and T. Seetawan Journal of Materials Science **61**, 3909–3918 (2026).
DOI:10.1007/s10853-025-12100-0

12. Fe-doping enhances the thermoelectric properties of Bi2Te3 thin films within a balance of oxidation states and magnetism
A. T. T. Pham, A. Vora-ud, C. Chananonnawathorn, P. Muthitamongkol, S. Ruamruk, S. Limwichean, M. Horprathum, R. Syariati, S. Park, F. Ishii, T. Seetawan, G. J. Snyder, and T. B. Phan Vacuum **244**, 114879 (2026).
DOI:10.1016/j.vacuum.2025.114879

ISHII, Kohei [B class; 400 (B), 80 (C)] ()
— *First-principles calculation of electronic structure considering electron-2-phonon interactions*

ISHIKAWA, Takahiro [C class; 2000 (B), 200 (C)] (130)
— *Exploration of hydride superconductors*

1. Evolutionary search for superconducting hydrides in the La-Pt-H ternary system under compression
T. Ishikawa, Y. Tanaka, and S. Tsuneyuki Phys. Scr. **101**, 105903 (2026).
DOI:10.1088/1402-4896/ae49c3

ISOBE, Masaharu [B class; 400 (B), 70 (C)] (355)
— *Non-reciprocal neighbor interaction and non-equilibrium phase transition in self-propelled hard polygon systems*

1. Crystallization and Motility-Induced Phase Separation in the Flow of Active Brownian Particles Around an Obstacle
K. Iwase and M. Isobe EPJ Web of Conferences **334** 01004 (2025).
DOI:10.1051/epjconf/202533401004

2. Self-organized spatial inhomogeneity in self-propelled quasi-elastic hard disk systems

D. Mugita, R. Kitagawa, N. Murase, and M. Isobe EPJ Web of Conferences **334** 01005 (2025).
DOI:10.1051/epjconf/202533401005

3. Cooperative phenomena in active matter systems with alternative interaction of neighbors
T. Nakamura, N. Murase, and M. Isobe EPJ Web of Conferences **334** 02001 (2025).
DOI:10.1051/epjconf/202533402001

4. Quantitative analysis of pedestrian counter-flow under congested conditions using floor field model
Y. Nakai and M. Isobe Proceedings of the 31th Symposium on Traffic Flow and Self-driven Particles, **31**, 13 (2025).

IWAZAKI, Ryuta [B class; 400 (B), 80 (C)] (185)
— *Novel quantum phases in organic Mott insulators based on first-principles calculations*

IZUMI, Yasuo [B class; 450 (B), 90 (C)] (176)
— *Theoretical Monitoring of the Behavior of Surface Intermediate Species on Semiconductor-Based Photocatalysts to Realize Highly-Selective CO_2 Photoreduction*

1. Charge Separation and/or Hot Spots: Clarification of Efficient CO2 Reduction over Ru-Ni Nanoparticles Compared to Photocatalysis on Ru- Ni-ZrO2 Composites
Masahito Sasaki, Tomoki Oyumi, Keisuke Hara, Hongwei Zhang, and Yasuo Izumi J. Am. Chem. Soc. 148, 13, 13570 (2026).
DOI:10.1021/jacs.5c17533

JANG, Seonghoon [C class; 2600 (B), 0 (C)] ()
— *Material Design for Mg-ion Cathode Materials with High Ion Conductivity*

JESCHKE, Harald [C class; 2200 (B), 0 (C)] (328)
— *Theoretical study of static and dynamic spin structure factors in 3D antiferromagnets*

1. Field-induced spin liquid in the decorated square-kagome antiferromagnet nabokoite $KCu_7TeO_4(SO_4)_5Cl$
M. G. Gonzalez, Y. Iqbal, J. Reuther, H. O. Jeschke Comm. Mater. **6**, 96 (2025).
DOI:10.1038/s43246-025-00806-2

2. The crystal structure, and magnetic and resonant properties of decorated spin kagome system $(CsCl)Cu_5As_2O_{10}$
I. V. Kornyakov, M. V. Likholetova, I. E. Lezova, S. V. Krivovichev, H. O. Jeschke, Y. Iqbal, A. V. Tkachev, S. V. Zhurenko, A. Gippius, L. V. Shvanskaya, A. Vasiliev J. Mater. Chem. C **14**, 3749 (2026).
DOI:10.1039/D5TC03217B

3. Origin of pressure-induced anomalies in the nodal-line ferrimagnet $Mn_3Si_2Te_6$
V. Venkatasubramanian, M. Shimizu, D. Guterding, H. O. Jeschke Comm. Mater. **7**, 94 (2026).
DOI:10.1038/s43246-026-01132-x

JIA, Xue [C class; 1400 (B), 300 (C)] (143)
— *Discover High-Performance Metal Carbide/Nitride Electrocatalysts Based on Catalysis Theory and Machine Learning*

1. Closed-Loop Framework for Discovering Stable and Low-Cost Bifunctional Metal Oxide Catalysts for Efficient Electrocatalytic Water Splitting in Acid
X. Jia, Z. Zhou, F. Liu, T. Wang, Y. Wang, D. Zhang, H. Liu, Y. Wang, S. Ye, K. Amezawa, L. Wei, and H. Li Journal of the American Chemical Society **147**, 22642 (2025).
DOI:10.1021/jacs.5c04079

JIE, Sun [C class; 2400 (B), 250 (C)] ()
— *Machine Learning for Screening Layered Materials with Ultrallow Thermal Conductivity*

JOSHI, Ashish [B class; 150 (B), 80 (C)] ()
— *Investigation of quantum skyrmions via neural quantum states*

KADARISMAN, Hana [B class; 300 (B), 0 (C)] (211)
— *First-principles study of nanodiamonds*

KAGESHIMA, Hiroyuki [C class; 3000 (B), 350 (C)] (104)
— *Study on physical properties of structural elementary excitations at solid surfaces and interfaces*

1. First-principles Study of Interstitial-Related Defects in Quartz
   H. Kageshima, T. Akiyama, K. Shiraishi J. Phys. Soc. Jpn. 94 (2025) 074707 (4 pages).
   DOI:10.7566/JPSJ.94.074707

2. Atomic Scale Insights into Si Transport Pathway in Si-oxide Film Based on Theoretical Investigation of Medium Density Eects
   H. Kageshima, T. Akiyama, K. Shiraishi e-J. Surf. Sci. Nanotechnol. 23 (2025) 306 (8 pages).
   DOI:10.1380/ejssnt.2025-043

3. First-principles study of excess Si transport in Si oxide on Si substrate using two-layer-oxide model for thermally oxidized interface
   H. Kageshima, I. Seo, T. Akiyama, K. Shiraishi Jpn. J. Appl. Phys. 65 (2026) 03SP18 (10 pages).
   DOI:10.35848/1347-4065/ae3d40

4. First-principles study on network effects of medium on excess Si transport in Si oxide films
   H. Kageshima, I. Seo, T. Akiyama, K. Shiraishi Mater. Sci. Semicond. Process. 209 (2026) 110582 (8 pages).
   DOI:10.7566/JPSJ.94.074707

KAIJU, Hideo [C class; 6000 (B), 650 (C)] (65)
— *Calculation of electronic structures and estimation of interfacial spin polarization in molecular spintronic devices*
— *Electronic structure analysis of molecular spintronic devices using first-principles calculation*

1. Observation of magnetoresistance effect in $Ni_{78}Fe_{22}$/tris-(8-hydroxyquinoline) erbium (Erq_3)/FeCo organic spin valves
   Mizuki Matsuzaka, Ryunosuke Miyamoto, Chika Hashimoto, Mari Taniguchi, Kotaro Kashima, Shun Dekura, Takumi Ueda, Yusuke Nomura, Tomoyuki Akutagawa, Kazuya Ando, Hideo Kaiju
   Journal of Magnetism and Magnetic Materials
   DOI:10.1016/j.jmmm.2025.173465

KANEKO, Ryui [DE class; 12500 (B), 1100 (C)] (223)
— *Variational Monte Carlo Study of the Impact of Multilayer Effects on Antiferromagnetism and Superconductivity*
— *Variational Monte Carlo study of ground states of a multilayer superconductor under pressure*

1. Seeding neural network quantum states with tensor network states
   R. Kaneko and S. Goto Phys. Rev. B **112**, 155163 (2025).
   DOI:10.1103/3rq4-2m5k

2. Adaptive interpolating quantum transform: A quantum-native framework for efficient transform learning
   G. Budiutama, S. Daimon, H. Nishi, R. Kaneko, T. Ohtsuki, and Y.-i. Matsushita Phys. Rev. A

112, 062410 (2025).
DOI:10.1103/vyr3-h9hq

KARIYADO, Toshikaze [B class; 350 (B), 0 (C)] (254)
— *Electronic structure engineering in low dimensional systems with artificial nanostructures*

1. Single-band square-lattice Hubbard model from twisted bilayer C568
T. Kariyado, A. Vishwanath, and Z.-X. Luo Phys. Rev. B **112**, 125159 (2025).
DOI:10.1103/73rf-cw9d

2. Spin States of Trioxotriangulene Controlled by SiO Bond Formation and Dissociation on $AuSi_x$ Surfaces
Z. Yuan, T. Kariyado, T. Murata, K. Sun, D. Li, O. Custance, Y. Morita, S. Kawai Nano Letters **25** 13040-13046 (2025).
DOI:10.1021/acs.nanolett.5c03477

KASAMATSU, Shusuke [C class; 3400 (B), 300 (C)] (100)
— *Thermodynamics of disordered crystalline systems considering phonons and charge ordering*

1. Mitigating proton trapping in cubic perovskite oxides via ScO_6 octahedral networks
Kota Tsujikawa, Junji Hyodo, Susumu Fujii, Kazuki Takahashi, Yuto Tomita, Nai Shi, Yasukazu Murakami, Shusuke Kasamatsu, and Yoshihiro Yamazaki Nature Mater. **24**, 1949 (2025).
DOI:10.1038/s41563-025-02311-w

KATAOKA, Yuta [C class; 2200 (B), 250 (C)] ()
— *Development of analytical method for hydrogen state by ab initio path integral molecular dynamics and machine learning*

KATO, Daiji [C class; 800 (B), 200 (C)] (164)
— *Scaling Up First-Principles Simulations of Plasma-Facing Material Damage Behavior Using Machine Learning*

KATO, Takeo [B class; 400 (B), 70 (C)] (353)
— *Numerical calculation of microwave response in a fractional quantum Hall droplet*

Data Repository
https://zenodo.org/records/18933586
DOI:10.5281/zenodo.18933586

KATO, Yasuyuki [B class; 500 (B), 90 (C)] (344)
— *Numerical study on transition between quantum spin liquids*

1. Large-N SU(4) Schwinger boson theory for coupled-dimer antiferromagnets
Shang-Shun Zhang, Yasuyuki Kato, E. A. Ghioldi, L. O. Manuel, A. E. Trumper, and Cristian D. Batista Phys. Rev. B **112**, 024410 (2025).
DOI:10.1103/qfmw-whbp

KAWAGUCHI, Kaishu [AB class; 600 (B), 50 (C)] ()
— *Investigation of Substrate Effects on Topological-Insulator Bi_2Te_3 Thin Films*
— *Spin-Polarized Band-Structure Analysis of Bi_2Te_3 Topological-Insulator Thin Films under Optical Excitation*

KAWAKATSU, Toshihiro [C class; 5000 (B), 0 (C)] (291)
— *Nonlinear particle-continuum switching in multiscale Smoothed-Particle Hydrodynamics (SPH) method*

KAWAMURA, Hikaru [C class; 1200 (B), 400 (C)] ()
— *Novel order in frustrated magnets*

KAWAMURA, Taira [B class; 400 (B), 40 (C)] (359)
— *A microscopic theory for charge imbalance in nonequilibrium superconductors*

1. Nonequilibrium electron distribution function in a voltage-biased metal wire: A nonequilibrium Green ' s function approach
   T. Kawamura, and Y. Kato J. Phys. Soc. Jpn. 95, 034702 (2026).
   DOI:10.7566/JPSJ.95.034702

2. Emergence of Charge-Imbalanced BCS State and Suppression of Nonequilibrium FFLO State in Asymmetric NSN Junctions
   T. Kawamura, and Y. Ohashi arXiv:2603.00435
   DOI:10.48550/arXiv.2603.00435

KINEFUCHI, Ikuya [C class; 3000 (B), 300 (C)] (313)
— *Study on gas separation mechanisms in facilitated transport membranes*

KITAO, Akio [C class; 4600 (B), 400 (C)] (289)
— *Efficient sampling simulation of the soft modes significantly contribute to protein properties*

1. Tandem Allosteric Effects of Reactant and Product that Promote Deacetylation Cycles in Sir2
   Z. Bai, D. P. Tran, A. Kitao Journal of Chemical Information and Modeling **65**, 11326 (2025).
   DOI:10.1021/acs.jcim.5c01755

2. Protein domain movement involved in binding of belinostat and HPOB as inhibitors of histone deacetylase 6 (HDAC6): a hybrid automated-interactive docking study
   G. Iakovou, L. Palmer, A. Ganesan, A. Kitao, S. D. Laycock, and S. Hayward Journal of Computer-Aided Molecular Design **39**, 52 (2025).
   DOI:10.1007/s10822-025-00636-x

3. RNA Binding Mechanism of the FUS Zinc Finger in Concert with Its Flanking Intrinsically Disordered Region
   S. Kijima and A. Kitao Journal of Chemical Information and Modeling **65**, 8262 (2025).
   DOI:10.1021/acs.jcim.5c01059

4. Interactive docking workshop: Docking the anticancer drug Belinostat to its cellular histone deacetylase (HDAC) target
   G. Iakovou, L. Palmer, A. Ganesan, A. Kitao, S. D. Laycock, and S. Hayward Journal of Chemical Education **102**, 2514 (2025).
   DOI:10.1021/acs.jchemed.4c01347

5. The strategy used by nave anti-PEG antibodies to capture flexible and featureless PEG chains
   Y. Liu, T. Mori, Y. Ito, K. Kuroki, S. Hayashi, D. Kohda, T. Shimizu, T. Ishida, S. R. Roffler, M. K. Kaneko, Y. Kato, T. Arimori, T. Teramoto, K. Takemura, K. Ishibashi, Y. Katayama, K. Maenaka, Y. Kakuta, A. Kitao, and T. Mori Journal of Controlled Release **380**, 396 (2025).
   DOI:10.1016/j.jconrel.2025.02.001

KITOH, Hirotaka [B class; 400 (B), 70 (C)] (191)
— *Electronic structure calculations and molecular dynamics simulations for fullerenes on a tungsten surface*

KOBAYASHI, Akito [B class; 450 (B), 80 (C)] (252)
— *Compensated Ferrimagnets with Spin Splitting based on inequivalent dimers in organic compounds*

KOBAYASHI, Katsuyoshi [B class; 400 (B), 70 (C)] (190)
— *Theoretical study on electronic properties of new nanoscale surfaces and interfaces*

KOBAYASHI, Nobuhiko [C class; 3400 (B), 350 (C)] (97)
— *Quantum transport theory by large scale first-principles electron transport calculations*

1. Evolution of electronic correlation in highly doped organic two-dimensional hole gas
   N. Kasuya, T. Furukawa, H. Ishii, N. Kobayashi, K. Hirose, H. Takayanagi, T. Okamoto, S. Watanabe, and J. Takeya Nat. Commun.16, 3214 (2025).
   DOI:10.1038/s41467-025-58215-5

2. Field emission from vertically aligned graphene edges at the apex of the pencil lead
   T. Igari, R. Tsuruta, Y. Nishiyama, M. Adachi, T. Myojin, K. Asanagi, M. Sasaki, N. Kobayashi, and Y. Yamada Sci. Rep. 15, 27456 (2025).
   DOI:10.1038/s41598-025-11895-x

KOBAYASHI, Yoshihiro [B class; 100 (B), 30 (C)] (378)
— *Molecular dynamics simulation of graphene-nanospacer stacking heterostructure properties*

1. Mechanical bistability and hysteresis in graphene-CNT hybrid systems: from atomistic simulations to macroscale structural responses
   M. Ding, N. Sakurai, M. Shen, T. Inoue, T. Matsuzaki, T. Mizuno, K. Suzuki, J. I. Enriquez, H. H. Halim, Y. Hamamoto, Y. Nishina, H.Y. Yoshikawa, Y. Morikawa, and Y. Kobayashi Submitted

KOGA, Akihisa [CD class; 6900 (B), 650 (C)] (229)
— *Analyzing ferromagnetic order in a particle doped SU(N) Fermi-Hubbard model using DMFT*
— *Numerical analysis of fermionic superfluidity with an interplay between dissipation and external fields in non-Hermitian SU(N) Hubbard models*
— *Magnetic phases near commensurate fillings in the SU(N) Fermi-Hubbard model*

1. Generalized Nagaoka ferromagnetism accompanied by flavor-selective Mott states in an SU(N) Fermi-Hubbard model
   J. Fujii, K. Yamamoto, and A. Koga Phys. Rev. B 113, 115132 (2026).
   DOI:10.1103/kx3p-phyq

2. Elliptical-rod geometries enhance photonic band gaps in disordered stealthy hyperuniform photonic crystals
   K. Asakura, K. Yamamoto, and A. Koga J. Phys. Soc. Jpn. 95, 024711 (2026).
   DOI:10.7566/JPSJ.95.024711

3. Itinerant ferromagnetism in an SU(3) Fermi-Hubbard model at finite temperature: A DMFT study
   J. Fujii, K. Yamamoto, and A. Koga Phys. Rev. B 112, 115136 (2025).
   DOI:10.1103/vpb4-4d54

4. Measurement-induced phase transitions for free fermions in a quasiperiodic potential
   T. Matsubara, K. Yamamoto and A. Koga Phys. Rev. B 112, 054309 (2025).
   DOI:10.1103/3zfd-3hqt

5. Quasiperiodically modulated honeycomb lattices and their magnetic properties
   A. Koga and T. Matsubara Phys. Rev. B 111, 214422 (2025).
   DOI:10.1103/7hsy-sct6

KOMIYA, Atsuki [C class; 1200 (B), 250 (C)] (147)

— *Numerical simulations of electron-lattice interactions under laser irradiation using time-dependent density-functional theory*

1. First-principles investigation of the relationship between laser irradiation intensity and non-thermal melting of α-quartz
   Mizuho Ono, Hiroki Gonome, Atsuki Komiya J. Appl. Phys. 138, 105103 (2025).
   DOI:10.1063/5.0279804

KOSHOJI, Ryotaro [C class; 5000 (B), 600 (C)] (280)

— *Ionic crystal structure search based on mathematical crystal chemistry*

— *Materials synthesis based on mathematical crystal chemistry*

Data Repository
Website for mathematical crystal chemistry
https://marici.mathematical-crystal-chemistry.solutions/optimal-solutions

KOURA, Akihide [C class; 1000 (B), 0 (C)] (163)

— *Ab initio study on static and dynamic properties of light metal alloys*

1. 機械学習ポテンシャルを用いたSiO¡sub¿2¡/sub¿メルトおよびガラスの大規模分子動力学シミュレーション
   若林大佑, 島村孝平, 下條冬樹, 高良明英日本結晶学会誌 **67**,121 (2025).
   DOI:10.5940/jcrsj.67.121

2. Structural Insights into Liquid Malic and Lactic Acids from First-Principles Simulations and X-ray Diffraction
   W. Sugimoto, K. Ito, H. Shimakura, S. Tahara, K. Ohara, A. Koura, K. Shimamura, and F. Shimojo J. Phys. Soc. Jpn. **95**, 014602 (2026).
   DOI:10.7566/JPSJ.95.014602

KUDO, Koji [CD class; 10200 (B), 0 (C)] (225)

— *Numerical study on a quantum anomalous Hall-superconductor hybrid*

— *Numerical study on a quantum anomalous Hall-superconductor hybrid: Creation of non-Abelian anyons*

— *Quantum anomalous Hall-superconductor hybrid: topological superconductivity*

1. Repulsive-Interaction-Driven Topological Superconductivity in a Landau Level Coupled to an s-Wave Superconductor
   K. Kudo, R. Nakai, H. Isobe, J. K. Jain, and K. Nomura arXiv:2510.04700
   DOI:10.48550/arXiv.2510.04700

KUNISADA, Yuji [C class; 6000 (B), 0 (C)] (69)

— *Designing of Ceramic Protective Coating and Grain Boundary to suppress hydrogen embrittlement of metallic materials*

— *Development of Ceramic Protective Coating for High Corrosion Resistance of Metallic Materials*

KURODA, Fumiaki [B class; 350 (B), 90 (C)] (198)

— *Development of a Surface Structure Exploration Program and Supporting Infrastructure*

KUROKI, Kazuhiko [C class; 4800 (B), 0 (C)] (232)

— *Theoretical designing of high T_c superconductivity at ambient pressure in multilayer nickelates and related materials*

1. TImprovement of the simplification method for the local two-particle full-vertex towards precise

frequency behavior
Myota Mizuno, Kazuhiko Kuroki, Masayuki Ochi Phys. Rev. B **111**, 205136 (2025)
DOI:10.1103/PhysRevB.111.205136

2. t-J model for strongly correlated two-orbital systems: Application to bilayer nickelate superconductors
Tatsuya Kaneko, Masataka Kakoi, Kazuhiko Kuroki Phys. Rev. B **112**, 075143 (2025)
DOI:10.1103/bsgt-sg2s

3. Doublon-Holon Pairing State in Photodoped Mott Insulators
Ryota Ueda, Madhumita Sarkar, Zala Lenarčič, Denis Golež, Kazuhiko Kuroki, Tatsuya Kaneko Phys. Rev. B **113**, L161109 (2026).
DOI:10.1103/dc6n-hrzj

4. Possible high thermoelectric power factor in alkali-metal-intercalated BC: anisotropic multiple valleys originating from the van Hove singularity of graphene
Ryutaro Enami, Kazuhiko Kuroki, Masayuki Ochi Phys. Rev. Mater. **9**, 084001 (2025).
DOI:10.1103/rqrv-7hqt

5. Optical control of the crystal structure in the bilayer nickelate superconductor $La_3Ni_2O_7$ via nonlinear phononics
Shu Kamiyama, Tatsuya Kaneko, Kazuhiko Kuroki, Masayuki Ochi Phys. Rev. B **112**, 094115 (2025).
DOI:10.1103/h6vj-fd4n

6. Theoretical study on the possibility of high s-wave superconductivity in the heavily hole-doped infinite layer nickelates
Hirofumi Sakakibara, Ryota Mizuno, Masayuki Ochi, Hidetomo Usui, Kazuhiko Kuroki Phys. Rev. B **111**, 224511 (2025).
DOI:10.1103/nl4m-n5dx

KUSAKABE, Koichi [C class; 3400 (B), 0 (C)] (103)
— *Electron excitation induced phase transformation of quantum materials*

1. Modulated Dirac bands and integer hopping ratios in a honeycomb lattice of phenalenyl-tessellation molecules
N. Morishita, K. Komatsu, M. Kitatani, and K. Kusakabe Physical Review B 111, 235117 (2025).
DOI:10.1103/PhysRevB.111.235117

2. Computational study of conformational interconversion of an amyloid β double layer system
Y. Oishi, M. Kitatani, K. Nakajima, H. Ogi, and K. Kusakabe RSC Advances, 15, 42395-42401, (2025).
DOI:10.1039/D5RA08004E

3. Real-space imaging of thermally and photo induced phase transition in quasi one dimensional organic complexes
K. Fukumoto, K. Onda, T. Tanaka, K. Kusakabe, E. Pyatenko, H. Yamochi, S. Adachi, S. Koshihara submitted to Phys. Rev. Res.

LEE, Minhyeok [C class; 2400 (B), 0 (C)] (326)
— *Multiphase-reactive simulations of aluminum particle combustion with detailed kinetics and interfacial phase change*

LI, Hao [E class; 2400 (B), 250 (C)] (115)

— Computational Screening of Magnetic Properties for Enhanced CO_2 Reduction Reaction (CO_2RR) Catalysts

1. HERO (Hessian-Engineered Relaxation Optimizer): Suppressing "Hessian pollution" for accelerated first-principles structural relaxation
   M. Li, P. Ma, L. Li, W. Yang*, and H. Li* CMC-Comput. Mater. Con. 2026, In Press.

2. Spin Effect Regulation as A Design Principle for M-N-C Catalysts for Oxygen Electrocatalysis
   H. Li, Z. Fu, Y. Yuan, D. Zhang, Y. Chen, H. Li*, and A. Cao* Chemical Science, 2026, In Press.

3. Unveiling the correlation between high-entropy alloy element systems and electrocatalytic activity
   X. Shan, F. Cai, Y. Tu, D. Zhang, Y. Pan, L. Chen, J. Liang, H. Gao, J. Xu, H. Li*, J. Li, E. Wang*. and M. Zhou* National Science Review, 2026, nwag161.
   DOI:10.1093/nsr/nwag161

4. Revealing Zn and Ga as effective promoters for Cu-catalyzed CO2 hydrogenation to methanol
   M. Ma, H. Li, A. Cao*, and J. Yan Journal of Energy Chemistry, 2026, In Press.

5. Data-Driven Paradigms for Advancing Alkali-Metal-Ion Battery Technologies
   H. Shao, N. Kumar, W.-H. Lai, H. Li, X. Jia, H.-K. Liu, and Y. Wang* Energy Storage Materials, 2026, 105044.

6. AI Agents: Opportunity, Hype, and the Way Through
   C. Zhao* and H. Li* AI Agent, 2026, 2, 3.
   DOI:10.20517/aiagent.2026.07

7. StableOx-Cat Agent: An AI Agent for Exploring Stable Metal Oxide Electrocatalysts
   X. Jia, D. Zhang, Y. Lu, Q. Wang, and H. Li* AI Agent, 2026, 2, 1.
   DOI:10.20517/aiagent.2026.03

8. Digital Materials Ecosystem: From Databases to AI Agents for Autonomous Discovery
   D. Zhang, X. Jia, Y. Wang, H. Liu, Q. Wang, S. H. Jang, D. Shah, S. Ye, H. B. Tran, and H. Li* Chemical Science, 2026, 17, 5782 (Invited Perspective; Front Cover Article).

9. Ligand-Intercalated MOFs Enable Reaction-Pathway Engineering in Biomass Electrooxidation via Steric and π- Electronic Microenvironment Control
   J. Chen, Z. Guo, J. Xie, L. Tang, S. Li, Y. Bu, C. Peng, M. Zhao, L. Zhang, J. Zhou, H. Liu*, H. Li*, and M. Li* Angewandte Chemie International Edition, 2026, e4762494.

10. Catalytic Strategies and Mechanisms for Enhancing MgH2 Solid-State Hydrogen Storage
    Z. Gao, X. Yang, Z. Zhuang, Y. Zhang, J. Cai, Y. Li, W. Fu, H. Li*, and W. Yang* Chem Catalysis, 2026, 6, 101692 (Invited Perspective).

11. Recent Development in Designing Electrocatalysts for Efficient and Selective Ammonia Oxidation Reaction
    Y. Deng, Z. Bao, Y. Huang, M. Cui, Y. Chen, H. Li*, and L. Wei* Advanced Energy and Sustainability Research, 2026, 7, e202600002 (Invited Review).

12. Accelerating Catalyst Materials Discovery with Large Artificial Intelligence Models
    D. Zhang, Y. Chen*, C. Liu, Y. Liu, H. Xin, J. Peng*, P. Ou*, and H. Li* Angewandte Chemie International Edition, 2026, e26150 (Invited Review; Cover Article).

13. Catalysis AI Agent Guides Discovering the Universal Design Principle of Cu-based Single-atom Alloy Catalysts for CO2 Electroreduction
    X. Wang, Z. Li, D. Zhang, H. Li*, H. Xu* and D. Cheng* Angewandte Chemie International

Edition, 2026, e24612.

14. Interface-Mediated Jahn–Teller Effect in a Structure-Reinforced $LiMnO_2$ Cathode
H. Liu, T. Shen, X. Zhu, M. Yang*, Y. Yao, J. Cheng, Y. Zhao, H. Li*, S. Li*, L. Gu, and H. Xia* J. Am. Chem. Soc. 2026, 148, 7388.
DOI:10.1021/jacs.5c20036

15. Coordination-Dependent Oxygen Reduction Reaction Activity of Single Atom Co-Nx-C Electrocatalysts
C. Liu, D. Zhang, J. Chen, F. She, F. Liu, Z. Yu, Z. Zhi, M. S. Levine, J. L. Sessler, Y. Chen, H. Li*, and L. Wei* J. Am. Chem. Soc. 2026, 148, 6569.
DOI:10.1021/jacs.5c20980

16. Boosting ammonia decomposition for hydrogen production over Co/CeO2 catalysts via Sr doping
L. Su, F. Zeng, J. Wang, Q. Qasim, X. Liu, J. Li, H. Li*, and W. Cen* Catal. Sci. Technol. 2026, In Press.

17. Strategically Advancing Semiconducting Phthalocyanines as High-Performance Electrocatalysts for Electrochemical CO2 Reduction
T. Liu*, X. Hou, D. Zhang, Y.Hirai, K. Ishibashi, Y. Matsuo, S. Ono, H. Li*, and H. Yabu* ACS Applied Electronic Materials, 2026, 8, 2187 (Invited Spotlight Review; Cover Article).

18. Enhancement of Methanol Yield in CO2 Hydrogenation by Promoting CO_2 Activation and Unlocking the RWGS + CO-Hydrogenation Pathway over Cu-La/ZrO_X Catalysts
J Yang, T. Gao, J. Yang, F. Xiao, S. Liu, N. Zhao* , D. Cao*, H. Li* ACS Catal. 2026, 16, 4773.
DOI:10.1021/acscatal.5c08427

19. Materials Databases: Foundations of Modern Digital Materials
Y. Zhuang, X. Yang, C. Zhang, X. Jia, D. Zhang, M. Li, T. Yao, J. Peng, Z. Gao, W. Yang*, and H. Li* Precision Chemistry, 2026, In Press (Invited Perspective).

20. Y-Induced Oxygen Vacancy Engineering and Local Electronic Reconstruction for Enhanced Ammonia Decomposition over $Ni_1Ce_{1-x}Y_xO_\alpha$
Z. Bao, H. Liu, Y. Zhang, Z. Wang, H. Li*, and H. Hu* Journal of Catalysis, 2026, 455, 116718
DOI:10.1016/j.jcat.2026.116718

21. AI-Driven Multi-Agent Collaborations for Accelerating Catalyst Design
H. Li* National Science Review, 2026, 13, nwag067 (Invited).
DOI:10.1093/nsr/nwag067

22. "DIVE" into Hydrogen Storage Materials Discovery with AI Agents
D. Zhang*, X. Jia, T. B. Hung, S. H. Jang, L. Zhang, R. Sato, Y. Hashimoto, T. Sato, K. Konno, S. Orimo*, and H. Li* Chemical Science, 2026, 17, 3031-3042 (Cover Article).

23. Atomic Eu-Mediated Acetonitrile Adsorption Configuration Switch Drives Long-Term, Ampere-Level Electrosynthesis of Ethylamine via Eu-Mediated Acetonitrile Adsorption Configuration Switching
H. Du, X. Wang, M. Li*, R. Lv, C. Wang, W. Xue, L. Li, D. Sun, Y. Tang, H. Li*, and G. Fu* Advanced Materials, 2026, 38, e21105.
DOI:10.1002/adma.202521105

24. Stepwise Acceleration of Water Dissociation and Hydrogen Spillover for Enhanced Overall Alkaline Hydrogen Evolution
T. Lu, J. Li, C. Wang, H. Liu, S. Ye, X. Jia, L. Zhang, D. Zhang, D. Sun, Y. Gu*, Q. Wang, B. Da, L. Wei, Y. Zhang*, H. Li*, and Y. Tang* ACS Catalysis, 2026, 16, 2827.

25. Tuning Stability of AB3-Type Alloys by Suppressing Magnetism
H. B. Tran*, T. Sato, R. Sato, H. Saitoh, S. Orimo*, and H. Li* Chemistry of Materials, 2026, 38, 497.

26. The Influence of Anion Effects on the Morphology of Copper-Based Hydroxides and Their Electrocatalytic Performance in Reduction of Nitrite to Ammonia
C. Sun, T. Wu*, X. Xing, L. Ding*,W. Xiong*, and H. Li* Ind. Eng. Chem. Res., 2026, 65, 4361.

27. Artificial Intelligence - Driven Discovery and Design of Solid-State Hydrogen Storage Materials
Y. Chu, Y. Li, Y. Lyu, D. Zhang, H. Li*, W. Yang*, J. Li, and L. Zhang* Green Energy Environ. 2026, In Press (Invited Review).

28. Recent Advances in the Application of Transition Metal-Based Catalysts in Electrocatalytic Ammonia Synthesis and C-N Bond Formation
S. Tu , J. Li , T. Wu* , X. Xing, W. Xiong*, and H. Li* Journal of Materials Chemistry A, 2026, 14, 1383.

29. Making Reactivity General for Machine-Learning Potentials
H. Li* Chem Catalysis, 2026, 6, 101572 (Invited).

30. Non-Directly Bonded Single-Atom Pairs Towards H2/CO Electrooxidation
T. Yang, H. Liu, H. Liu, W. Zhao, J. Ge, W. Wang, S. Yang, M. Tang, K. Wei, K. Wang, Z. Qi, X. Wang*, H. Li*, and J. Ge* Science Bulletin, 2026, 71, 399.

31. Roadmap for Transforming Heterogeneous Catalysis with Artificial Intelligence
H. Xin*, J. R. Kitchin*, N. Lpez*, N. M. Schweitzer*, N. Artrith, F. Che, L. C. Grabow, G. Gunasooriya, H. J. Kulik, T. Laino, H. Li, S. Linic, A. Medford, R. Meyer, J. Peng, C. Phillips, J. Qian, L. Qi, W. Shaw, Z. W. Ulissi, S. Wang, and X. Wang Nature Catalysis, 2026, 9, 102.

32. Universal Catalyst Design Framework for Electrochemical Hydrogen Peroxide Synthesis Facilitated by Local Atomic Environment Descriptors
Z. Liu, Y. Liu, Y. Zhang, Y. Deng, Z. Zheng, R. Knibbe, T. Gao, M. Li, Z. Wang, B. Zhang, X. Jia, D. Zhang, H. Liu, X. Shao, Z. Gao, L Wei*, H. Li*, and W. Yang* Angewandte Chemie International Edition, 2026, 65, e18027 (Cover Article).

33. Covalent Bridges Enabling Layered C60 as an Exceptionally Stable Anode in Lithium-Ion Batteries
S. Wang, H. Liu, Y. Lei, D. Li, Y. Fan, L. Hong, X. Guo, M. Wang, Z. Huang, Y. Cheng, X. Yang, J. Zhang, H. Li*, and G. Wang* J. Am. Chem. Soc. 2025, 147, 47663.

34. 2D Topological Electrocatalysts with SpinOrbit Coupling: Interplay Between The “Electrochemical” and “Topological” Surface States
H. Liu*, T. B. Hung, Y. Wang, D. Zhang, Y. Lu, and H. Li* Journal of Physical Chemistry Letters, 2025, 16, 12892.

35. Atomic Eu Substitution in Cu2O Tailors C1 and C2+ Product Selectivity by Frustrated Deep Hydrogenation in Electrochemical CO2 Reduction
Y. Liu, X. Wang, Z. Mao, J. Zhang, M. Li, D. Sun, Y. Tang, H. Li*, and G. Fu* Journal of the American Chemical Society, 2025, 147, 45808.

36. Selective Electrocatalytic Reduction of Nitrate for the Synthesis of Hydroxylamine with Cu-ZnO/N-C Catalyst
J. Li, Y. Wang, T. Wu, X. Xing, L. Li, W. Xiong*, and H. Li* Chemical Engineering Science, 2025, 323, 123204.

37. Machine Learning-Driven Advances in Environmental Pollutant Management
Z. Qiu, Z. Zhuang, X. Jia, H. Li, C. Chen, and B. Yu* Journal of Environmental Chemical Engineering, 2025, 13, 120441.

38. Physically Interpretable Descriptors Drive the Materials Design of Metal Hydrides for Hydrogen Storage
S.-H. Jang*, D. Zhang, H. B. Tran, X. Jia, K. Konno, R. Sato, S. Orimo*, and H. Li* Chemical Science, 2025, 16, 23111- 23120

39. Atomically Ordered RuGa Intermetallic Electrocatalyst Enables High-Efficiency Nitrate-to-Ammonia Conversion
Y.-Z. Yu, Q.-L. Jiang, Y. Cheng, S. Li, T. Li, K.-Z. Xue, Y. Xu, S. Cheng, H. J. Sun, T. Wang, J. Xu,* X. Su, Y. Chen, B. Da, H. Li*, and Z.-Y. Wu* Advanced Functional Materials, 2025, e24120.

40. Synergistic MultiPhysics Catalysis Enabled by LotusRootInspired Flow Fields in Proton Exchange Membrane Fuel Cells
Y. Zhou, Z. Miao*, H. Li*, K. Meng, B. Chen, M. Chen, H. Luo, Y. Guan, Y. Duan, Q. Ding, D. Wu, J. Li, and X. Tian* Journal of Materials Chemistry A, 2025, 13, 40821.

41. Theory-Guided Design of Non-Precious Single-Atom Catalyst for Electrocatalytic Chlorine Evolution
K. Ma, L. Yang, X. Yang, C. Zhang, D. Zhang, L. Zhang, L. Wei, C. Ye*, H. Li*, and W. Yang* Advanced Functional Materials, 2025, 36, e25210.

42. Design of Metal-Supported MgO Catalysts for Electrochemical CO2 Reduction to Formic Acid via the MottSchottky Effect
S. Zhao, Y. Wang, H. Liu, X. Jia, Y. Zhang, L. Zhang, B. Da, Q. Wang, H. Zheng*, H. Li*, and W. Li* Journal of Catalysis, 2025, 453, 116502.

43. Simultaneous Electrocatalytic Oxidation and Hydrogenation of Biomass-Derived Aldehydes on Single- Atom Ru Catalysts
Y. Wang, B. Liu, Y. Duan, B. Da, Z. Hu, H. Wen, W. Bu, H. Luo, S. Zhang, H. F. Garces, C. Wang, T. Mu, H. Li*, and K. Yan* Advanced Energy Materials, 2025, 15, e04502.

44. Cloud Synthesis: A Global Closed-Loop Feedback Powered by Autonomous AI-Driven Catalyst Design Agent
D. Zhang, X. Jia, H. Liu, Y. Wang, S. Ye, Q. Jiang, Y. Wang, Z. Guo, L. Zhang, L. Wei, W. Yang, H. Liu, S. Zhao, H. Xu, D. Cheng, Y. Hashimoto, T. Tomai, and H. Li* AI Agent, 2025, 1, 2.
DOI:10.20517/aiagent.2025.02

45. Probing the Reactivity of In-Situ Formed Oxygen Vacancies of Non-Noble Lead Oxides for Anodic Propylene Oxidation
J. Ge, T. Wang, X.-L. Zhang, H. Sun, R. Wang, P.-C. Yu, X. Sun, S.-P. Sun, H. Liu, Y. Liu, C.-L. Zhang, B. Da, Y.- R. Zheng,* M.-R. Gao,* and H. Li* Catal. Sci. Technol. 2025, 15, 7228.

46. Decoding pH- Dependent Electrocatalysis through Electric Field Models and Microkinetic Volcanoes
S. Ye, Y. Wang, H. Liu, D. Zhang, X. Jia, L. Zhang, Y. Zhang, A. Kumatani, H. Shiku*, and H. Li* Journal of Materials Chemistry A, 2025, 13, 37821 (Invited Perspective; Front Cover Article)

47. Ampere-Level Electrosynthesis of CO via Well-Defined Pyridinic-N Incorporated Cobalt Phthalocyanine
T. Liu*, X. Hou, D. Zhang, Y. Hirai, K. Ito, K. Ishibashi, Y. Matsuo, J. Yoshida, S. Ono, H. Li*,

and H. Yabu* Small, 2025, e07824.

48. Designing Interfacial Edge Microenvironments of Cobalt Phosphide Quantum Dots/Graphitic Carbon Nitride to Modulate Electron Delocalization for Ultrafast Photocatalytic Hydrogen Evolution
X. Hu, Y. Zeng*, H. Liu*, B. D, H. Li, B. Hong, X. Peng, and X. Wang Chemical Engineering Journal, 2025, 523, 168790.

49. Artificial Intelligence Technology in Environmental Research and Health: Development and Prospects
Z. Guo, L. Huang*, J. Yan, H. Zhang*, X. Jia*, M. Li, and H. Li* Environmental International, 2025, 23, 109788.

50. Temperature Dependent Mechanism Evolution Effect Enables Stabilized RhRu3Ox for Water Oxidation in Proton Exchange Membrane Electrolyzer
M.-R. Qu, H. Liu, S.-H. Feng, X.-Z. Su, J. Xu, H.-L. Duan, R.-Q. Liu, Y.-Y. Qin, W.-S. Yan, S. Zhu*, R. Wu*, H. Li*, and S.-H. Yu* Nature Communications, 2025, 16, 9261.

51. High-Density W Single Atoms in Two-Dimensional Spinel Break the Structural Integrity for Enhanced Oxygen Evolution Catalysis
Y. Wang, B. Jia*, W. Qin, Y. Wang, S. Liu, Y. Qin, Y. Zhao, L. Liu, D. Zhang, H. Liu, H. Zhong, J. Liu, J. Tu, Y. Liu, H. Wu, D. Zhang, J. Fan, X. Qu, H. Li*, and M. Qin* J. Am. Chem. Soc. 2025, 147, 32249.

52. Selective Epitaxial Growth of MOF-on-MOF-derived Core-shell $Fe_2O_3/CoFe_2O_4$ Nanocomposites for Efficient Electrochemical Detection of Multiple Heavy Metal Ions
J. Guo, S. Tu, L. Li, X. Xing, W. Xiong*, and H. Li* Ind. Eng. Chem. Res., 2025, 64, 19075.
DOI:10.1021/acs.iecr.5c02521

53. Modulating Surface-Active Hydrogen for Facilitating Nitrate-to-Ammonia Electroreduction on Layered Double Hydroxides Nanosheets
B. Liu, Y. Wang, H. Wen, Y. Wang, H. Liu, B. Da, K. Li, H. Luo, H. Li*, and K. Yan* Advanced Functional Materials, 2025, e19238.

54. Unveiling Multilayer Cobalt Phthalocyanine/Carbon Core-Shell Structures as Efficient Catalytic Units for CO2-to-CO Electroreduction
T. Liu*, D. Zhang, Y. Chu, K. Ohashi, Y. Hirai, K. Ito, K. Ishibashi, Y. Matsuo, J. Yoshida, S. Ono, K. Kamiya, H. Li*, and H. Yabu* Applied Catalysis B: Environment and Energy, 2025, 381, 125852.

55. AI Agent-Defining the Next Era of Intelligent Agents
H. Li* AI Agent, 2025, 1, 1.
DOI:10.20517/aiagent.2025.01

56. Application of An Explainable Machine Learning to CO2 Methanation for Optimal Design Nickel-Based Catalysts
J. Zhang, X. Jia*, H. Li, F. Xiao, Q. Wang*, and N. Zhao* ACS Sustainable Chem. Eng. 2025, 13, 14278.

57. Hydrophobically Modified Cu_2O Nanocube for Selective CO_2 Electroreduction to C_{2+} Products
C. Li, Z. Guo, X. Mao, Y. Shen, S. Yang, Y. Jiang, P. Tang, H. Li*, H. Li*, C. Li* AIChE Journal, 2025, 71, e70049.
DOI:10.1002/aic.70049

58. Insights Into Giant Magnetocaloric Effect in $BiCu_3Cr_4O_{12}$ with Charge-Spin-Lattice Coupling
H. B Tran*, H. Li*, M. Goto, K. Sato, and Y. Shimakawa J. Mater. Chem. A, 2025, 13, 34286.
DOI:10.1039/D5TA03354C

59. C60 Fullerene as the Active Site for CO2 Electroreduction
S.-W. Ying, Y. Wang, P. Du, Q. Wang*, C. Yue, D. Zhang, Z.-C. Chen, J.-W. Zheng*, S.-Y. Xie*, and H. Li* Angewandte Chemie International Edition, 2025, 64, e202511924 (Editor's Choice; Cover Article).

60. Reinforcing the Chemical Bonding in Pt3Ni Catalysts via Metallic Interface-Directed Activation for Durable Fuel Cells
M. Chen, C. Wu, Z. Miao*, H. Li, H. Zhang, Q. Liu, J. He, Y. Zhou, D. Wu*, J. Li, R. Li, and X. Tian* Advanced Functional Materials, 2025, e12164.

61. The Key Steps and Distinct Performance Trends of Pyrrolic vs. Pyridinic M-N-C Catalysts in Electrocatalytic Nitrate Reduction
Q. Jiang, M. Gu, S. Pei, T. Wang, F. Liu, X. Yang, D. Zhang, Z. Wu, Y. Wang*, L. Wei*, and H. Li* J. Am. Chem. Soc. 2025, 147, 26029.

62. Unraveling the Potential-Dependent Selectivity of Propylene Electrooxidation: The Role of Electrochemistry-Induced Reconstruction
D. Li , P. Sun, D. Zhang, H. Li*, H. Xu*, and D. Cao* J. Am. Chem. Soc. 2025, 147, 24900.

63. Closed-Loop Framework for Discovering Stable and Low-Cost Bifunctional Metal Oxide Catalysts for Efficient Electrocatalytic Water Splitting in Acid
X. Jia, Z. Zhou, F. Liu, T. Wang, Y. Wang, D. Zhang, H. Liu, Y. Wang, S. Ye, K. Amezawa*, L. Wei*, and H. Li* J. Am. Chem. Soc. 2025, 147, 22642 (Cover Article).

64. Rare Earths Evoked Gradient Orbital Coupling in Electrocatalysis: Recent Advances and Future Perspectives
X. Wang, M. Li, Y. Tang, H. Li*, and G. Fu* Progress in Materials Science, 2025, 155, 101539.

65. Furfural Electrovalorisation to Hydrofuroin with Near-Unity Faradaic Efficiency on a Single-Atom Zinc Catalyst
J. Chen, S. Ye, F. She, X. Yang, F. Liu, Z. Yu, Z. Zheng, M. Hong, Q. Wang, Y. Chen, H. Li*, and L. Wei* EES Catalysis, 2025, 3, 1062.

66. The Hidden Engine of AI in Electrocatalysis: Databases and Knowledge Graphs at Work
D. Zhang and H. Li* Mol. Chem. Eng. 2025, 1, 100003 (Invited Editorial; Cover Article).

67. Preview: Polymer Solubility Dictates the Fate of Polymer Chains
H. Li* Newton, 2025, 100191 (Invited Preview).

68. Bridging Theory and Experiment: Machine Learning Potential-Driven Insights into pH-Dependent CO2 Reduction on Sn-Based Catalysts
Y. Wang, Z. Wu, Y. Jiang, D. Zhang, Q. Wang*, C. Wang, H. Li*, X. Jia, J. Fan*, and H. Li* Advanced Functional Materials, 2025, e06314 (Cover Article).

69. Advancing Electrochemical Nitrate Reduction: Overcoming Rate-Limiting Bottlenecks with Copper/Cobalt Catalysts
J. Li, Y. Wang, X. Xing, Y. Wang, W. Xiong*, and H. Li* Advanced Functional Materials, 2025, 35, e13717.

70. Dynamic Evolution of Self-Renewal Fe- N-C Catalysts for Acidic Oxygen Reduction Reaction
F. Liu, L. Lai, Z. Guo, F. She, J. Prabowo, H. Li*, L. Wei*, and Y Chen* EES Catalysis, 2025, 3, 1358.

71. A Materials Map Integrating Experimental and Computational Data via Graph-Based Machine

Learning for Enhanced Materials Discovery
Y. Hashimoto*, X. Jia, H. Li, and T. Tomai APL Machine Learning, 2025, 3, 036104.

72. Chlorine-Dopant Dynamically Stabilizes Cu0/Cu+ Active Sites for Selective CO2 Electroreduction to Multicarbon Products
C. Li, Z. Guo, J. Cui, T. Zhang, Z. Liu, X. Mao, Y. Shen, S. Yang, Y. Jiang, P. Tang, H. Li*, H. Li*, and C. Li* AIChE Journal, 2025, 71, e18934.

73. Data-Driven Strategies for Designing Multicomponent Molten Catalysts to Accelerate Industrialization of Methane Pyrolysis
Y. Chen*, X. Huang, Y. He, Q. Liu, J. Du, W. Yang, W. Wang, D. Zhang, X. Jia, H. Wang, Y. Tang*, Q. Yu, S. K. Kim*, and H. Li* ACS Catalysis, 2025, 15, 11003.

74. Phosphorus-Mediated Oxygen Vacancy Engineering in Cu2O for Highly Selective CO2 Electroreduction to Multi-carbon Products
X. Mao, Z. Guo, S. Yang, Y. Shen, L. Wei, C. Li, H. Li*, H. Li*, and C. Li* ACS Nano, 2025, 19, 23, 21669.

LIU, Heng [E class; 2500 (B), 600 (C)] ()
— *Explore the pH-dependent surface state and oxygen evolution reaction performance for transition metal nitrides*

MAEHIRA, Takahiro [B class; 300 (B), 60 (C)] (207)
— *Electronic Structure of Rhenium*

MAKINO, Takayuki [B class; 400 (B), 70 (C)] (188)
— *Optical properties of transition-metal monoxides based on coherent potential approximation*

1. Hubbard energy dependence of electronic structures in rare-earth monoxides
M. Tago, T. Kurachi, and T/ Makino Jpn. J. Appl. Phys. 64 09SP18 (2025).
DOI:10.35848/1347-4065/adfee3

2. Sensitivity enhancement of surface plasmon resonance sensor employing 2D black phosphorus: an analytical insight
A. Saha, B. Dey, Md. Sherajul Islam, M. Tago, and T. Makino Jpn. J. Appl. Phys. 64 11SP13 (2025).
DOI:10.35848/1347-4065/ae1143

MASAKI, Yusuke [B class; 400 (B), 70 (C)] (352)
— *Tensor-network approach to phase transition of quantum chiral spin model*

MATSUSHITA, Katsuyoshi [C class; 400 (B), 0 (C)] (366)
— *Study of Self-transport and Clogging of Cells in Tissue Pipeline*

MATSUSHITA, Yu-Ichiro [E class; 13000 (B), 1800 (C)] (44)
— *Development of an HPC/Quantum Hybrid Platform for High-Precision Defect Analysis to Accelerate Materials Innovation*
— *High-precision calculation of semiconductor defects using an HPC/quantum hybrid computer*

1. Tensor-decomposition technique for qubit encoding of maximal-fidelity Lorentzian orbitals in real-space quantum chemistry
T. Kosugi, X. Huang, H. Nishi, and Y. Matsushita Phys. Rev. A **5**, 052615 (2025).
DOI:10.1103/PhysRevA.111.052615

2. Practical rule for trimming the DFT-1/2 self-interaction: Band gap, absolute band alignment,

and defect properties of semiconductors
C. Homma, R. Akashi, Y. Nishiya, S. Tsuneyuki, and Y. Matsushita Phys. Rev. B **112**, 115111 (2025).
DOI:10.1103/mp93-55g3

3. Towards improved quantum machine learning for molecular force fields
Y. Couzini, S. Daimon, H. Nishi, N. Ito, Y. Harazono, and Y. Matsushita Phys. Rev. A **112**, 062442 (2025).
DOI:10.1103/5s9m-h7yb

4. Adaptive interpolating quantum transform: A quantum-native framework for efficient transform learning
G. Budiutama, S. Daimon, H. Nishi, R. Kaneko, T. Ohtsuki, and Y. Matsushita Phys. Rev. A **112**, 062410 (2025).
DOI:10.1103/vyr3-h9hq

5. Advancing N-type doping in semiconductors through hydrogen-defect interactions
A. Kiyoi, Y. Nishiya, Y. Matsushita, and T. Umeda Comm. Materials **7**, 8 (2026).
DOI:10.1038/s43246-025-00955-4

6. Logical quantum phase estimation for x-ray absorption spectra
H. Nishi, T. Kosugi, S. Hirose, T. Okayama, and Y. Matsushita Phys. Rev. Applied **25**, 034026 (2026).
DOI:10.1103/cwj3-xmsg

MINAMI, Susumu [B class; 950 (B), 180 (C)] ()
— *First-principles study for mechanical control of magnetic thermoelectric properties in topological magnets*
— *High-throughput study of strain-induced anomalous Nernst effect*

MISAWA, Masaaki [B class; 350 (B), 0 (C)] (210)
— *Computational study on nanoscale surface/interface structural design based on functional materials*

1. Dendritic WS2 Nanoribbon Networks Grown in Interfacial Confinement Space: Edge-Rich Architectures for Enhanced Hydrogen Evolution
H. Suzuki, K. Hirata, Y. Takahashi, S. Fujii, M. Misawa, T. Tokunaga, I. Nakaya, Y. Senda, Y. Hayashi, Y. Takahashi Small Structures **7**, e202500542 (2025)
DOI:10.1002/sstr.202500542

MISAWA, Takahiro [E class; 18500 (B), 1700 (C)] (219)
— *Analysis of the mechanism of pressure-induced superconductivity in molecular solids*Exotic superconductivity in the doped Kitaev spin liquid

MITARAI, Yoko [C class; 1000 (B), 300 (C)] (149)
— *Phase transformation and electric state of high entropy alloys*

MIURA, Yoshio [C class; 1200 (B), 0 (C)] ()
— *Theoretical study on spin related phenomenon at interfaces of ferromagnetic materials*

MIZUGUCHI, Tomoko [C class; 400 (B), 0 (C)] (364)
— *Role of counterions in ion-mediated permeation of hydrophobic ions into lipid bilayers*

MIZUKAMI, Wataru [C class; 4400 (B), 0 (C)] (295)
— *Creating a quantum computing database for sensor materials*

1. Enhancing quantum computations with the synergy of auxiliary field quantum Monte Carlo and computational basis tomography
   Viktor Khinevich, Wataru Mizukami Phys. Rev. Research **7**, 043344 (2025).
   DOI:10.1103/rbhc-dkh1

2. Integrating Classical and Quantum Software for Enhanced Simulation of Realistic Chemical Systems
   Tomoya Shiota, Klaas Gunst, Toshio Mori, Toru Shiozaki, Wataru Mizukami arXiv:2506.18877
   DOI:10.48550/arXiv.2506.18877

3. Symmetry-Adapted State Preparation for Quantum Chemistry on Fault-Tolerant Quantum Computers
   Viktor Khinevich, Wataru Mizukami arXiv:2601.08533
   DOI:10.48550/arXiv.2601.08533

4. Doubling the size of quantum selected configuration interaction based on seniority-zero space and its application to QC-QSCI-AFQMC
   Yuichiro Yoshida, Takuma Murokoshi, Rika Nakagawa, Chihiro Mori, Naoya Kuroda, Shigeki Furukawa, Hanae Tagami, Wataru Mizukami arXiv:2602.07912
   DOI:10.48550/arXiv.2602.07912

5. Expanding Universal Machine Learning Interatomic Potentials to 97 Elements Towards Nuclear Applications
   Naoya Kuroda, Kenji Ishihara, Tomoya Shiota, Wataru Mizukami arXiv:2603.03223
   DOI:10.48550/arXiv.2603.03223

MOCHIZUKI, Yasuhide [C class; 2400 (B), 250 (C)] (113)
— *Theoretical prediction of negative thermal expansion behavior from molecular dynamics calculations using machine learning potential and experimental verification*

1. Discovery of Biaxial Negative Thermal Expansion in KNbSi2O7 from Computations and Experiments
   H. Koiso, S. Kawasoe, J. Zhang, T. Isobe, A. Nakajima, and Y. Mochizuki* J. Phys. Chem. C 129, 9509 (2025).
   DOI:10.1021/acs.jpcc.5c01247

2. Reply to Comment on “Thermal expansion and phase stability of BF3 (B = Sc, Y, La, Al, Ga, In) from first principles”
   H. Koiso, S. Yoshida, T. Nagai, T. Isobe, A. Nakajima, and Y. Mochizuki Phys. Rev. B 112, 226102 (2025).
   DOI:10.1103/njgh-v8dh

MOID, Mohammad [B class; 200 (B), 50 (C)] ()
— *Impact of Electrostatic Forces on the Crystallization Process of Water Droplets*

MORI, Hatsumi [D class; 2500 (B), 0 (C)] ()
— *First-principles NEB calculations of proton tautomeric conduction pathways based on Neutron diffraction*

MORIKAWA, Yoshitada [E class; 17000 (B), 2450 (C)] (42)
— *Theoretical study on chemical reaction processes at surfaces and interfaces using density functional theory and machine learning methods*

1. O Coadsorption Effects on Water-Gas Shift Reaction over Cu Clusters on Cu(111): Insights from Machine Learning Force Field and Microkinetic Modeling
   M. F. Anshor, H. H. Halim, and Y. Morikawa Phys. Chem. Chem. Phys. in press.
   DOI:10.1039/d5cp05031f

2. Predicting reactive graphene edge-adsorbed Pt single-atom catalyst structures for oxygen reduction via machine learning-enhanced DFT calculations
   B. A. C. Tan, N. A. Sofi, P. N. Thanh, K. I. M. Rojas, S. E. P. P. Masan, Y. Hamamoto, I. Hamada, and Y. Morikawa Phil. Trans. R. Soc. A, **384**, 20240555 (2026).
   DOI:10.1098/rsta.2024.0555

3. Clarifying Photodetachment in Al_{13}^- Anions and Photoionization in Al13 Neutrals Using Diffusion Monte Carlo
   M. R. Chiong III, A. Nakajima, and Y. Morikawa J. Phys. Chem. A **130**, 1851 (2026).
   DOI:10.1021/acs.jpca.6c00226

4. Bridging the Pressure Gap in Hydrogenation of CO2 to Formate on Cu(100) by Machine-learning Molecular Dynamics and First-Principles Microkinetic Modeling
   W. O. N. F. Rajaelo †, H. H. Halim †, M. F. Anshor, Y. Yamada, S. Ramadhani, F. A. Mubarok, S. E. M. Putra, A. L. Ivansyah, T. D. K. Wungu, Suprijadi, Y. Morikawa*, and F. Muttaqien*, † These authors contributed equally ACS Catal., **16**, 5068 (2026).
   DOI:10.1021/acscatal.5c09279

5. Enhancing Atomic Structure Exploration: The Scaled-LCB and Similarity-based Structure Sharing
   S. E. P. P. Masan, T. N. Pham, K. I. M. Rojas, B. A. C. Tan, F. Rusydi, Y. Hamamoto, and Y. Morikawa, J. Ceram. Soc. Jpn. **133**, 602 (2025).
   DOI:10.2109/jcersj2.25083

MORITA, Satoshi [B class; 450 (B), 80 (C)] (350)
— *Development of tensor renormalization group method for random spin systems*

1. TeNeS-v2: Enhancement for Real-Time and Finite Temperature Simulations of Quantum Many-Body Systems
   Y. Motoyama, T. Okubo, K. Yoshimi, S. Morita, T. Aoyama, T. Kato, and N. Kawashima Comput. Phys. Commun. **315**, 109692 (2025).
   DOI:10.1016/j.cpc.2025.109692

2. Tensor renormalization group calculations of partition-function ratios
   S. Morita and N. Kawashima J. Phys. Soc. Jpn. **95**, 044001 (2026).
   DOI:10.7566/JPSJ.95.044001

Data Repository

Tensor Renormalization Group Calculations of Partition-Function Ratios
https://datarepo.mdcl.issp.u-tokyo.ac.jp/repo/63

MOTOME, Yukitoshi [C class; 9200 (B), 800 (C)] (226)
— *Theoretical study of strongly correlated quantum properties by mathematical information science*

1. Quantum reservoir probing of quantum phase transitions
   K. Kobayashi and Y. Motome Nature Communications **16**, 3871 (2025).
   DOI:10.1038/s41467-025-58751-0

2. Topological Majorana flat bands in the Kitaev model on a Bishamon-kikko lattice

K. Fukui and Y. Motome Physical Review B **112**, 14411 (2025).
DOI:10.1103/ztny-z9yb

3. Three-dimensional topological superstructure of magnetic hopfions threaded by meron strings in easy-plane magnets
S. Kasai, K. Shimizu, S. Okumura, Y. Kato, and Y. Motome Physical Review B **112**, 184424 (2025).
DOI:10.1103/l11y-9gnq

4. Spin-liquid and spin-glass behavior in quantum spin models with all-to-all p-spin interactions
S. Wadashima and Y. Motome Physical Review B **112**, 214204 (2025).
DOI:10.1103/r5d6-2cby

5. Edge of Many-Body Quantum Chaos in Quantum Reservoir Computing
K. Kobayashi and Y. Motome Physical Review Letters **136**, 040602 (2026).
DOI:10.1103/j2qj-vwcl

6. Controlling Knot Topology in Magnetic Hopfions via Spin-orbit Torque
S. Kasai, S. Okumura, and Y. Motome, accepted for publication in APS Open Science

7. Nonequilibrium dynamics of magnetic hopfions driven by spin-orbit torque
S. Kasai, S. Okumura, and Y. Motome, accepted for publication in Physical Review B

8. Kitaev Meets AKLT: Competing Quantum Disorder in Spin-3/2 Honeycomb Systems
S. Ikegami, K. Fukui, R. Pohle, and Y. Motome submitted to Physical Review B

MURAMATSU, Mayu [B class; 500 (B), 0 (C)] ()
— *Development of a FEM-MD Coupling Analysis Method*
— *Development of a MD-FEM Coupling Analysis Method*

MURAOKA, Azusa [C class; 2800 (B), 0 (C)] (110)
— *Theoretical Study Aiming at Novel Renewable Energy Materials Using First-Principles Calculations*

MURASHIMA, Takahiro [C class; 4200 (B), 350 (C)] (293)
— *Molecular dynamics simulation studies of soft matters*

1. Identifying the Threshold Chain Length for Stress Overshoot in Ring-Linear Polymer Blends under Uniaxial Elongation: The Role of Multiple Threading
T. Murashima, K. Hagita and T. Kawakatsu arXiv:2603.25505 (2026).
DOI:10.48550/arXiv.2603.25505

NADA, Hiroki [BC class; 4250 (B), 0 (C)] (296, 297)
— *A Metadynamics Simulation Study on the Mechanism of Ice VI Formation*
— *Investigation of Unknown Ice Phases Using Large-Scale Metadynamics Simulations With Unsupervised Machine Learning*

1. Multiple freezing-melting pathways of high-density ice at room temperature
Y.-H Lee, J. K. Kim, Y.-J. Kim, M. Kim, Y. C. Cho, R. J. Husband, E. Ehrenreich-Petersen, R. Bauer, F. Lehmkuhler, H.-P. Liermann, C. Strohm, K. Appel, M. Tang, Z. Konopkova, T. Eklund, K. Amann-Winkel, E. F. O ' Bannon, Z. Jenei, C.-. Yoo, H. Marquardt, H. Nada, and G. W. Lee Nat. Mater. **25**, 302 (2026).
DOI:10.1038/s41563-025-02364-x

NAKAGAWA, Naoko [C class; 4600 (B), 200 (C)] ()
— *Thermodynamics of phase separation and molecular association*

NAKAGAWA, Takeshi [B class; 900 (B), 170 (C)] (339)
— *Structural analysis of two dimensional boride using electron diffraction and DFT*
— *Surface structural analysis of single layer thin films using TensorLEED and DFT*

1. Structural investigation of pristine and Mn-intercalated flat-honeycomb bismuthene on Ag(111)
   Ziyong Zhang , Xiaobin Chen, and Takeshi Nakagawa Phys. Rev. B 113, 035436
   DOI:10.1103/nflc-z372

2. Large Hole Borophene Formation on Ni surface via Edge-Orientation Control
   X. Chen, I. Yamamoto, K. Takahashi, and T. Nakagawa, submitted

NAKAI, Fumiaki [B class; 400 (B), 0 (C)] (362)
— *Vibrated Granular System: Relation Between Viscoelastic Relaxation and Particle Dynamics*

1. Dislocation Glides in Granular Media
   F. Nakai, T. Uneyama, Y. Sasaki, K. Yoshii, and H. Katsuragi Phys. Rev. Lett. 135, 048202 (2025).
   DOI:10.1103/7g7s-c157

2. Dislocation glides in monolayered granular media: Effect of lattice constant
   F. Nakai, T. Uneyama, Y. Sasaki, K. Yoshii, and H. Katsuragi EPJ Web Conf. 340, 04008 (2025).
   DOI:10.1051/epjconf/202534004008

3. Anomalous phonon dispersion near yielding in athermal crystals
   F. Nakai, M. Otsuki, K. Saitoh, H. Katsuragi EPJ Web of Conferences
   DOI:10.48550/arXiv.2603.26825

Data Repository
Dataset for "Anomalous phonon dispersion near yielding in athermal crystals"
https://zenodo.org/records/19244125
DOI:https://doi.org/10.5281/zenodo.19244125

Dataset for "Dislocation Glides in Granular Media"
https://zenodo.org/records/14942701
DOI:https://doi.org/10.5281/zenodo.14942701

NAKAMURA, Kazuma [C class; 1000 (B), 0 (C)] (161)
— *Ab initio electronic structure analysis for Ca5Ir3O12*
— *Ab initio electronic structure calculation for grain boundary in transition metal oxides*

1. Hidden Markov model analysis of fluorescence blinking in fluorescently labeled DNA
   T. Furuta, S. Fan, T. Takada, Y. Kondo, M. Fujitsuka, A. Maruyama, K. Kawai, K. Nakamura Sci. Rep. **16**, 11306 (2026).
   DOI:10.1038/s41598-026-40876-x

2. 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

NAKAMURA, Kohji [C class; 2800 (B), 0 (C)] (109)
— *Material search and functional creation for interfacial spin-orbitronics*

1. Interface Design for Concurrent Realization of High Perpendicular Magnetic Anisotropy and Low

Magnetic Damping in Fe/MgO
Y. N. Apriati, M. Tsuchida, M. Arifin, K. Nakamura IEEE Transactions on Magnetics **62**, 4400107 (2025).
DOI:10.1109/TMAG.2025.3620412

2. Tensor representation of four-magnon interactions Hamiltonian and magnon decay rates suppression by magnetic dipolar interactions in antiferromagnetic insulator NiO
A. Gumarilang, K. Nawa, K. Nakamura Physical Review B **113**, 024411 (2026).
DOI:10.1103/kfmn-wfkg

3. Role of Rashba spinorbit coupling for voltage-controlled magnetic anisotropy at magnetic tunnel junction interface Fe/MgO
Y.-N. Apriati, M. Tsuchida, K. Nawa, K. Nakamura Applied Physics Letters **128**, 042401 (2026).
DOI:10.1063/5.0304651

4. Tailoring Spin-Exchange Interactions and Topological Magnons in 2D Ferromagnetic van der Waals CrI_3/As via Multiple Stacking Orders
A. Gumarilang, K. Nakamura Physical Review Materials **10**, 024407 (2026).
DOI:10.1103/kd5v-grhn

NAKANO, Hiroki [C class; 2800 (B), 300 (C)] (318)
— *Numerical study on low-energy states of quantum spin systems*

1. Numerical Diagonalization Study of the Phase Boundaries of the S=2 Heisenberg Antiferromagnet on the Orthogonal Dimer Lattice
H. Nakano, T. Sakai, and Y. Hosokoshi J. Phys. Soc. Jpn. 95, 033704 (2026).
DOI:10.7566/JPSJ.95.033704

2. The Haldane Gap of the $S = 7$ Antiferromagnetic Chain
H. Nakano and T. Sakai J. Low Temp. Phys. 222, 69 (2026).
DOI:10.1007/s10909-026-03406-7

NAKANO, Hiroyoshi [C class; 8000 (B), 800 (C)] (267)
— *Development of a numerical solver for three-dimensional fluctuating hydrodynamics*
— *Numerical study of the upper critical dimension of nonequlibrium critical phenomena*

1. Symmetry-based nonlinear fluctuating hydrodynamics in one dimension
Y. Minami, H. Nakano, and K. Saito Phys. Rev. Lett. **136** 187101 (2026).
DOI:10.1103/2z9s-5d7w

2. Dissipation anomaly in gradient-driven nonequilibrium steady states
H. Nakano, and Y. Minami arXiv:2511.17851
DOI:10.48550/arXiv.2511.17851

3. Looking at bare transport coefficients in fluctuating hydrodynamics
H. Nakano, Y. Minami, and K. Saito arXiv:2502.15241
DOI:10.48550/arXiv.2502.15241

NAKASHIMA, Takeru [B class; 250 (B), 0 (C)] (212)
— *Development of the real-space topology of crystals: Fundamental research for materials discovery based on homotopy of real-space crystals.*

NAKAYAMA, Akira [C class; 2400 (B), 250 (C)] (112)
— *Multiscale simulation for liquid/oxide interface based on first-principles calculations*

NARUSE, Takuya [B class; 300 (B), 60 (C)] (205)
— *Development of On-the-fly Machine Learning Potentials in High-Accuracy Phonon Calculations*

NASU, Joji [C class; 1800 (B), 150 (C)] (242)
— *Numerical analysis of excitation spectra and thermal responses arising from quasiparticles in insulating magnets*

1. Formulation of the spin Nernst effect for spin-nonconserving insulating magnets
   S. Koyama and J. Nasu Phys. Rev. B **112**, 014447 (2025).
   DOI:10.1103/8xgc-d9ch

2. Controlling discrete time crystals via single-site operations in zero-field diamond quantum simulators
   N. Egawa, K. Mizuta, and J. Nasu Phys. Rev. B **111**, 144311 (2025).
   DOI:10.1103/PhysRevB.111.144311

3. Magnetic-Field Effect on Excitonic Condensation Emergent in Extended Falicov-Kimball Model
   N. Ohta and J. Nasu J. Phys. Soc. Jpn. **94**, 054702 (2025).
   DOI:10.7566/JPSJ.94.054702

NIKI, Kaori [C class; 1400 (B), 400 (C)] (139)
— *Electronic state calculations under photoinduced reactions*

1. Femtosecound concerted rotation of molecules on a 2D material interface
   K. Baumgrtner, M. Nozaki, M. Reuner, N. Wind, M. Haniuda, C. Metzger, M. Heber, D. Kutnyakhov, F. Pressacco, L. Wenthaus, K. Hara, K. Chordiya, C.-H. Min, M. Beye, F. Reinert, F. Roth, S. Kr Mahatha, A. Madsen, T. Wehling, K. Niki, D.P. Gorelova, K. Rossnagel, M. Scholz
   Nat. Commun C, 17, 2110 (2026).
   DOI:10.1038/s41467-026-69801-6

NISHIDATE, Kazume [C class; 600 (B), 0 (C)] (175)
— *Surface electronic structure of double perovskite*

1. Electrophoretic deposition films and photocatalytic activities for doubleperovskite oxide $Ba_2Ce(Bi,Sb)O_6$
   H. Sakou, K. Hata, M. Matsukawa, M. Arakida, K. Nishidate, S. Aisawa, K. Akiba, and D.C. Roy
   J Mater Sci: Mater Electron **36**, 1800 (2025).
   DOI:10.1007/s10854-025-15846-0

Data Repository
Computer simulation with C
http://web.cc.iwate-u.ac.jp/ñisidate/main.pdf

NISHIGUCHI, Kazutaka [B class; 300 (B), 60 (C)] (203)
— *First-principles study of point defects in perovskite photocatalyst $PbTiO_3$*

NISHIKAWA, Yoshihiko [C class; 3400 (B), 0 (C)] (309)
— *Numerical study on finite-time non-equilibrium phase transitions*

NOGUCHI, Hiroshi [C class; 4800 (B), 400 (C)] (287)
— *structure formation of biomembrane*

1. Dynamic modes of active Potts models with factorizable numbers of states
   H. Noguchi Phys. Rev. Res. 7, 033243 (2025).
   DOI:10.1103/w1fg-6qmv

2. Coarsening dynamics for spiral and disordered waves in active Potts models
H. Noguchi Phys. Rev. E 113, 054108 (2026).
DOI:10.1103/sc5g-rpvs

3. Spiral, target, stripe, and disordered waves in active six-state Potts models
H. Noguchi arXiv:2604.22353
DOI:10.48550/arXiv.2604.22353

Data Repository
Data of Monte Carlo Simulations of Active Potts Models
https://isspns-gitlab.issp.u-tokyo.ac.jp/hiroshi.noguchi/activePotts

NOGUCHI, Yoshifumi [C class; 7800 (B), 750 (C)] (57)
— *Development of full-frequency electron-hole interaction kernel*
— *Development of self-interaction-corrected GWΓ method*

1. Significance of self-interaction corrections in the GWΓ method
T. Isago, Y. Noguchi, and K. Ohno Phys. Rev. B, **111**, 195146 (2025).
DOI:10.1103/PhysRevB.111.195146

NOMURA, Yusuke [E class; 13000 (B), 1000 (C)] (221)
— *Study on nickelate superconductors using transformer-based wave functions*

1. Strong-coupling high- superconductivity in doped correlated band insulators
Yusuke Nomura, Motoharu Kitatani, Shiro Sakai, and Ryotaro Arita Phys. Rev. B **112**, L020504 (2025).
DOI:10.1103/dygc-94fq

NOZAWA, Kazuki [C class; 1600 (B), 500 (C)] (133)
— *First-principles study of surface atomic structure and chemical properties of intermetallic compounds*

1. Creation of novel Pd single-atom catalysts using complex intermetallic compound $Al_{13}Fe_4$
M. Hanaoka, S. Iwado, K. Nozawa, M. Aoyama, S. Ohhashi, N. Fujita, and S. Kameoka Applied Materials Today, ¥bf 46, 102878 (2025).
DOI:10.1016/j.apmt.2025.102878

2. Toward Accurate Modeling of Aperiodic Surfaces: Cluster-Based DFT Analysis of Pentacene on Cu(111) Surface
M. Sato and K. Nozawa Materials Transactions, in press

NUNOURA, Teppei [B class; 600 (B), 0 (C)] (174)
— *Interface characterization and performance optimization of Ni/CeO_2-Al_2O_3 catalysts: A combined DFT and experimental study*
— *Theoretical study on catalytic hydrogenolysis mechanism of lignin structural units over Ni/CeO_2-Al_2O_3 based on first-principle calculations*

OBATA, Masao [B class; 750 (B), 180 (C)] (168)
— *Development of quasiparticle self-consistent GW calculation code and its application to interfacial materials*
— *Development of quasiparticle self-consistent GW calculation code and its application to metals and magnetic materials*

1. Efficient implementation of the quasiparticle self-consistent GW method on GPU
Masao Obata, Takao Kotani, Tatsuki Oda Comp. Mat. Sci. 260, 114190 (2025).
DOI:10.1016/j.commatsci.2025.114190

OCHI, Masayuki [C class; 5000 (B), 0 (C)] (76)
— *Development of the optimization method for the long-range correlation factor in the first-principles wave-function theory*

1. Theoretical study on the possibility of high T_c $s\pm$-wave superconductivity in heavily hole-doped infinite layer nickelates
   H. Sakakibara, R. Mizuno, M. Ochi, H. Usui, and K. Kuroki Phys. Rev. B **111**, 224511 (2025).
   DOI:10.1103/nl4m-n5dx

2. Possible high thermoelectric power factor in alkali-metal-intercalated BC_3: Anisotropic multiple valleys originating from the van Hove singularity of graphene
   R. Enami, K. Kuroki, and M. Ochi Phys. Rev. Mater. **9**, 084001 (2025).
   DOI:10.1103/rqrv-7hqt

ODA, Masato [B class; 400 (B), 0 (C)] ()
— *Diffusion reactions of large defects in GaN and GaN/AlN*

ODA, Tatsuki [C class; 7000 (B), 750 (C)] (60, 61)
— *Analyses on electronic structure and magnetic anisotropy in high-performance spintronics magnetic materials and development/application in quasi-particle self-consistent GW code*
— *Development/application in quasi-particle self-consistent GW and analyses on magnetic anisotropy in spintronics magnetic materials*

1. Layer-resolved Rashba spin-orbit coupling of ferromagnetic interface from a first-principles study
   I. Pardede, M. Obata, D. Yoshikawa, T. Kanagawa, N. Ikhsan, and T. Oda Key Engineering Materials, **1015**, 23 (2025).
   DOI:10.4028/p-3gsPr4

2. Efficient implementation of the quasiparticle self-consistent GW method on GPU
   M. Obata, T. Kotani, and T. Oda Computational Materials Science, **260**, 114190 (2025).
   DOI:10.1016/j.commatsci.2025.114190

3. Role of magnetic ordering on transformation properties of Heusler Ni_2MnGa magnetic shape memory alloy
   J. Lutinec, M. Obata, P. Sedlk, J. Hamrle, H. Seiner, O. Heczko, and T. Oda J. Phys.: Condens. Matter, **38**, 015502 (2026).
   DOI:10.1088/1361-648X/ae2a9a

4. Machine learning band gap predictions: linking quasiparticle self-consistent GW and LDA-derived partial density of states
   S. Takano, T. Kotani, M. Obata, K. Sato, H. Saito, and T. Oda Jpn. J. Appl. Phys., **65**, 031002 (2026).
   DOI:10.35848/1347-4065/ae3bc0

5. Optical and electronic spectra in a transparent transition-metal oxide $LiTi_2O_4$ from first-principles quasiparticle self-consistent GW calculations
   H. Niwa, M. Obata, T. Kotani, and T. Oda Phys. Rev. B, **113**, 155114 (2026).
   DOI:10.1103/hsmv-pgd7

OHKUBO, Yuji [B class; 850 (B), 0 (C)] (169)
— *Calculation of adsorption energy of fluorinated molecules on chromate conversion coating layer containing hydroxyl groups using DFT+U method*
— *Calculation of adsorption energy of fluorinated molecules on chromate conversion coating layer using*

DFT+U method

OHMURA, Satoshi [C class; 3600 (B), 100 (C)] (98, 99)
— *Ab Initio Molecular Dynamics Study of the Structural Instability of Ettringite under Dehydration and Rehydration Conditions*
— *Ab initio molecular-dynamics study on self-healing in cement-based hydrated minerals*

1. Local structure and mechanical properties of 1.1 nm tobermorite under compression and recompression using ab initio molecular dynamics simulations
   I. KANEMASU, and S. OHMURA High Pressure Reserch, 1-9 (2026).
   DOI:10.1080/08957959.2026.2660933

OHNISHI, Masato [E class; 21500 (B), 1900 (C)] (40)
— *Construction of anharmonic phonon property database using first-principles calculations*
— *Data creation for higher-order anharmonic phonon properties*

1. 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 npj Computational Materials
   DOI:10.1038/s41524-026-02033-w

Data Repository
Phonix
https://huggingface.co/phonix-db
DOI:10.57967/hf/8233

OHNO, Kaoru [C class; 4400 (B), 400 (C)] (78)
— *Improvement and application of all-electron mixed basis program*

1. Significance of Self-Interaction Corrections in GWΓ Method
   Tamao Isago, Yoshifumi Noguchi, and Kaoru Ohno Phys. Rev. B **111**, 195146 (2025).
   DOI:10.1103/PhysRevB.111.195146

2. First-Principles Self-Interaction Free GWΓ Simulations for First Ionization Potentials and Electron Affinities
   Tamao Isago, Yoshifumi Noguchi, and Kaoru Ohno J. Chem. Phys. **164**, 144110 (2026).
   DOI:10.1063/5.0317103

3. Temperature-dependent electron-capture decay rate of ^{7}Be in a Nb crystal
   Riichi Kuwahara, Tsutomu Ohtsuki, Hidetoshi Yamaguchi, Takashi Hashimoto, Yasuo Wakabayashi, Seiya Hayakawa, Daid Kahl, Shigeru Kubono, Kentaro Hirose, and Kaoru Ohno Phys. Rev. C **113**, 113, 044617 (2026).
   DOI:10.1103/kgsv-fgs4

OHSAWA, Kazuhito [C class; 1200 (B), 0 (C)] (154)
— *Study of interaction between radiation damage and lattice defect*

OHTSUKI, Tomi [C class; 5200 (B), 450 (C)] (279)
— *Critical behavior of measurement induced transition*

1. Universal Stochastic Equations of Monitored Quantum Dynamics
   Z. Xiao, T. Ohtsuki, K. Kawabata Phys. Rev. Lett. **134**, 140401 (2025).
   DOI:10.1103/PhysRevLett.134.140401

2. Predicting unmeasured asymmetry time spectra in μSR experiments using Random Forest
K.F. Chin, M.R. Omar, T.L. Yoon, Y. Komiyama, D.P. Sari, W.N. Zaharim, T. Ohtsuki, T. Adachi, T. Goto, I. Watanabe J. Magn. Magn. Mat. **629**, 173320 (2025).
DOI:10.1016/j.jmmm.2025.173320

3. Adaptive interpolating quantum transform: A quantum-native framework for efficient transform learning
G Budiutama, S Daimon, H Nishi, R Kaneko, T Ohtsuki, Y Matsushita Phys. Rev. A **112**, 062410 (2025).
DOI:10.1103/vyr3-h9hq

OKUBO, Tsuyoshi [C class; 9600 (B), 850 (C)] (264)
— *Novel phenomena in frustrated magnets*

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

2. TeNeS-v2: Enhancement for Real-Time and Finite Temperature Simulations of Quantum Many-Body Systems
Y. Motoyama, T. Okubo, K. Yoshimi, S. Morita, T. Aoyama, T. Kato, and N. Kawashima Computer Physics Communications **315**, 109692 (2025).
DOI:10.1016/j.cpc.2025.109692

3. Thermal Hall transport in Kitaev spin liquids
T. Okubo, J. Nasu, T. Misawa, and Y. Motome arXiv:2507.16558
DOI:10.48550/arXiv.2507.16558

4. Plastic tensor networks for interpretable generative modeling
K. O. Akamatsu, K. Harada, T. Okubo, and N. Kawashima Machine Learning: Science and Technology **7**, 015014 (2026).
DOI:10.1088/2632-2153/ae3048

OKUMURA, Hisashi [C class; 5000 (B), 400 (C)] (286)
— *Molecular dynamics simulation of disease-causing protein aggregates*

ONO, Atsushi [B class; 600 (B), 100 (C)] (247)
— *Analysis of nonlinear response functions through real-time evolution*

1. Extracting Nonlinear Dynamical Response Functions from Time Evolution
A. Ono Phys. Rev. Lett. **135**, 026401 (2025).
DOI:10.1103/qsxr-c2pq

2. Temporal modulation of second harmonic generation in ferroelectrics by a pulsed electric field
A. Ono Phys. Rev. B **112**, 115146 (2025).
DOI:10.1103/xsrf-t1hj

ONO, Shota [B class; 1300 (B), 240 (C)] (145, 146)
— *A novel framework for predicting non-van der Waals 2D materials*
— *Prediction of quasi-2D materials in non-layered materials based on stacking fault and cleavage energy calculations*
— *What can be mixed with noble metals to enhance their brightness?*

1. Composition-dependent ultrafast luminescence in Cu-Ni alloys: Combined experimental and ab initio study
   T. Suemoto, H. Morino, S. Ono, T. Okuno, T. Suzuki, K. Okazaki, S. Tani, and Y. Kobayashi Phys. Rev. B **112**, 035138 (2025).
   DOI:10.1103/xn1s-28z3

2. Framework for identifying nonvan der Waals two-dimensional materials
   S. Ono Phys. Rev. B **112**, 075403 (2025).
   DOI:10.1103/crw6-zvpx

Data Repository
Crystal structure and thin film energy for non-van der Waals 2D materials
https://zenodo.org/records/16187681
DOI:doi.org/10.5281/zenodo.16187681

ONO, Tomoya [C class; 11000 (B), 950 (C)] (46)
— *First-principles study on functionality of electronic devices*

1. Theoretical investigation of interface atomic structure of graphene on NiFe alloy substrate
   N. Matsumoto, R. Endo, M. Uemoto, and T. Ono J. Appl. Phys. **138**, 104305 (2025).
   DOI:10.1063/5.0283881

2. Effects of inserted methylene groups on structure and flexibility of molecule junction system
   M. Furushima, T. Tahara, M. Uemoto, Y. Majima, and T. Ono Jpn. J. Appl. Phys. submitted.

OSHIKAWA, Masaki [B class; 450 (B), 80 (C)] ()
— *Elucidation of conformal field theory on closed manifolds by tensor network*

OSHIYAMA, Atsushi [C class; 4000 (B), 350 (C)] ()
— *Clarification of Microscopic Mechanisms of Semiconductor Epitaxial Growth and Device-Interface Formation by Large-Scale Quantum-Theory-Based Computations*

OTSUKI, Junya [C class; 8000 (B), 300 (C)] (228)
— *Dynamical mean-field calculation of non-linear electric conductivity under magnetic toroidal ordering*
— *Study of multipolar fluctuations and cross-correlated responses by dynamical mean-field theory*

1. From localized $4f$ electrons to anisotropic exchange interactions in ferromagnetic $CeRh_6Ge_4$
   S. Itokazu, A. Kirikoshi, H. O. Jeschke, and J. Otsuki Commun. Mater. **6**, 269 (2025).
   DOI:10.1038/s43246-025-00998-7

2. Multipolar fluctuations from localized $4f$ electrons in $CeRh_2As_2$
   K. Numa, E. Matsuda, A. Kirikoshi, and J. Otsuki Phys. Rev. B **113**, 115141 (2026).
   DOI:10.1103/nw88-plgx

OTSUKI, Michio [B class; 550 (B), 90 (C)] (343)
— *Shape dependence of dynamic friction in viscoelastic materials*

OYA, Yutaka [C class; 3600 (B), 200 (C)] (305)
— *Evaluation of Self-Healing Performance and Microscopic Damage in Vitrimers via Molecular Simulations*

1. Molecular Mechanism of Disulfide Bond Healing and Network Repair in Epoxy Vitrimers Revealed by Quantum Chemical and Molecular Dynamics Simulations
   T. Uyama, N. Kishimoto, Y. Oya, T. Murashima and J. Koyanagi Polymers **18**, 861 (2026).
   DOI:10.3390/polym18070861

OZEKI, Yukiyasu [C class; 3400 (B), 500 (C)] (303)
— *Deepening studies for critical universality with high precision dynamical scaling analysis*
— *High precision study on critical phenomena by relaxation analysis of fluctuations using machine learning*

PETERS, Robert [C class; 2200 (B), 350 (C)] (238)
— *Nonequilibrium phenomena in strongly correlated systems*
1. The toric code under antiferromagnetic isotropic Heisenberg interactions
W. Jang, R. Peters, T. Posske arXiv:2603.05707 (under review).

PHUNG, Manh Quan [C class; 600 (B), 0 (C)] ()
— *Density Functional Theory Investigation of Sodium Intercalation and Ion Migration Mechanisms in Next-Generation Battery Electrode Materials*

POHLE, Rico [C class; 2200 (B), 250 (C)] (241)
— *Dynamical properties of spin nematic phases*
1. Electron-phonon coupled Langevin dynamics for Mott insulators
R. Pohle, Y. Motome, T. Tadano, and S. Hoshino preprint (arXiv:2507.19764)
DOI:10.48550/arXiv.2507.19764

RAEBIGER, Hannes [C class; 4000 (B), 350 (C)] (85)
— *High-entropy MXenes and MAX-phase materials*
1. Prediction of superconductivity in haeckelite compounds using first-principles calculations
K. Hamidi, M. Keivanloo, M. Sandoghchi, M. R. Mohammadizadeh, H. Raebiger, K. Hongo, R. Maezono, K. Ohno, and M. Khazaei iScience **28**, 113219 (2025).
DOI:10.1016/j.isci.2025.113219

2. Diverse surface reconstructions in MAX phases
M. Khazaei, M. Bagheri, A. Ranjbar, S. Bae, R. Khaledialidusti, Y. Mochizuki, T. D. Kühne, K. Shudo, H. Raebiger, H.-P. Komsa, and H. Hosono Nanoscale **17**, 24184 (2025).
DOI:10.1039/D5NR02421H

SAKAGUCHI, Norihito [C class; 7600 (B), 0 (C)] (62)
— *Reduction of Rare Metals in Fuel Cell and Formic Acid Decomposition Catalysts*
1. Real-Space Observation of Spin-Induced Lattice Distortion of O_2 Monolayers Revealed by Atomic Force Microscopy
M. Kimura, Y. Kunisada, and Y. Sugimoto ACS Nano **20**, 2633 (2026).
DOI:10.1021/acsnano.5c11357

2. Tailoring Catalytic Properties via Light-Element Doping into Graphene Supports
Y. Kunisada, K. Sato, and N. Sakaguchi Vacuum and Surface Science **69**, 135 (2026).
DOI:10.1380/vss.69.135

SAKAI, Shiro [B class; 450 (B), 90 (C)] (347)
— *Numerical simulation of disordered hyperuniform electron systems*

SAKAI, Toru [C class; 5600 (B), 300 (C)] (275, 277)
— *Magnetization Process of the S=3/2 Antiferromagnetic Chain*
— *Numerical Study on the Magnetization Process of the S=1 Spin Ladder*

1. Translational-Symmetry-Broken Magnetization Plateaux of the $S = 3/2$ Anisotropic Antiferromagnetic Chain
T. Kawatsu, H. Suzuki, M. Hashimoto, K. Doi, T. Houda, R. Furuchi, H. Nakano, K. Okamoto, T. Sakai Journal of the Physical Society of Japan, 94, 064701 (2025).
DOI:10.7566/JPSJ.94.064701-1-7

2. Possible Spin Gap Transition of ESR at the Magnetization Plateau of the Distorted Diamond Spin Chain
T. Sakai Applied Magnetic Resonance, 56, 1499 (2025).
DOI:10.1007/s00723-025-01788-7

3. Translational Symmetry Broken Magnetization Plateau of the S=1/2 Anisotropic Spin Ladder with Ferromagnetic Rung Interaction
T. Sakai, K. Doi, K. Okamoto, K. Okunishi, M. Hashimoto, T. Houda, R. Furuchi, and H. Nakano Journal of Physics: Conference Series, 3161, 012004 (2026).
DOI:10.1088/1742-6596/3161/1/012004

4. Magnetization Plateau of the S=1/2 Distorted Diamond Spin Chain with Ferromagnetic Interaction
M. Hashimoto, K. Doi, T. Houda, R. Furuchi, H. Nakano, K. Okamoto, T. Sakai Journal of Physics: Conference Series, 3161, 012006 (2026).
DOI:10.1088/1742-6596/3161/1/012006

5. Field-Induced Spin Nematic Liquid of the S=1/2 Kondo Necklace Spin Chain
R. Hasegawa, Y. Hamazaki, T. Kawatsu, H. Suzuki, T. Houda, H. Nakano, K. Okamoto and T. Sakai AIP Advances 16, 025102 (2026).
DOI:10.1063/9.0000960

6. Magnetization plateau of the S = 1 spin ladder with anisotropies
Y. Hamazaki, R. Hasegawa, T. Kawatsu, H. Suzuki, T. Houda, H. Nakano, K. Okamoto and T. Sakai AIP Advances 16, 025302 (2026).
DOI:10.1063/9.0000956

7. Spin nematic phase of the ferromagnetic dimer system on the Shastry-Sutherland lattice
T. Sakai AIP Advances 16, 025006 (2026).
DOI:10.1063/9.0000952

8. Magnetization Plateaus of the Antiferromagnetic Chain with Competing Anisotropies
T. Sakai, T. Houda, T. Kawatsu, H. Suzuki, R. Hasegawa, Y. Hamazaki, H. Nakano, K. OKamoto Journal of Low Temperature Physice. 222, 1 (2026).
DOI:10.1007/s10909-025-03333-z

9. The Haldane Gap of the S = 7 Antiferromagnetic Chain
H. Nakano and T. Sakai Journal of Low Temperature Physics. 222, 69 (2026).
DOI:10.1007/s10909-026-03406-7

10. Spin excitation of the Heisenberg antiferromagnet with frustration: from the bounce-lattice antiferromagnet through the maple-leaf-lattice antiferromagnet to the exact-dimer system
H. Nakano and T. Sakai to appear in Zeitschrift für Naturforschung A

SAKAKIBARA, Hirofumi [CD class; 7700 (B), 730 (C)] (58)
— Study of unconventional multi-orbital and -layer superconductors in first-principles
— Theoretical exploration of ambient pressure superconducting materials based on multilayer mixed anion nickel oxide systems

1. Theoretical study on the possibility of high T_c $s\pm$-wave superconductivity in heavily hole-doped infinite layer nickelates
H. Sakakibara, R. Mizuno, M. Ochi, H. Usui, K. Kuroki Phys. Rev. B 111, 224511 (2025).
DOI:10.1103/PhysRevB.109.L201124

SAKASHITA, Tatsuya [B class; 150 (B), 140 (C)] ()
— *Development of integrated interface of eigensolvers Rokko and application to quantum spin systems*

SASAKI, Takehiko [C class; 3600 (B), 600 (C)] (87, 88)
— *Study on poisoning of Pt nanoparticles with sulfur by first principles calculations*
— *Study on surface diffusion of adsorbed hydrogen atoms on Ru(001)*
1. Cyclic Voltammetry − Synchronized Operando HERFD-XANES and RIXS Analyses of Adsorbed Structures and Bonding States of Active Oxygen Species on Pt Nanoparticle Electrocatalysts in PEFC
H. Ariga-Miwa, T. Sasaki, T. Sakata, K. Higashi, T. Yoshida, O. Sekizawa, T. Kaneko, T. Uruga, and Y. Iwasawa ACS Catal. **15**, 9856 (2025).
DOI:10.1021/acscatal.5c01160

SATO, Naoki [AC class; 3300 (B), 50 (C)] (106)
— *Complementary analysis of chemical pressure and lattice dynamics in complex crystal structures*
— *Effects of anomalous chemical bonding and local structures on thermal transport and thermoelectric properties*

SATO, Ryuhei [C class; 2400 (B), 0 (C)] (124)
— *Understanding the super high-pressure synthesis of superhydride by machine-learning MD simulation*
1. Surface melting–driven hydrogen absorption for high-pressure polyhydride synthesis
Ryuhei Sato, Lewis J. Conway, Di Zhang, Chris J. Pickard, Kazuto Akagi, Kartik Sau, Hao Li, and Shin-ichi Orimo Proceedings of the National Academy of Sciences USA 122, e2413480122 (2025).
DOI:10.1073/pnas.2413480122

2. Visualizing Concerted Ion Migration of Superionic Conductors via Directed Graphs
Ryuhei Sato, Yasunobu Ando, Kartik Sau, and Yasushi Shibuta Chemistry of Materials 38, 287 (2026)..
DOI:10.1021/acs.chemmater.5c02374

3. Competing Hydrogenation Pathways to Metastable CaH_6 Revealed by Machine-Learning-Potential Molecular Dynamics
Ryuhei Sato, Peter I. C. Cooke, Maelie Causse, Hung Ba Tran, Seong Hoon Jang, Di Zhang, Hao Li, Shin-ichi Orimo, Yasushi Shibuta, Chris J. Pickard arXiv:2603.08950
DOI:10.48550/arXiv.2603.08950

SATO, Shunsuke [C class; 3600 (B), 0 (C)] (15)
— *Microscopic investigation on light-induced nonlinear and ultrafast phenomena in semiconductors*
1. Polarized Houston State Framework for Nonequilibrium Driven Open Quantum Systems
Shunsuke A. Sato, Hannes Hübener, Umberto De Giovannini, Angel Rubio arXiv:2507.20160
DOI:10.48550/arXiv.2507.20160

SATO, Takeshi [B class; 400 (B), 70 (C)] (351)
— *Phase structure and rheology in polymer blends: A molecular dynamics simulation study*

SAU, Kartik [C class; 2200 (B), 0 (C)] (129)
— *Designing Advanced Hydride Materials Toward Next-Generation Battery, Hydrogen Storage and Heat Management Systems using Computer Simulation*

SEINO, Kaori [C class; 3600 (B), 550 (C)] (91)
— *First-principles study of surface and defect systems for power-electronics materials II*

1. Atomic and electronic structures of point defects related to vacancy-mediated mechanism of Mg diffusion in GaN
   K. Seino , K. Shiraishi, and A. Oshiyama Jpn. J. Appl. Phys. **64**, 121004 (2025).
   DOI:10.35848/1347-4065/ae2174

2. Diffusion mechanisms via vacancies of a magnesium acceptor in gallium nitride
   K. Seino, K. Shiraishi, and A. Oshiyama Phys. Rev. B **113**, 045201 (2026).
   DOI:10.1103/ybl9-fqwz

SEKI, Yuya [B class; 350 (B), 60 (C)] ()
— *Analysis of Ising model in statistical-mechanical informatics*

SEO, Insung [C class; 1200 (B), 0 (C)] (152)
— *First-principles study on magnetocrystalline anisotropy of $RFe_{12}X$*

1. Lithiation of Epitaxial Monolayer Borophene
   Kamal, Sherif ; Seo, Insung; Cojocariu, Iulia; Jugovac, Matteo; Locatelli, Andrea; Gohda, Yoshihiro; Kralj, Marko; Mente, Tevfik; Petrovi, Marin In revision

SHIMADA, Takahiro [B class; 1050 (B), 190 (C)] (150)
— *Ab initio DFT study of lattice defect electronic structures for emergent polar skyrmions*
— *First-principles lattice defects engineering for polar skyrmions and their lattices*

SHIMAMURA, Kohei [C class; 2000 (B), 250 (C)] (126)
— *Improving Stability of Molecular Dynamics Simulation using Machine-Learning Interatomic Potentials II*

SHIMIZU, Koji [C class; 8000 (B), 800 (C)] (56)
— *Analysis of Atomic and Ionic Behavior in Complex Structures Using First-Principles Calculations and Machine Learning*
— *Atomic and Ionic Behavior Analysis in Complex Structures via First-Principles Calculations and Machine Learning*

1. 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. **23**, 188 (2025).
   DOI:10.1380/ejssnt.2025-028

2. Charge States of Ions around Σ 5(310)/[001] Grain Boundary in Cubic-ZrO2 Revealed by First-Principles Calculations
   S. Arai, K. Shimizu, A.K.A. Lu, H. Masuda, H. Yoshida, S. Watanabe e-J. Surf. Sci. Nanotechnol. **23**, 323 (2025).
   DOI:10.1380/ejssnt.2025-044

3. Reactivity of high-entropy alloy CoCuFeMnNi surface toward CO adsorption and CO2 conversion processes: A combined density functional theory and machine learning study
   E.R. Beronio, M. Palmero, H.O. Tubalinal, A.N. Hipolito, T. Chookajorn, K. Shimizu, A.A. Padama Surf. Interfaces **82**, 108457 (2026).
   DOI:10.1016/j.surfin.2026.108457

4. Study of the ion mobility in defect-laden ZrO2 under an electric field using neural network with predictions for Born effective charges
   A.K.A. Lu, N. Maekawa, A. Ikeda, K. Shimizu, H. Masuda, H. Yoshida, S. Watanabe Phys. Rev. Mater. under review.

5. Exploring the low-temperature synthesis pathway of lithium ionic conductor garnet-type solid electrolytes
   K. Onoue, A. Nasu, Y. Douchi, S. Mori, H. Kobayashi, K. Shimizu, M. Matsui ACS Appl. Energy Mater. under review.

6. Distance-Insensitive Graph Neural Networks and Multi-Task Learning for Accurate Prediction of Adsorption Energies on Alloy Nanoclusters
   K. Otsuka, A.K.A. Lu, K. Shimizu, S. Watanabe Computer. Mater. Sci. under review.

SHIMIZU, Makoto [C class; 5200 (B), 0 (C)] (230)
— *Spin fluctuations and superconductivity in UTe2 under pressure*
— *Spin fluctuations and superconductivity in heavy-fermion systems*

SHIMOJO, Fuyuki [C class; 3200 (B), 300 (C)] (101)
— *First-Principles Molecular-Dynamics Study of Structural and Electronic Properties of Disordered Materials under Extreme Conditions*

1. Bonding nature of Cu^{2+} in distorted tetragonal pyramidal coordination in clinoclase and callaghanite
   Masaaki Misawa, Akira Yoshiasa, Fuyuki Shimojo, Makoto Tokuda, Satoko Ishimaru, Kazumasa Sugiyama J. Mineral. Petrol. Sci. **120**, 240925 (2025).
   DOI:10.2465/jmps.240925

2. Intermolecular Correlations in Liquid Racemic Lactic Acid: A Comparison with Liquid L-Lactic Acid
   K. Ito, H. Shimakura, S. Tahara, K. Ohara, A. Koura, K. Shimamura, and, and F. Shimojo J. Phys. Soc. Jpn. **94**, 044604 (2025).
   DOI:10.7566/JPSJ.94.044604

3. Structural Insights into Liquid Malic and Lactic Acids from First-Principles Simulations and X-ray Diffraction
   Wataru Sugimoto, Kai Ito, Hironori Shimakura, Shuta Tahara, Koji Ohara, Akihide Koura, Kohei Shimamura, and Fuyuki Shimojo J. Phys. Soc. Jpn. **95**, 014602 (2026).
   DOI:10.7566/JPSJ.95.014602

SHIMOKAWA, Tokuro [C class; 9400 (B), 850 (C)] (266)
— *Multipartite entanglement in quantum frustrated magnets*

SHINAOKA, Hiroshi [B class; 500 (B), 90 (C)] ()
— *Parallelizing quantics tensor cross interpolation*

SHINODA, Wataru [E class; 28000 (B), 2200 (C)] (258)
— *Large-Scale Molecular Simulations of Soft Matter Using All-Atom and Coarse-Grained Models*
— *Large-scale Molecular Simulation of Soft Materials using All-Atom and Coarse-Grained Model*

1. SPICA Force Field for Nucleic Acids and Its Application to Lipid Nanoparticles
   Akhil Pratap Singh, Hiroki Tanaka, Yusuke Miyazaki, Wataru Shinoda J. Phys. Chem. B **129**, 7939 (2025).
   DOI:10.1021/acs.jpcb.5c01729

2. In Silico Study of Ionizable Lipid Nanoparticles Using the SPICA Force Field
Akhil Pratap Singh, Hiroki Tanaka, Yusuke Miyazaki, Shusaku Nagano, Wataru Shinoda J. Chem. Theory Comput. **21**, 6226 (2025).
DOI:10.1021/acs.jctc.5c00498

3. Unraveling the Molecular Mechanism of Transient Multilamellar Formation in Ethanol-Modified Vesicle Solutions
Kana Shibata, Masatoshi Maeki, Manabu Tokeshi, Wataru Shinoda Langmuir **41**, 13372 (2025).
DOI:10.1021/acs.langmuir.5c01139

4. A Melittin-Derived Peptide with Improved Cytosolic Delivery Efficiency through Caveolae-and Actin-Mediated Endocytosis
Yoshimasa Kawaguchi, Naoki Tamemoto, Yusuke Uehata, Yusuke Miyazaki, Wataru Shinoda, Shiroh Futaki Chem. Pharm. Bull. **73**, 896 (2025).
DOI:10.1248/cpb.c25-00479

5. Molecular Insight into the Hepatitis B Virus: Coarse-Grained Simulations of the EnvelopeCapsid Complex
Ryo Urano, Wataru Shinoda J. Phys. Chem. Lett. **17**, 77 (2026).
DOI:10.1021/acs.jpclett.5c03156

6. Asymmetry and Heterogeneity in the Plasma Membrane
Teppei Yamada, Wataru Shinoda Biophys. J. **125**, 387 (2026).
DOI:10.1016/j.bpj.2025.06.026

7. Hydrophobicity-Governed Protein Adsorption on Poly (ω-methoxyalkyl acrylate) Surfaces: A Coarse-Grained Molecular Dynamics Study
Hari OS Yadav, An-Tsung Kuo, Shingo Urata, Kosuke Funahashi, Yutaka Imamura, Wataru Shinoda J. Chem. Theory Comput. **21**, 10561 (2025).
DOI:10.1021/acs.jctc.5c01218

8. Structural insights into a citrate transporter that mediates aluminum tolerance in barley
Tran Nguyen Thao, Namiki Mitani-Ueno, Ryo Urano, Yasunori Saitoh, Peitong Wang, Naoki Yamaji, Jian-Ren Shen, Wataru Shinoda, Jian Feng Ma, Michihiro Suga Proc. Natl. Acad. Sci. U.S.A. **122**, e2501933122 (2025).
DOI:10.1073/pnas.2501933122

9. Membrane Pore Formation Unveiled by ∞ RETIS Path Sampling: From Thinning to Flip-Flop
Daniel Tianhou Zhang, Lukas Baldauf, Grzegorz Lazarski, Titus S van Erp, Wataru Shinoda J. Chem. Theory Comput. **22**, 3072 (2026).
DOI:10.1021/acs.jctc.5c01814

10. Design of Liquid Electrolytes for Next-Generation Batteries Based on Analysis of Ion Dynamics
Keisuke Shigenobu, Seiji Tsuzuki, Wataru Shinoda, Kazuhide Ueno BUNSEKI KAGAKU **74**, 427 (2025).
DOI:10.2116/bunsekikagaku.74.427

11. Discrepant lithium transference numbers due to heterogeneous speciation
Frederik Philippi, Yuna Matsuyama, Simon Buyting, Taku Sudoh, Keisuke Shigenobu, Wataru Shinoda, Monika Schnhoff, Masayoshi Watanabe, Kazuhide Ueno Phys. Chem. Chem. Phys. **27**, 15185 (2025).
DOI:10.1039/D5CP00222B

12. Polymer‐Assisted Supercooled Lithium Salts: Nonflammable Single‐Ion Conducting Liquid Elec-

trolytes for Next - Generation Batteries
Taku Sudoh, Keisuke Shigenobu, Frederik Philippi, Choji Niwamura, Yosuke Ugata, Yuna Matsuyama, Shinji Kondou, Seiji Tsuzuki, Saki Sawayama, Kenta Fujii, Wataru Shinoda, Kazuhide Ueno Adv. Energy Mater. **16**, e05229 (2026).
DOI:10.1002/aenm.202505229

SHINOHARA, Yasushi [C class; 1000 (B), 0 (C)] (160)
— *First-principles simulations for time-resolved diffraction imaging of crystalline solids*

SHIOMI, Junichiro [E class; 21000 (B), 1600 (C)] ()
— *Analysis of phonon transport properties in surface modified systems*
— *Disorder-Driven Phonon Engineering for Advanced Thermal Management in Twisted and Amorphous Materials*

SHIRAI, Tatsuhiko [B class; 350 (B), 0 (C)] (371)
— *Scrambling in long-range interacting quantum systems*

1. Out-of-time-order correlator computation based on a discrete truncated Wigner approximation
   T. Shirai, and T. Mori Phys. Rev. B **112**, 014309 (2025).
   DOI:10.1103/lxwb-ql9q

SHIRAISHI, Kenji [C class; 10300 (B), 0 (C)] (50, 51)
— *Clarification of Atomic Level Operation Mechanism of New Vibration-Powered Generator Using Si/SiO2 Interfaces*
— *Theoretical Studies on the Electron Traps in a-SiN for Flash Memory Application*

1. Space-induced floating electronic states in non-stoichiometric amorphous silicon nitride for memory devices applications
   M. Boero, K. Shiraishi, T. Nagahashi, F. Nanataki, and A. Oshiyama Phys. Rev. Materials **9**, 084601(2025).
   DOI:10.1103/mc16-76ck

SHUDO, Ken-Ichi [B class; 400 (B), 80 (C)] (184)
— *Band tuning of ZnO with varied impurity*

SUGINO, Osamu [C class; 2400 (B), 200 (C)] (119)
— *Mechanism of fast ion conductivity*

1. Elucidation of superionic conduction in K2NiF4-type BaLi oxyhydride from a first-principles molecular dynamics study
   J. Haruyama, F. Takeiri, G. Kobayashi, and O. Sugino J. Mater. Chem. A, 14, 8332 (2026).
   DOI:10.1039/D5TA08063K

SUMITA, Shuntaro [B class; 550 (B), 0 (C)] (345)
— *Theoretical study on cooperative phenomena between magnetism and superconductivity in electron systems with multiple degrees of freedom*

1. Phase-modulated superconductivity via altermagnetism
   S. Sumita, M. Naka, and H. Seo Phys. Rev. B **112**, 144510 (2025).
   DOI:10.1103/3k12-2467

SUMIYA, Yosuke [B class; 1000 (B), 180 (C)] ()
— *Elucidation of principles for the polymer adhesion based on first-principle calculations*
— *Theoretical elucidation of adhesion principle in polymers based on first-principle calculations*

SUN, Rongyan [B class; 650 (B), 0 (C)] (173)
Elucidation of Chemical Reaction Mechanisms at the Frictional Interface in Plasma-assisted Polishing via First-Principles Calculations
— *Elucidation of Interfacial Chemistry in Plasma-Assisted Polishing Using First-Principles Calculations*

1. Plasma-assisted polishing with silicon and silica plates: Comparison of interaction mechanism and achievement of atomically flat surfaces on single- and polycrystalline diamond
   J. Dong, S. Sugihara, K. Fujiwara, R. Sun, Y. Ohkubo, J. Wang, T. Suga, and K. Yamamura
   Journal of Materials Processing Technology, 348, 119187 (2025).
   DOI:10.1016/j.jmatprotec.2025.119187

SUWA, Hidemaro [C class; 3400 (B), 350 (C)] (234)
— *Novel magnetic order induced by spin-charge coupling in bilayer systems*

1. Thermally quenched metastable phase in the Ising model with competing interactions
   H. Oike, H. Suwa, Y. Takahashi, and F. Kagawa Phys. Rev. B 112, 064409 (2025).
   DOI:10.1103/ydc4-cfrm

2. Contrasting magnetic behavior in MnSc2X4 (X=S,Se) spinel compounds investigated by magnetoelastic studies
   J. Grumbach, J. Sourd, M. Deeb, A. Miyata, H. Suwa, T. Gottschall, A. Hauspurg, S. Chattopadhyay, M. Rotter, S. Granovsky, L. Prodan, V. Tsurkan, S. Zherlitsyn, M. Doerr, and J. Wosnitza
   Phys. Rev. B 112, 214415 (2025).
   DOI:10.1103/479d-4jvy

3. Unified Description of Spin-Lattice Coupling and Thermodynamics in the Pyrochlore Heisenberg Antiferromagnet
   M. Gen, H. Suwa, S. Imajo, C. Dong, H. Ueda, M. Tachibana, A. Ikeda, K. Kindo, and Y. Kohama
   Phys. Rev. Lett. 136, 116702 (2026).
   DOI:10.1103/8c73-l4nk

SUZUKI, Takafumi [C class; 1400 (B), 250 (C)] (335)
— *Temperature dependence of specific heat in an extended Kitaev model on a honeycomb lattice*

SUZUKI, Takehito [B class; 100 (B), 30 (C)] (376)
— *Analysis of phase transition in complexity of sentences based on combinatory categorial grammar*
— *Understanding the characteristics of sentence production based on differences in language acquisition methods*

SUZUKI, Yuji [C class; 5800 (B), 650 (C)] (67)
— *Simulation of Metal Nitriding by Ammonia Flame*

1. Molecular dynamics simulation of nitrogen diffusion in iron and iron nitrides using ab initio data trained machine learning potentials
   Peijie Feng, Aditya Dilip Lele, Minhyeok Lee, Yiguang Ju, Yuji Suzuki Physical Chemistry Chemical Physics **28**, 9341 (2026).
   DOI:10.1039/D6CP00172F

2. Prediction of Nitrogen Diffusion into Iron-Based Materials under High Temperature
   Peijie Feng, Minhyeok Lee, Yuji Suzuki 62nd NHTS/HTSJ Int. Heat Transf. Symp., Okinawa, Japan, IGS15-2-01, (2025).

TADA, Kohei [C class; 400 (B), 300 (C)] (171)
— *Establishment of guidelines for controlling open-shell nature of molecules by solids*

1. Efficient Hydrogenation of Nitrobenzene to Aniline over a Palladium Carbide Nanocube Catalyst
   S. Yamaguchi, M. Sarmiento-Diaz, T. Kawakami, K. Tada, T. Mitsudome, and T. Mizugaki ACS Appl. Nano Mater. **8**, 13886 (2025).
   DOI:10.1021/acsanm.5c02582

2. Toward a deeper understanding of HNi3C interactions: rule-based insights
   K. Tada, K. Matsuyama, S. Yamaguchi, R. Kishi, T. Mizugaki, and Y. Kitagawa Phys. Chem. Chem. Phys. **28**, 1118 (2026).
   DOI:10.1039/d5cp02869h

3. Local structural evolutions of the Na23(Mn23Ni13)O2 with two different crystallinities during Na extraction/insertion using in situ PDF analysis
   R. Kataoka, A. Machida, K. Tada, N. Taguchi, and N. Takeichi Electrochim. Acta **549**, 148038 (2026).
   DOI:10.1016/j.electacta.2025.148038

4. A theoretical study of singly occupied molecular bands and their magnetic character in one-dimensional trioxotriangulene chains
   Y. Kitano, K. Tada, R. Hirota, T. Kawakami, R. Kishi, and Y. Kitagawa Bull. Chem. Soc. Jpn. **99**, uoag036 (2026).
   DOI:10.1093/bulcsj/uoag036

5. Stabilization of isolated Fe atoms on a 1-nm-thick MgO/Fe(001) insulating surface via critical tunneling for a robust quantum spin platform
   T.K. Yamada, N.K.M. Nazriq, and K. Tada Appl. Surf. Sci. Adv. **33**, 100965 (2026).
   DOI:10.1016/j.apsadv.2026.100965

6. Impact of the surface energy of the layered Na2/3(Mn2/3Ni1/3)O2 on the structural change at higher state of charge
   R. Kataoka, Y. Kitano, K. Tada, Y. Kitagawa, and N. Takeichi J. Alloy Comp., under review

7. Controlling the Ligand Spin of Surface-Adsorbed Double-Decker Phthalocyaninato Complexes: Suggestions Based on Theoretical Calculations
   R. Hirota, K. Tada, K. Ikenaga, K. Katoh, R. Kishi, and Y. Kitagawa J. Phys. Chem. C, under review

8. Rechargeable battery reaction mechanisms of tribromotrioxotriangulene crystal investigated by density functional theory calculations
   Y. Kitano, K. Tada, T. Kawakami, R. Kishi, and Y. Kitagawa J. Phys. Chem. C, under review

TADA, Yasuhiro [C class; 2200 (B), 250 (C)] (240)
— *Study of quantum many-body systems under external fields*

1. Diagnosing energy gap in quantum spin liquids via polarization amplitude
   T. Yokoyama and Y. Tada arXiv:2602.12990

TAHARA, Shuta [B class; 300 (B), 60 (C)] ()
— *Structure and ionic diffusion of liquid AgI-RbI system*

TAKAHASHI, Jun [E class; 13000 (B), 1000 (C)] (262)
— *Physical and Computational Phase Diagrams for Quantum and Classical Spin Models*

1. Plastic tensor networks for interpretable generative modeling

Katsuya O Akamatsu*, Kenji Harada, Tsuyoshi Okubo, and Naoki Kawashima Mach. Learn.: Sci. Technol. 7 015014 (2026).
DOI:10.1088/2632-2153/ae3048

TAKAYAMA, Akari [B class; 400 (B), 0 (C)] ()
— *Structure analysis of atomic layer alloy with Rashba-type superconductor studied by TRHEPD*

TAKEMORI, Nayuta [C class; 200 (B), 100 (C)] (374)
— *Superconductivity properties in 12-fold symmetrical quasicrystals*

1. Photonic band gap properties of two-dimensional quasiperiodic tiling approximants
   Nayuta Takemori and Akiji Yamamoto J. Phys.: Condens. Matter **37**, 355701 (2025).
   DOI:10.1088/1361-648X/adfbb9

TAMAYA, Tomohiro [C class; 3200 (B), 350 (C)] (307)
— *Polarized Spin Magnetization Accumulation on Semiconductor Surfaces Under Intense Light Irradiation*

TANAKA, Katsuhiro [B class; 900 (B), 170 (C)] (156)
— *First-principles calculation of tunnel magnetoresistance effect with antiferromagnetic materials*
— *Study on control of magnetic and transport properties of antiferromagnets from first-principles*

1. *Ab initio* study of magnetoresistance effect in $Mn_3Sn/MgO/Mn_3Sn$ antiferromagnetic tunnel junction
   K. Tanaka, Y. Toga, S. Minami, S. Nakatsuji, T. Nomoto, T. Koretsune, and R. Arita Phys. Rev. Materials **10**, 044405 (2026).
   DOI:10.1103/xt7z-sf3x

TANAKA, Shu [B class; 450 (B), 80 (C)] (348)
— *Physical properties of Ising machines*

1. Machine Learning Supported Annealing for Prediction of Grand Canonical Crystal Structures
   Y. Couzini, Y. Seki, Y. Nishiya, H. Nishi, T. Kosugi, S. Tanaka, Y. Matsushita J. Phys. Soc. Jpn. **94**, 044802 (2025).
   DOI:10.7566/JPSJ.94.044802

2. Improving the efficiency of quantum annealing with controlled diagonal catalysts
   T. Hattori and S. Tanaka Phys. Rev. A **113**, 022433 (2026).
   DOI:10.1103/vff6-cf7c

3. Quantitative analysis of the effectiveness of mid-anneal measurement in quantum annealing
   K. Takahashi and S. Tanaka J. Phys. Soc. Jpn. **95**, 034002 (2026).
   DOI:10.7566/JPSJ.95.034002

4. Utilizing intermediate states in quantum annealing for multi-objective optimization
   K. Takahashi and S. Tanaka J. Phys. Soc. Jpn. **95**, 053001 (2026).
   DOI:10.7566/JPSJ.95.053001

TANAKA, Tomonori [B class; 850 (B), 160 (C)] (158)
— *Application of the Magnetic Interaction Parameter Calculation Program to Skyrmion Systems*
— *Development of a non-perturbative calculation tool for magnetic coupling parameters*

1. General spin models from noncollinear spin density functional theory and spin-cluster expansion
   T. Tanaka and Y. Gohda arXiv:2512.04458
   DOI:10.48550/arXiv.2512.04458

TATAN, Alpin [AB class; 500 (B), 130 (C)] (183)
— *First-principles studies of magnetic tunnel junctions with non-collinear antiferromagnets*
— *Foundational first-principles studies of magnetic tunnel junctions*

TATETSU, Yasutomi [C class; 2600 (B), 300 (C)] (108)
— *Computational study on the stability of magnetic ordered alloy nanoparticles*

TEN-NO, Seiichiro [C class; 4000 (B), 350 (C)] (83)
— *Material design of in perovskite photocatalysts using first-principles calculations*

TERAO, Takamichi [B class; 600 (B), 130 (C)] (342)
— *Self-organization and dynamics in dendrimer polyelectrolytes*

1. Repulsive interactions between oppositely charged macroions in asymmetric multivalent salt solutions: Ion-valence and many-body effects
   M. Eguchi, and T. Terao J. Mol. Liq. 437 128377 (2025).
   DOI:10.1016/j.molliq.2025.1283

TEZUKA, Masaki [C class; 4000 (B), 350 (C)] ()
— *Scrambling in Sachdev-Ye-Kitaev-like strongly correlated models*

TODO, Synge [C class; 4800 (B), 400 (C)] ()
— *Simulation of quantum many-body systems by tensor network and sampling*

TOHYAMA, Takami [C class; 3000 (B), 0 (C)] (235)
— *Photoinduced nonequilibrium dynamics in the charge-ordered phase of doped Mott insulators*

1. Easy-axis Heisenberg model on the triangular lattice: From a supersolid to a gapped solid
   M. Ulaga, J. Kokalj, T. Tohyama, and P. Prelovsek Phys. Rev. B **111**, 174442 (2025).
   DOI:10.1103/PhysRevB.111.174442

2. Optical absorption activated by an ultrashort half-cycle pulse in metallic and superconducting states of the Hubbard model
   K. Shinjo, S. Sota, S. Yunoki, and T. Tohyama Phys. Rev. B **111**, 235125 (2025).
   DOI:10.1103/q1fw-tdk1

3. Low-energy photoexcitations inside the Mott gap in doped Hubbard and t-J ladders
   S. Chandra, K. Shinjo, S. Sota, S. Yunoki, and T. Tohyama Phys. Rev. B **113**, 045127 (2026).
   DOI:10.1103/pt16-43yd

TRAN BA, Hung [E class; 2600 (B), 300 (C)] (324)
— *Quantum Corrections to Classical Heisenberg Model for Giant Magnetocaloric Hydrogen Liquefaction*

1. Realistic finite temperature simulations for magnetic and transport properties of ferromagnets
   H. B. Tran and H. Li J. Mater. Chem. C **13**, 11393 (2025).
   DOI:10.1039/d5tc01141h

2. Insights into giant magnetocaloric effects in $BiCu_3Cr_4O_{12}$ with charge–spin–lattice coupling
   H. B. Tran, H. Li, M. Goto, K. Sato, and Y. Shimakawa J. Mater. Chem. A **13**, 34286 (2025).
   DOI:10.1039/d5ta03354c

3. 2D topological electrocatalysts with spin–orbit coupling: interplay between electrochemical and topological surface states
   H. Liu, H. B. Tran, Y. Wang, D. Zhang, Y. Lu, and H. Li J. Phys. Chem. Lett. **16**, 12892 (2025).

DOI:10.1021/acs.jpclett.5c03589

TSUJI, Naoto [B class; 500 (B), 80 (C)] (250)
— *Development of the nonequilibrium dynamical mean-field theory with tensor train methods*

TSUJI, Yuta [C class; 3200 (B), 600 (C)] (96)
— *Exploration of High-Entropy Oxide Catalysts Using First-Principles Calculations and Machine Learning*First-Principles Computational Approach to the Oxygen Evolution Reaction

1. Understanding the transition from reversed to conventional conductance decay in single-molecule wires from the effective Hamiltonian and frontier orbital perspective
K. Okazawa, Y. Tsuji, and K. Yoshizawa Bull. Chem. Soc. **98**, uoaf040(2025).
DOI:10.1093/bulcsj/uoaf040

2. A ferroelectric proton conductor with colossal polarization induced by in-plane symmetry breaking in a two-dimensional coordination polymer
Y. Song, Y. Tsuji, K. Sugimoto, T. Kikuchi, Y. Shi, Y. Murakami, K. Hiramatsu, B.L. Ouay, M. Ohba, and R. Ohtani Chem. Sci. **16**, 13413 (2025).
DOI:10.1039/d4sc08700c

3. First-Principles Calculation on the Adsorption of Ethylene-Acrylic Acid Molecules on Chromium Oxide Surfaces
H. Iwai,and Y. Tsuji ACS Omega **10**, 29578 (2025).
DOI:10.1021/acsomega.5c03021

4. Identifying Active Sites of IrOx Catalysts for OER: A Combined Operando XAS, SEIRAS, and Theoretical Study
N. Thakur, Y. Ren, M. Kumar, T. Uchiyama, M. Fujita, I. Arima, M. ishida, Y. Wu, Y. Tsuji, H. Imai, M. Matsumoto, Y. Zhuang, K. Yamamoto, T. Matsunaga, K. Ohara, M. Matsumoto, Y. Orikasa, Y. Kuroda, S. Mitsushima, and Y. Uchimoto J. Am. Chem. Soc. **147**, 30613 (2025).
DOI:10.1021/jacs.4c18510

5. Reversible and Massive Structural Transformation in MeltableCyanido-bridged Coordination Polymer Crystals
Y. Iwai, S. Kimura, M. Nakaya, T. Nakane, A. Kawamoto, G. Kurisu, Y. Tsuji, K. Hirai, K. Kimoto, O.Cretu, F.Takeiri, K. Sugimoto, B.L. Ouay, M. Ohba, and R. Ohtani Chem. Eur. J. **31**, e02640 (2025).
DOI:10.1002/chem.202502640

6. Discovery of Stable Short-Range Order in High-Entropy Oxides Assisted with Bayesian Optimization
T. Ueno, and Y. Tsuji J. Chem. Theory Comput. **21**, 11697 (2025).
DOI:10.1021/acs.jctc.5c01284

7. Co3O4-FeOOH as a heterojunction electrocatalyst for highly-efficient hydrazine-assisted water electrolysis and pollutant degradation
L. Dai, Y. Tsuji, H. Iwai, Q. Quan, D. Song, X. Liu, J. Liu, T. Yanagida, J.C. Ho and S. Yip Appl. Surf. Sci. **721**, 165458 (2026).
DOI:10.1016/j.apsusc.2025.165458

8. Navigating the Bio-Inspired Structure-Function Landscape: Spectroscopy Driven Finding of Hidden Radical Oxidation in Co-porphyrinic Porous Organic Polymer
B. Boro, C. Biswas, T.H. Vuong, S. Nandy, A. Shrotri, Y. Tsuji, J. Rabeah and J. Mondal Small Methods **10**, e01981 (2026).
DOI:10.1002/smtd.202501981

9. Facet-Selective Electrostatic Assembling of 2D MXene ontoAnisotropic Single-Crystal Metal Oxides for EnhancedPhotocatalysis
S. Kashiwaya, S.N. Myakala , S. Nekita, Y. Tsuji, Y. Niu, X. Liu, L. Qin, M. Sharma, A. Zakharov, L. Hultman, D. Eder, H. Saito, A. Cherevan and J. Rosen Adv. Mater. **38**, e19087 (2026).
DOI:10.1002/adma.202519087

TSUKAHARA, Noriyuki [B class; 350 (B), 80 (C)] (199)
— *The trapping mechanism of guest adsorbed molecules by porous metal-organic films on metal surfaces*

1. Microscopic Observation of the Oligomerization Process of HCOOH Molecules Confined by a 2D Metal-Organic Network on Cu(111)
Noriyuki Tsukahara and Jun Yoshinobu Small **21**, e05213 (2025).
DOI:10.1002/smll.202505213

TSUNEYUKI, Shinji [C class; 5800 (B), 0 (C)] (70)
— *Advancement and application of methods for predicting dielectric properties and structure exploration of materials*

1. 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 Phys. Rev. B ¥bf 111, 165149 (2025).
DOI:10.1103/PhysRevB.111.165149

2. 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 Phys. Rev. B ¥bf 111, 134516 (2025).
DOI:10.1103/PhysRevB.111.134516

3. Practical rule for trimming the DFT-1/2 self-interaction: Band gap, absolute band alignment, and defect properties of semiconductors
C Homma, R Akashi, Y Nishiya, S Tsuneyuki, Y Matsushita Phys. Rev. B ¥bf 112, 115111 (2025).
DOI:10.1103/mp93-55g3

4. Evolutionary search for superconducting hydrides in the La-Pt-H ternary system under compression
T. Ishikawa, Y. Tanaka, and S. Tsuneyuki Physica Scripta ¥bf 101, 105903 (2026).
DOI:10.1088/1402-4896/ae49c3

5. Search for high-pressure phases of yttrium via a data assimilation approach
Y. Kubo, T. Ishikawa, Y. Tanaka, Y. Nakamoto, M. Sakata and S. Tsuneyuki submitted

TU, Wei-Lin [B class; 400 (B), 70 (C)] (253)
— *Development of Fermi machine and finite temperature tensor network algorithm*

1. Probing the Dynamical Structure Factor of Quantum Spin Chains via Low-Temperature Gibbs States with Matrix Product State Subspace Expansion
T. Takahashi, W.-L. Tu, J.-Y. Chen, and Y. Nomura arXiv:2601.09326 (2026).
DOI:10.48550/arXiv.2601.09326

Data Repository

Dataset for "Probing the Dynamical Structure Factor of Quantum Spin Chains via Low-Temperature Gibbs States with Matrix Product State Subspace Expansion"

https://zenodo.org/records/18408712
DOI:10.5281/zenodo.18408711

UCHIDA, Takashi [B class; 200 (B), 60 (C)] (375)
— *Spontaneous formation of multiple-Q orders in two-dimensional Hubbard models*

UEMURA, Naoki [C class; 4600 (B), 550 (C)] (75)
— *The effect of added elements on the slip system of magnesium*

1. Density Functional Theory Study of the Role of Molybdenum in Weakening Hydrogen Effect on bcc Iron: A Comparison with Carbon and Nitrogen Effects
   S. Kato, N. Uemura, M. Vijendran, and R. Matsumoto ISIJ Int. **66**, 702 (2026).
   DOI:10.2355/isijinternational.ISIJINT-2025-390

UMEBAYASHI, Yasuhiro [AB class; 500 (B), 140 (C)] (181)
— *Interaction between Electrodes and Electrolytes in Li-S Batteries Studied by Classical Molecular Dynamics and First-Principles Calculations*
— *Molecular Dynamics and First-Principles Study of Cathode-Electrolyte Interfaces in Lithium-Sulfur Batteries*

USUI, Hidetomo [B class; 450 (B), 80 (C)] (178)
— *Theoretical exploration of goniopolar high-performance thermoelectric materials*

1. $Rb(Cd,Zn)_4As_3$ as a new n-type Zintl phase thermoelectric compound
   K. Ono, Y. Goto, H. Usui, M. Murata, S. Tsutsui, K. Kuroki, Y. Kamihara, and C.-H. Lee Acta Mater. **307**, 121968 (2026).
   DOI:10.1016/j.actamat.2026.121968

VENGAYIL KRISHNAN, Vishnu [B class; 500 (B), 60 (C)] ()
— *Yielding and aging of colloidal gels*

WANG, Tianyi [C class; 2200 (B), 250 (C)] ()
— *Exploring Transition Metal Oxide Catalysts for Nitrogen Reduction Reactions*

WANG, Yinqiao [C class; 800 (B), 150 (C)] ()
— *Exploring the Phase Behavior and Glassy Dynamics of Sticky Spheres*

WATANABE, Hiroshi [C class; 8200 (B), 300 (C)] (269)
— *Molecular dynamics study on analysis and control of Rayleigh-Plateau instability*
— *Molecular dynamics study on the interface instability with perturbations*

1. Molecular dynamics study of Rayleigh-Plateau instability at liquid-liquid interfaces
   S. Kikuchi and H. Watanabe Phys. Rev. Fluids **11**, 023901 (2026).
   DOI:10.7566/JPSJ.93.114601

Data Repository
Simulation data of the Rayleigh-Taylor instability
https://isspns-gitlab.issp.u-tokyo.ac.jp/kaityo256/rt-instability-data

WATANABE, Hiroshi [B class; 500 (B), 80 (C)] (248)
— *Study on the Novel Mechanism of Superconductivity in Nickel Oxides*

1. Hierarchical structure of primary and hybridization-induced superconducting correlations in bilayer nickelates
   H. Watanabe, H. Sakakibara, and K. Kuroki arXiv:2603.13604

WATANABE, Satoshi [C class; 8200 (B), 800 (C)] (54)
— *Analyses on correlation between material properties and atomic structures in complex structures via ab-initio-based methods*

1. Construction of Machine Learning Potentials toward the Exploration of Alloy Cluster Catalysts
   K. Miyamoto, K. Shimizu, A. K. A. Lu, S. Watanabe e-Journal of Surface Science and Nanotechnology **23**, 188 (2025).
   DOI:10.1380/ejssnt.2025-028

2. Charge States of Ions around Σ 5 (310)/[001] Grain Boundary in Cubic-ZrO2 Revealed by First-principles Calculations
   S. Arai, K. Shimizu, A. K. A. Lu, H. Masuda, H. Yoshida, S. Watanabe e-Journal of Surface Science and Nanotechnology **23**, 323-327 (2025).
   DOI:10.1380/ejssnt.2025-044

3. Study of the ion mobility in defect-laden ZrO_2 under an electric field using neural network with predictions for Born effective charges
   A. K. A. Lu, N. Maekawa, A. Ikeda, K. Shimizu, H. Masuda, H. Yoshida, S. Watanabe Phys. Rev. Mater., submitted.

YAMADA, Atsuo [C class; 3600 (B), 350 (C)] (95)
— *Exploration of novel rechargeable battery materials using first-principles calculations and machine learning*

1. Kinetic Suppression of Anion Intercalation into Cathode Conductive Carbon in High-Voltage Lithium Batteries
   K. Nakamura, N. Takenaka, S. Hagiwara, M. Otani, A. Yamada ACS Appl. Mater. Interfaces. **17**, 61439 (2025).
   DOI:10.1021/acsami.5c14007

2. Prerequisite of Oxygen Local Environment for Facile Proton Intercalation into Transition-Metal Oxides
   S. Park, S. Nishimura, J. Li, A. Kitada, S. Lee, W.-S. Yoon, A. Yamada J. Am. Chem. Soc. **148**, 7931 (2026).
   DOI:10.1021/jacs.5c22803

YAMADA, Atsushi [C class; 1000 (B), 200 (C)] ()
— *Analyses of the superconductivity in Hubbard models and their applications to strongly correlated electron systems.*

YAMAGUCHI, Naoya [C class; 1200 (B), 350 (C)] (144)
— *Development of First-principles Berry Phase Calculation codes for Application to Large Systems*

1. First-principles study of interface states in diamond(111)/Al2O3 with different terminations
   Y. Zhang, N. Yamaguchi, X. Zhang, M. Saito and N. Tokuda, and F. Ishii Surf. Interfaces **72**, 107147
   DOI:10.1016/j.surfin.2025.107147

2. First-principles study of electric-dipole-induced Rashba spin-splitting in Janus WSSe
   S. A. Putri, M. A. U. Absor, N. Yamaguchi, and F. Ishii Jpn. J. Appl. Phys. **64**, 10SP21
   DOI:10.35848/1347-4065/ae00cf

3. First-principles study of thickness-dependent vertical polarization in multilayer hexagonal boron nitride

N. M. Chadiza, H. P. Kadarisman, N. Yamaguchi, and F. Ishii Jpn. J. Appl. Phys. **64**, 11SP09
DOI:10.35848/1347-4065/ae0e2b

4. Capacitance profile of graphene via effective screening medium method: first-principles study
A. Sohib, N. Yamaguchi, and F. Ishii Jpn. J. Appl. Phys. **64**, 11SP11
DOI:10.35848/1347-4065/ae0cd3

5. The effect of interlayer coupling on thermoelectricity in atomically thin CaGe2: a first-principles study
A. A. Ghiffari, R. Syariati, Y. Morishima, N. Yamaguchi, and F. Ishii Jpn. J. Appl. Phys. **64**, 11SP31
DOI:10.35848/1347-4065/ae11bf

6. Band Unfolding in Finite Nanostructures: Visualizing Dirac, SpinValley, and Rashba Features
N. Yamaguchi, S. Yunitasari, W. Amalia, C.-C. Lee, T. Ozaki, and F. Ishii Nano Lett. **25**, 17725
DOI:10.35848/1882-0786/ae241f

Data Repository
layerAHC
https://isspns-gitlab.issp.u-tokyo.ac.jp/n-yamaguchi/layerAHC

GMBU.jl
https://isspns-gitlab.issp.u-tokyo.ac.jp/n-yamaguchi/GMBU.jl

Code for the Giant Molecule Band Unfolding
https://zenodo.org/records/17815785
DOI:10.5281/zenodo.17815785

YAMAMOTO, Go [C class; 3800 (B), 400 (C)] (298)
— *Machine Learning and Molecular Dynamics-Based Prediction of Optimal Structures for High-Strength MWCNT Yarns*

YAMASHITA, Tomoki [C class; 4000 (B), 350 (C)] (82)
— *Material Design Using Crystal Structure Prediction and First-Principles Calculations*

YAMAUCHI, Kunihiko [C class; 2600 (B), 0 (C)] (118)
— *Spintronics applications based on spin-splitting phenomena in altermagnets*

1. Spin-degenerate bulk bands and topological surface states associated with Dirac nodal lines in RuO2
T. Osumi, K. Yamauchi, S. Souma, S. Paul, A. Honma, K. Nakayama, K. Ozawa, M. Kitamura, K. Horiba, H. Kumigashira, C. Bigi, F. Bertran, T. Oguchi, T. Takahashi, Y. Maeno, and T. Sato Physical Review B **113**, 085116 (2026).
DOI:10.1103/wvs6-hqfv

YANAGISAWA, Susumu [BC class; 4450 (B), 0 (C)] (81)
— *First-principles investigation in search for organic materials in two-dimensional perovskite photovoltaics*
— *First-principles investigation of organic materials as candidates for materials of two-dimensional perovskite solar cells*
— *First-principles investigation on the electron-phonon coupling in organic semiconductor crystals*First-principles study on the mechanism of charge transfer at organic-electrode interfaces

1. Fingerprinting weak electronic interaction at a van derWaals interface: Fano signatures in a pentacene monolayer on graphite

Y. Hasegawa, T. Yamaguchi, M. Meissner, T. Ueba, F. Bussolotti, S. Ideta, K. Tanaka, S. Yanagisawa and S. Kera Phys. Rev. B **112**, 085301 (2025).
DOI:10.1103/2k7h-h8jm

YANAGISAWA, Takashi [B class; 700 (B), 140 (C)] (245)
— *Study of optimized many-body wave functions in strongly correlated electron systems*

1. Superconductivity and Inhomogeneous charge-ordered state in the two-dimensional Hubbard model – Off-Diagonal Wave Function Monte Carlo Studies of Hubbard Model IV–
T. Yanagisawa J. Phys. Soc. Jpn. 94, 074708 (2025).
DOI:10.7566/JPSJ.94.074708

YASUDA, Chitoshi [C class; 1000 (B), 0 (C)] (340)
— *Enhancement of correlation functions due to deficit in quantum spin systems*

1. Classical Ground-State Phase Diagram of the Multiple-Spin Exchange Model on a Honeycomb Lattice
C. Yasuda and Y. Chibana J. Phys. Soc. Jpn. **94**, 084704 (2025).
DOI:10.7566/JPSJ.94.084704

YASUDA, Yusuke [BC class; 5000 (B), 470 (C)] (282, 284)
— *MD Simulations on Single-Molecule Reactors based on Bottlebrush Polymers*
— *Study on structure-properties relationship in uniform/dynamic polymer networks via precise graph structure analysis*

1. Coarse-grained molecular dynamics simulations of slide-ring gels under finite deformation: influence of sliding ring rearrangement on softness and extensibility
Y. Yasuda, K. Mayumi, M. Toda, H. Yokoyama, H. Morita, and K. Ito Soft Matter **21**, 4573 (2025).
DOI:10.1039/D5SM00003C

YASUHARA, Sou [C class; 2600 (B), 0 (C)] (117)
— *Investigation of polarization switching in Li2GeO3*

1. Ferroelectric behavior of divalent cation-doped LiGaO2 with a distorted wurtzite-type structure
Sou Yasuhara, Yuto Tomizawa, Kazuki Okamoto, Masaki Tozuka, Ayato Nakagawa, Shintaro Yasui, Hiroshi Funakubo and Takuya Hoshina Jpn. J. Appl. Phys. 64 08SP02 (2025),
DOI:10.35848/1347-4065/adefe9

YOKO, Akira [C class; 4200 (B), 250 (C)] ()
— *Adsorption effects on electronic states of ultrasmall metal oxides*
— *Electronic state and new properties of ultrasmall metal oxides*

YOSHIDA, Tsuneya [C class; 3400 (B), 0 (C)] ()
— *Topology of strongly correlated electrons with dissipation*

YOSHIMI, Kazuyoshi [C class; 2600 (B), 100 (C)] (236)
— *Verification of the Effects of van der Waals interactions in Organic Materials by First-Principles Calculations toward Materials Design*

1. 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, and Y. Uwatoko Phys. Rev. Materials **9**, L021801 (2025).
DOI:10.1103/PhysRevMaterials.9.L021801

2. Ambient-Pressure Organic Dirac Electron State in α-$(BETS)_2AuCl_2$
T. Kobayashi, K. Yoshimi, A. Nishimoto, S. Michimura, and H. Taniguchi J. Phys. Soc. Jpn. **95**, 043701 (2026).
DOI:10.7566/JPSJ.95.043701

Data Repository
Data for "Pressure-induced topological changes in Fermi surface of two-dimensional molecular conductor β'-$(BEDT\text{-}TTF)_2ICl_2$"
https://isspns-gitlab.issp.u-tokyo.ac.jp/k-yoshimi/betap-ET2ICl2

Data for "Ambient-Pressure Organic Dirac Electron State in α-$(BETS)_2AuCl_2$"
https://isspns-gitlab.issp.u-tokyo.ac.jp/k-yoshimi/alpha-bets2-aucl2

YUHARA, Junji [B class; 300 (B), 60 (C)] (202)
— *Structural analysis of metal oxide quasicrystal thin films*

ZHANG, Di [C class; 1600 (B), 300 (C)] (136)
— *Exploring high Ionic Conductivity Solid-State Electrolytes using Machine-Learning Driven Genetic Algorithms and Metadynamic Simulations*

1. 2D Topological Electrocatalysts with Spin–Orbit Coupling: Interplay between the "Electrochemical" and "Topological" Surface States
H. Liu, H. B. Tran, Y. Wang, D. Zhang, Y. Lu, and H. Li J. Phys. Chem. Lett. **16**, 12892 (2025).
DOI:10.1021/acs.jpclett.5c03589

2. Ampere-Level Electrosynthesis of CO via Well-Defined Pyridinic-N Incorporated Cobalt Phthalocyanine
T. Liu, X. Hou, D. Zhang, Y. Hirai, K. Ishibashi, Y. Matsuo, J. Yoshida, S. Ono, H. Li, and H. Yabu Small **21**, e202507824 (2025).
DOI:10.1002/smll.202507824

3. C60 Fullerene as the Active Site for CO2 Electroreduction
S.-W. Ying, Y. Wang, P. Du, Q. Wang, C. Yue, D. Zhang, Z.-C. Chen, J.-W. Zheng, S.-Y. Xie, and H. Li Angew. Chem. Int. Ed. **64**, e202511924 (2025).
DOI:10.1002/anie.202511924

4. High-Density W Single Atoms in Two-Dimensional Spinel Oxide Break the Structural Integrity for Enhanced Oxygen Evolution Catalysis
Y. Wang, B. Jia, W. Qin, Y. Wang, S. Liu, Y. Qin, Y. Zhao, L. Liu, D. Zhang, H. Liu, H. Zhong, J. Liu, J. Tu, Y. Liu, H. Wu, D. Zhang, J. Fan, X. Qu, H. Li, and M. Qin J. Am. Chem. Soc. **147**, 32249 (2025).
DOI:10.1021/jacs.5c12122

5. Stepwise Acceleration of Water Dissociation and Hydrogen Spillover for Enhanced Overall Alkaline Hydrogen Evolution
T. Lu, J. Li, C. Wang, H. Liu, S. Ye, X. Jia, L. Zhang, D. Zhang, D. Sun, Y. Gu, Q. Wang, B. Da, L. Wei, Y. Zhang, H. Li, and Y. Tang ACS Catal. **16**, 2827 (2026).
DOI:10.1021/acscatal.5c08576

6. Universal Catalyst Design Framework for Electrochemical Hydrogen Peroxide Synthesis Facilitated by Local Atomic Environment Descriptors
Z. Liu, Y. Liu, Y. Zhang, Y. Deng, Z. Zheng, R. Knibbe, T. Gao, M. Li, Z. Wang, B. Zhang, X. Jia, D. Zhang, H. Liu, X. Shao, Z. Gao, L. Wei, H. Li, and W. Yang Angew. Chem. Int. Ed. **65**, e202518027 (2026).
DOI:10.1002/anie.202518027

○ A class

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

AKIYAMA, Ryota [A class; 100 (B), 50 (C)] ()
— *Exploration of topological properties in natural minerals in Japanese mines*

AONISHI, Toru [A class; 100 (B), 50 (C)] ()
— *Image Analysis and Feature Extraction for Fusion Reactor Materials*

DEKURA, Shun [A class; 100 (B), 50 (C)] ()
— *Calculation of the electronic states of vapochromic HOF involving structural modulation*

HAN, Jihae [A class; 100 (B), 50 (C)] (187, 400)
— *Reductive decomposition mechanism of electrolyte at electrode/electrolyte interface by first-principles*

HATANO, Naomichi [A class; 100 (B), 50 (C)] ()
— *Dynamics of quantum walkers interacting with a localized spin*

HAZE, Masahiro [A class; 100 (B), 50 (C)] ()
— *Role of atomic steps in the transport properties of monolayer films*

KAMEYAMA, Ryohei [A class; 100 (B), 50 (C)] ()
— *Electronic-Structure Design and Mechanism Discovery in Molecular Crystals and Interfaces*

KAWAGUCHI, Kaishu [A class; 100 (B), 50 (C)] (409)
— *Investigation of Substrate Effects on Topological-Insulator Bi_2Te_3 Thin Films*

KAWAI, Kosuke [A class; 100 (B), 50 (C)] ()
— *Exploring anionic redox reactions induced by zinc-ion insertion/extraction*

KISHIDA, Ippei [A class; 100 (B), 50 (C)] ()
— *First-principles calculations of ionics in Li-gradient compounds and their application to battery materials*

KONISHI, Yusuke [A class; 100 (B), 50 (C)] ()
— *Computational Materials Exploration of High-Entropy REBCO Compounds*

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

MASUDA, Go [A class; 100 (B), 50 (C)] ()
— *Molecular Simulation of Polymer-Carbon Fiber Interfaces for Advanced Matrix Design*

MATSUNAGA, Noriaki [A class; 100 (B), 50 (C)] ()
— *Study of Electronic States in Low-Dimensional Organic Conductors*

MATSUURA, Keisuke [A class; 100 (B), 50 (C)] ()
— *Investigation of the origin of low-temperature hysteresis broadening in the antiferromagnetic-ferromagnetic phase transition*

MORITA, Katsuhiro [A class; 100 (B), 50 (C)] ()
— *MPI parallelization for finite-temperature quantum calculations*

1. Chemically tunable quantum magnetism on the anisotropic triangular lattice in rhenium oxyhalides
   M. Gen, D. Hirai, K. Morita, K. Nawa, S. Kogane, N. Matsuyama, T. Yajima, M. Kawamura, K. Deguchi, A. Koda, M. Kofu, S. Ohira-Kawamura, T. J. Sato, A. Matsuo, K. Kindo, Y. Kohama, and Z. Hiroi Nat Commun 16, 9938 (2025).
   DOI:10.1038/s41467-025-65913-7

OHKOSHI, Shin-Ichi [A class; 100 (B), 50 (C)] ()
— *Theoretical studies on the physical properties of novel functional phase transition materials*

OSADA, Wataru [A class; 100 (B), 50 (C)] ()
— *The effect of electronic states of the Pd/Cu(111) single atom alloy catalyst on its catalytic activity*

OSADA, Wataru [A class; 100 (B), 50 (C)] ()
— *The effect of electronic states of the Pd/Cu(111) single atom alloy catalyst on its catalytic activity 2*

ROY, Tufan [A class; 100 (B), 50 (C)] ()
— *First-principles and machine-learning study of magneto-transport phenomena in Kagome magnets and Heusler alloys for spintronics applications*

SATO, Naoki [A class; 100 (B), 50 (C)] (106, 435)
— *Complementary analysis of chemical pressure and lattice dynamics in complex crystal structures*

SEKI, Shinichiro [A class; 100 (B), 50 (C)] ()
— *Search of antiferromagnets hosting non-relativistic splitting based on DFT calculation*

SHIMADA, Toshihiro [A class; 100 (B), 50 (C)] ()
— *Electronic structure calculation of organic crystals with polarity*

TATAN, Alpin [A class; 100 (B), 50 (C)] (183, 443)
— *Foundational first-principles studies of magnetic tunnel junctions*

UDAGAWA, Masafumi [A class; 100 (B), 50 (C)] ()
— *Conserved charge and critical phenomena in geometrically frustrated systems*

UMEBAYASHI, Yasuhiro [A class; 100 (B), 50 (C)] (181, 446)
— *Molecular Dynamics and First-Principles Study of Cathode-Electrolyte Interfaces in Lithium-Sulfur Batteries*

UMEYAMA, Daiki [A class; 100 (B), 50 (C)] ()
— *Research on the band structure design and semiconductor properties of hybrid materials*

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

1. Development of a virtual CFD model for regulating temperature in a liquid tank
   uthorJ. Wang, F. Xu, Y. Sakai, H. Takahashi, R. Zhang, H. Kanayama, D. Satou, and Y. Kansha
   The 35th European Symposium on Computer Aided Process Engineering (ESCAPE—35), July 6-9, 2025, Ghent, Belgium

WAIZUMI, Hiroki [A class; 100 (B), 50 (C)] ()
— *First-principles study on surface structure and electronic states of layered chalcogenides under molecular adsorption*

ZUSHO, Yu [A class; 100 (B), 50 (C)] ()
— *Molecular dynamics modeling of repair behavior in self-healing composite materials*

□ SCCMS Projects

FUKUSHIMA, Tetsuya [4000 (B), 400 (C)] (381)
— *Data Generation for Magnetic Properties at Finite Temperature*

1. Impact of Lattice Distortions on Magnetocrystalline Anisotropy and Magnetization in $(Nd_{1-x}Pr_x)_2Fe_14B$ Alloys
   H. Okumura, T. Miyake, T. Fukazawa, N. Sakuma, Y. Suzuki, T. Shoji, H. Akai, M. Ogura, and T. Fukushima arXiv:2512.07285
   DOI:10.48550/arXiv.2512.07285

MATUBAYASI, Nobuyuki [2000 (B), 200 (C)] (384)
— *Chiral Effects on Aqueous Solubility of Polypeptides Explored by Molecular Simulations*

MISAWA, Takahiro [4000 (B), 400 (C)] (219)
— *Estimation of the Hamiltonians of quantum spin liquid candidate material using Bayesian optimization*

MIYAKE, Takashi [2000 (B), 0 (C)] (383)
— *First-principles study of magnetic materials using KKR Green's function method*

1. Covariance Linkage Assimilation method for Unobserved Data Exploration
   Yosuke Harashima, Takashi Miyake, Ryuto Baba, Tomoaki Takayama, Shogo Takasuka, Yasuteru Shigeta, Yuichi Yamaguchi, Akihiko Kudo, and Mikiya Fujii Phys. Rev. Materials **9**, 093803 (2025).
   DOI:10.1103/8tjv-wtx5

2. Liquid structure of SmFe12-based alloys
   Kengo Nishio, Takehide Miyazaki, Taro Fukazawa, Tetsuya Fukushima and Takashi Miyake Computational Materials Science **256**, 113947 (2025).
   DOI:10.1016/j.commatsci.2025.113947

SHIMAZAKI, Tomomi [2000 (B), 100 (C)] (385)
— *Theoretical study on proton behavior in fuel cell material based on first-principles method*

1. Theoretical study of Lewis base passivation of p-type surface defects in IBr mixed-halide tin perovskites
   Emi Kino, Makito Takagi, Takumi Naito, Masanori Tachikawa, Koichi Yamashita, Tomomi Shimazaki J. Chem. Phys, **163**, 104703 (2025).
   DOI:10.1063/5.0285545

2. Theoretical study on the analyzability of modified convex regression for radical reaction
   Tomomi Shimazaki, Masanori Tachikawa Phys. Chem. Chem. Phys., **28**, 2499 (2026).
   DOI:10.1039/d5cp03946k

3. Rolling two-dimensional covalent organic framework (COF) sheets into one-dimensional electronic and proton-conductive nanotubes
   Zhuowei Li, Rajendra Prasad Paitandi, Yusuke Tsutsui, Wakana Matsuda, Masaki Nobuoka, Bin Chen, Samrat Ghosh, Takayuki Tanaka, Masayuki Suda, Tong Zhu, Hiroshi Kageyama, Yoshihiro Miyake, Hiroshi Shinokubo, Makito Takagi, Tomomi Shimazaki, Masanori Tachikawa, Katsuaki Suzuki, Hironori Kaji, Yasunobu Ando, Takahiro Ezaki, Shu Seki Proceedings of the National Academy of Sciences, **122**, e2424314122 (2025).
   DOI:10.1073/pnas.2424314122

YAMAJI, Youhei [5000 (B), 500 (C)] (386)

— *AI numerical spectroscopy for analyzing emergent structures of quantum entanglement in correlated quantum materials*

1. Photoemission microscope tomography for polycrystalline metals
   Y. Yamaji, S. Tsuda, and K. Yaji Science and Technology of Advanced Materials: Methods **6** 2611609 (2026).
   DOI:10.1080/27660400.2025.2611609

2. Unified Description of Cuprate Superconductors by Fractionalized Electrons Emerging from Integrated Analyses of Photoemission Spectra and Quasiparticle Interference
   S. Sakai, Y. Yamaji, F. Imoto, T. Tamegai, A. Kaminski, T. Kondo, Y. Kohsaka, T. Hanaguri, and M. Imada Phys. Rev. X **16** 011018 (2026).
   DOI:10.1103/mww7-32gn