4 PUBLICATION LIST

Example:

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

— *Project title*

1. First paper
   Names of Authors, etc.
2. Second paper
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□ ISSP Joint Research Projects

○ B–E classes

AKASHI, Ryosuke [B class; 600 (B), 100 (C)] (180)

— *Renormalized charge-spin fluctuations from first principles*

1. Semiconducting Electronic Structure of the Ferromagnetic Spinel $HgCr_2Se_4$ Revealed by Soft-X-Ray Angle-Resolved Photoemission Spectroscopy
   Hiroaki Tanaka, Andrei V Telegin, Yurii P Sukhorukov, Vladimir A Golyashov, Oleg E Tereshchenko, Alexander N Lavrov, Takuya Matsuda, Ryusuke Matsunaga, Ryosuke Akashi, Mikk Lippmaa, Yosuke Arai, Shinichiro Ideta, Kiyohisa Tanaka, Takeshi Kondo, Kenta Kuroda Physical Review Letters **130**, 186402 (2023).
   DOI:10.1103/PhysRevLett.130.186402

AOYAMA, Kazushi [B class; 500 (B), 100 (C)] (342)

— *Field-induced chirality in breathing-kagome antiferromagnets*

ARAI, Munehito [C class; 6400 (B), 0 (C)] (266)

— *Development of a general method for rationally improving enzymatic activity*

— *Rational design of novel proteins for drug discovery*

1. Accurate prediction of protein folding mechanisms by simple structure-based statistical mechanical models
   K, Ooka, and M. Arai Nature Communications **14**, 6338 (2023).
   DOI:10.1038/s41467-023-41664-1

2. Crucial residue for tuning thermal relaxation kinetics in the biliverdin-binding cyanobacteriochrome photoreceptor revealed by site-saturation mutagenesis
   T. Suzuki, M. Yoshimura, M. Arai, and R. Narikawa J Mol Biol. **436**, 168451 (2024).
   DOI:10.1016/j.jmb.2024.168451

ARAKI, Takeaki [B,C class; 5200 (B), 670 (C)] (275, 276, 277)

— *Physical origin of forming ferroelectric nematic phase*

— *Study on Johari-Goldstein relaxation mode in glass-forming liquids*

— *Topological and mechanical properties of colloidal gels*

ARIMA, Kenta [B class; 800 (B), 0 (C)] (177)
— *Analysis of interface reaction between functional graphene and semiconductor surface*
— *Simulation of electronic structures of functional graphene sheets with wrinkles*

1. First-principles simulations of scanning tunneling microscopy images exhibiting anomalous dot patterns on armchair-edged graphene nanoribbons
   Junhuan Li, Kouji Inagaki, and Kenta Arima, Physical Review Research, **6**, 013252 (2024).
   DOI:10.1103/PhysRevResearch.6.013252

ARUGA, Tetsuya [B class; 400 (B), 100 (C)] ()
— *Electronic structure and conductivity of novel indium thin film on semiconductor surface*

ASANO, Yuta [E class; 16000 (B), 1550 (C)] (259)
— *Large-scale molecular dynamics simulation of ultrasonic cavitation*
— *Molecular dynamics simulation of ultrasound cavitation*

BIN, Xu [C class; 5000 (B), 650 (C)] (96)
— *Elucidating the Thermal Transport Mechanisms at Semiconductor Interfaces*
— *Thermal transport across heterojunction between 2D materials and substrate*

BUI, VANPHO [C class; 1600 (B), 0 (C)] (158)
— *Study on the removal mechanism of Copper Oxide processing in catalyst-referred etching method*

CAMPOS, Dos [C class; 2200 (B), 0 (C)] (143)
— *Exploring the Role of Neutral Molecules in All-solid-state Battery Electrolytes*

DEKURA, Shun [B,C class; 2200 (B), 100 (C)] (139)
— *First-principles calculations for phase stabilities and electronic structures of As-incorporated organoelemental materials*
— *First-principles calculations on the electronic states of novel organic semiconductors with extended hydrogen-bonding networks*
— *Unveiling the proton conduction pathways based on proton tautomerism in anhydrous molecular crystals by first-principles NEB calculations*

1. Precise Control of the Molecular Arrangement of Organic Semiconductors for High Charge Carrier Mobility
   R. Akai, K. Oka, S. Dekura, K. Yoshimi, H. Mori, R. Nishikubo, A. Saeki, N. Tohnai J. Phys. Chem. Lett. **14**, 34613467 (2023).
   DOI:10.1021/acs.jpclett.3c00334

EGAMI, Yoshiyuki [C class; 6000 (B), 300 (C)] (88)
— *First-principles electron-transport study on 2-dimensional SiC materials*
— *First-principles study on electron transport properties in molecule-adsorbed atomic layered materials*

1. GPU acceleration of conjugate gradient method obtaining Green's function for transport-property calculation
   T. Akamatsu, M. Uemoto, Y. Egami, and T. Ono, Comp. Phys. Commun. **295**, 108989 (2024).
   DOI:10.1016/j.cpc.2023.108989

FUCHIZAKI, Kazuhiro [C class; 2000 (B), 0 (C)] (305)
— *Kinetics of phase transition and polyamorphism*

1. Can weight hysteresis in a neural network judge the continuity/discontinuity of a phase transition?
   K. Nakamura and K. Fuchizaki, J. Phys. A: Math. Theor. **56**, 305002 (2023).
   DOI:10.1088/1751-8121/ace13e

FUJI, Kana [B class; 200 (B), 90 (C)] ()
— *Numerical studies on morphogenesis of organoids using a multicellular phase field model*

FUJI, Yohei [B class; 800 (B), 170 (C)] (321)
— *Dynamics of monitored quantum systems with symmetry*
— *Numerical study for stability of measurement-induced critical phenomena*

FUJII, Susumu [C class; 3000 (B), 0 (C)] (125)
— *Analysis of phonon-assisted ionic transport in solid electrolytes*

1. Discovery of unconventional proton-conducting inorganic solids via defect-chemistry-trained, interpretable machine learning
   S. Fujii, Y. Shimizu, J. Hyodo, A. Kuwabara, and Y. Yamazaki, Adv. Energy Mater., 2301892 (2023).
   DOI:10.1002/aenm.202301892

FUJIMOTO, Yoshitaka [C class; 1400 (B), 0 (C)] (160)
— *First-principles calculations of electronic transport of graphene*
— *Transport study of graphene layers*

1. Formation, structure, electronic and transport properties of nitrogen defects in graphene and carbon nanotubes
   Y. Fujimoto: submitted to Micromachine.

2. Modulation Doping and Quantum Transport in Double-Walled Boron-Nitride Nanotubes
   Y. Fujimoto and S. Saito: submitted to Physical Review Letters.

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

FUJINO, Tomoko [C class; 1800 (B), 400 (C)] (237)
— *Electronic structures for highly conducting oligomer conductors in single crystals*

1. Metallic State of a Mixed-sequence Oligomer Salt that Models Doped PEDOT Family
   K. Onozuka, T. Fujino, R. Kameyama, S. Dekura, K. Yoshimi, T. Nakamura, T. Miyamoto, T. Yamakawa, H. Okamoto, H. Sato, T. Ozaki, and H. Mori, J. Am. Chem. Soc. **145**, 15152 (2023).
   DOI:10.1021/jacs.3c01522

2. Single-crystalline oligomer-based conductors modeling the doped poly(3,4-ethylenedioxythiophene) family
   T. Fujino, R. Kameyama, K. Onozuka, K. Matsuo, S. Dekura, K. Yoshimi, and H. Mori, Faraday Discuss. **250**, 348 (2024).
   DOI:10.1039/D3FD00134B

FUJISAKI, Takaya [B class; 300 (B), 60 (C)] (202)
— *Search for optimal composition of reforming catalysts for high efficiency of fuel cells with direct biogas supply*

FUJISHIRO, Hiroki [C class; 2400 (B), 0 (C)] (137)
— *Strained Band-Structure Engineering for Antimonide-Based Terahertz Transistors*

FUJITA, Takatoshi [C class; 2600 (B), 0 (C)] (132)
— *First-Principles Investigation of Energy-Conversion Processes in Biological and Material Systems*

1. Ab Initio Study of Charge Separation Dynamics and PumpProbe Spectroscopy in the P3HT/PCBM Blend
   Takatoshi Fujita, Takeo Hoshi J. Phys. Chem. B 127 (2023) 7616.
   DOI:10.1021/acs.jpcb.3c02458

FUKUDA, Jun-ichi [B class; 800 (B), 180 (C)] (320)
— *Calculation of ordered structures, dynamics and optical properties of soft materials*

FUKUDA, Masahiro [B class; 400 (B), 100 (C)] (192)
— *Electronic stress tensor density analysis for material surfaces*

1. Electronic band structure change with structural transition of buckled Au_2X monolayers induced by strain
   Masahiro Fukuda, and Taisuke Ozaki, Phys. Chem. Chem. Phys., **26**, 3367 (2024)
   DOI:10.1039/D3CP03135G

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Structural identification of silicene on the Ag(111) surface by atomic force microscopy
https://isspns-gitlab.issp.u-tokyo.ac.jp/masahiro.fukuda/root13_silicene_on_Ag111
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Atomic arrangement of Si adatom on the Silicene/Ag(111) surface
https://isspns-gitlab.issp.u-tokyo.ac.jp/masahiro.fukuda/T4_silicene_Si_adatom_on_Ag111
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FUKUI, Ken-ichi [C class; 2800 (B), 100 (C)] (301)
— *Analyses on the Potential-dependent Dynamics of Ionic Liquid Forming Electric Double Layer Facing the Electrodes*

FUKUMOTO, Yoshiyuki [B class; 800 (B), 0 (C)] (327, 328)
— *Impact of direction of the Dzyaloshinskii-Moriya vector on the magnon dispersion of the q=0 state in Kagome-lattice systems*
— *Numerical study of dynamical structure factors based on spinon operator representation of Heisenberg antiferromagnets*

1. A Series Expansion Study for Large Negative Quantum Renormalization of Magnon Spectra in the S =1/2 Kagome-Lattice Heisenberg Antiferromagnet $\{Cs_2Cu_3SnF_{12}\}$
   Singo Kogure, Masashi Takeda, Katsuhiro Morita, Yoshiyuki Fukumoto, Mutsuki Saito, and Hidekazu Tanaka: J. Phys. Soc. Jpn. 92, 113703, (2023).
   DOI:10.7566/JPSJ.92.113703

GOHDA, Yoshihiro [C class; 8800 (B), 900 (C)] (64)
— *Electron theory of magnetocrystalline anisotropy*
— *Phonon effects in phase equilibria*

1. Clarification of origin of positive excess volume of PdFe binary alloys by using first-principles calculations and HAXPES
   M. Watanabe, Y. Takagi, T. Tanaka, Y. Gohda, M. Adachi, M. Uchikoshi, T. Nakamura, M.

Takata, and H. Fukuyama, Acta Mater. **267**, 119718 (2024).
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2. Strain-induced specific orbital control in a Heusler-alloy-based interfacial multiferroics
J. Okabayashi, T. Usami, A.M. Yatmeidhy, Y. Murakami, Y. Shiratsuchi, R. Nakatani, Y. Gohda, and K. Hamaya, NPG Asia Mater. **16**, 3 (2024).
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3. Unidirectional Nano-Modulated Binding and Electron Scattering in Epitaxial Borophene
S. Kamal, I. Seo, P. Bampoulis, M. Jugovac, C.A. Brondin, T. Menteş, I. Šarić-Janković, A. Matetskiy, P. Moras, P. Sheverdyaeva, T. Michely, A. Locatelli, Y. Gohda, M. Kralj, M. Petrović, ACS Appl. Mater. Interfaces 15, 57890 (2023).
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4. Metastable Co3Mn/Fe/Pb(Mg1/3Nb2/3)O3-PbTiO3 multiferroic heterostructures
Y. Murakami, T. Usami, R. Watarai, Y. Shiratsuchi, T. Kanashima, R. Nakatani, Y. Gohda and K. Hamaya, J. Appl. Phys. 134, 224101 (2023).
DOI:10.1063/5.0180644

5. Unveiling the Origin of Large Coercivity in (Nd, Dy)-Fe-B Sintered Magnets
X. Tang, J.N. Li, H. Sepehri-Amin, A. Bolyachkin, A. Martin-Cid, S. Kobayashi, Y. Kotani, M. Suzuki, A. Terasawa, Y. Gohda, T. Ohkubo, T. Nakamura, and K. Hono, NPG Asia Mater. 15, 50 (2023).
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6. Strain-induced magnetic anisotropy in Heusler alloys studied from first principles
A.M. Yatmeidhy and Y. Gohda, Appl. Phys. Express 16, 053001 (2023).
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7. Subphase exploration for SmFe12-based permanent magnets by Gibbs energies obtained with first-principles cluster-expansion method
S. Enomoto, S. Kou, T. Abe, and Y. Gohda, J. Alloys Compd. 950, 169849 (2023).
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GOHLKE, Matthias [C class; 1000 (B), 200 (C)] (313)
— *Ground state and dynamical properties of the J_1J_2K-Heisenberg model on the square lattice*

GONOME, Hiroki [C class; 3800 (B), 600 (C)] (209)
— *Study of the principle of photothermal conversion by ab initio calculations*

HAGITA, Katsumi [C class; 1400 (B), 500 (C)] (307)
— *Physical properties of crosslinked polymer networks through network topology analysis*

1. All-atom molecular dynamics simulations of poly(ethylene glycol) networks in water for evaluating negative energetic elasticity
K. Hagita, S. Nagahara, T. Murashima, T. Sakai, N. Sakumichi, Macromolecules **56**, 8095 (2023).
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HAMADA, Ikutaro [C class; 7400 (B), 500 (C)] (78)
— *Density functional theory study of adsorption and reaction of molecules on metal surfaces*

1. Oxygen Reduction Reaction on Single-Atom Catalysts From Density Functional Theory Calculations Combined with an Implicit Solvation Model
A. F. Z. Abidin and I. Hamada J. Phys. Chem. C 127, 13623 (2023).
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2. Electronic and optical properties of the hydrogen boride sheet from the many-body perturbation theory
L. T. Ta, Y. Morikawa, and I. Hamada J. Phys.: Condens. Matter 35, 435002 (2023).
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HAMAGUCHI, Satoshi [C class; 6200 (B), 750 (C)] ()
— *Development of atomic interaction models for reactive sputtering simulation by machine learning*
— *Surface reaction analyses for atomic layer processes*

HAMAMOTO, Yuji [C class; 1200 (B), 0 (C)] (164)
— *Structure search of the T phase in silicene on the Ag(111) surface by Gaussian process regression*
1. Stability of Pd_xO_y Particles Supported on Strontium Titanate Perovskite under Three-Way Catalyst Operating Conditions: Implications for Sintering Resistance
T. N. Pham, B. A. C. Tan, Y. Hamamoto, K. Inagaki, I. Hamada, and Y. Morikawa ACS Catal. **14**, 1443 (2024).
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2. Machine-learned search for the stable structures of silicene on Ag(111)
Y. Hamamoto, T. N. Pham, M. K. Bisbo, B. Hammer, and Y. Morikawa Phys. Rev. Materials **7**, 124002 (2023).
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HARADA, KENJI [C class; 800 (B), 500 (C)] (310)
— *Application of tensor networks in tensor data analysis*

HARASHIMA, Yosuke [C class; 1000 (B), 0 (C)] (168)
— *Materials exploration using materials informatics*
1. Finite temperature effects on the structural stability of Si-doped HfO_2 using first-principles calculations
Y. Harashima, H. Koga, Z. Ni, T. Yonehara, M. Katouda, A. Notake, H. Matsui, T. Moriya, M. K. Si, R. Hasunuma, A. Uedono, and Y. Shigeta, Appl. Phys. Lett. **122**, 262903 (2023).
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HARUYAMA, Jun [C class; 3000 (B), 500 (C)] (15)
— *Electrochemical reaction analysis using density functional calculation + implicit solvation model 5*
1. First-principles study of water adsorption monolayer on Pt(111): Adsorption energy and second-order nonlinear susceptibility
J. Haruyama, T. Sugimoto, and O. Sugino, Phys. Rev. Mater. **7**, 115803 (2023).
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QE input for H20 adsorption monolayer system on Pt(111)
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HATANO, Naomichi [B class; 500 (B), 100 (C)] (341)
— *Numerical Simulation of A Novel Model of Two-Dimensional Quantum Active Particle*

HAYAMI, Satoru [C class; 3400 (B), 450 (C)] (290)
— *Search for magnetic skyrmion by machine learning*
1. Anisotropic spin model and multiple-Q states in cubic systems

R. Yambe and S. Hayami Physical Review B **107**, 174408 (2023).
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2. Field direction dependent skyrmion crystals in noncentrosymmetric cubic magnets: A comparison between point groups (O, T) and $T_{\rm d}$
S. Hayami and R. Yambe Physical Review B **107**, 174435 (2023).
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3. Antiferro Skyrmion Crystal Phases in a Synthetic Bilayer Antiferromagnet under an In-Plane Magnetic Field
S. Hayami Journal of Physical Society of Japan **92**, 084702 (2023).
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4. Magnetic bubble crystal in tetragonal magnets
S. Hayami and Y. Kato Physical Review B **108**, 024426 (2023).
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5. Unconventional Hall effect and magnetoresistance induced by metallic ferroaxial ordering
S. Hayami, R. Oiwa, and H. Kusunose Physical Review B **108**, 085124 (2023).
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6. Checkerboard bubble lattice formed by octuple-period quadruple-Q spin density waves
S. Hayami Physical Review B **108**, 094415 (2023).
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7. Chern insulating state with double-Q ordering wave vectors at the Brillouin zone boundary
S. Hayami Physical Review B **108**, 094416 (2023).
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8. Uniform and Staggered electric axial moment in zigzag chain
S. Hayami Physical Review B **108**, 094106 (2023).
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9. Time-reversal switching responses in antiferromagnets
S. Hayami and H. Kusunose Physical Review B **108**, L140409 (2023).
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10. Chiral charge as hidden order parameter in URu_2Si_2
S. Hayami and H. Kusunose Journal of Physical Society of Japan **92**, 123703 (2023).
DOI:10.7566/JPSJ.92.123703

11. Multiple-q Dipole-Quadrupole Instability in Spin-1 Triangular-Lattice Systems
S. Hayami and K. Hattori Journal of Physical Society of Japan **92**, 124709 (2023).
DOI:10.7566/JPSJ.92.124709

12. Three-sublattice antiferro-type and ferri-type skyrmion crystals in magnets without the Dzyaloshinskii-Moriya interaction
S. Hayami Physical Review B **109**, 014415 (2024).
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13. Hybrid skyrmion and anti-skyrmion phases in polar C_{4v} systems
S. Hayami Physical Review B **109**, 054422 (2024).
DOI:10.1103/PhysRevB.109.054422

HIDA, Kazuo [B class; 500 (B), 100 (C)] (339)
— *Numerical Study of One Dimensional Frustrated Quantum Spin Systems*

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

HIGUCHI, Yuji [C class; 5600 (B), 700 (C)] (272)
— *Rotational diffusion of water molecules on phospholipid bilayers*
— *Self-assembly processes of amphiphilic molecules and their structural controls*

1. Coarse-grained molecular dynamics simulation of cation distribution profiles on negatively charged lipid membranes during phase separation
   Yuji Higuchi, Klemen Bohinc, Jurij Rečsčič, Naofumi Shimokawa, and Hiroaki Ito, Soft Matter **19**, 3640 (2023).
   DOI:10.1039/d3sm00222e

2. Quasi-elastic neutron scattering reveals the relationship between the dynamical behavior of phospholipid headgroups and hydration water
   Md. Khalidur Rahman, Takeshi Yamada, Norifumi L. Yamada, Mafumi Hishida, Yuji Higuchi, and Hideki Seto, Struct. Dyn. **10**, 044701 (2023).
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3. Lateral Transport of Domains in Anionic Lipid Bilayer Membranes under DC Electric Fields: A Coarse-Grained Molecular Dynamics Study
   Hiroaki Ito, Naofumi Shimokawa, and Yuji Higuchi, J. Phys. Chem. B **127**, 8860 (2023).
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4. Absorption of water molecules on the surface of stereocomplex-crystal spherulites of polylactides: An in-situ FT-IR spectroscopy investigation
   Tomoka Kokuzawa, Shunryu Hirabayashi, Yuka Ikemoto, Junsu Park, Ryohei Ikura, Yoshinori Takashima, Yuji Higuchi, and Go Matsuba, Polymer **298**, 126922 (2024).
   DOI:10.1016/j.polymer.2024.126922

HINUMA, Yoyo [B class; 300 (B), 0 (C)] (207)
— *Reactivity analysis of high entropy alloys for catalyst informatics*

HIRATA, Kenji [C class; 800 (B), 0 (C)] ()
— *First-principles investigation of electronic state and piezoelectric property in oxide-based phosphor*

HIYAMA, Miyabi [B class; 400 (B), 0 (C)] (351)
— *Theoretical study for absorption and fluorescence spectra of firefly bioluminescence substrate analogs*

1. Experimental and Theoretical Study for Core Excitation of Firefly Luciferin in Carbon K - Edge Spectra
   Y. Kudo, F. Kumaki, M. Nagasaka, J-i. Adachi, Y. Noguchi, N. Koga, H. Itabashi, and M. Hiyama, J. Phys. Chem. A **128**, 611 (2024).
   DOI:10.1021/acs.jpca.3c07504

HO, Ngoc [C class; 1400 (B), 400 (C)] (155)
— *Electronic and transport properties of transition metal monosilicides for thermoelectric applications: KKR-CPA calculations*

1. Insight into Scattering Mechanisms and Transport Properties of AgCuS for Flexible Thermoelectric Applications
   Nam, Ho Ngoc and Phung, Quan Manh and Suzuki, Katsuhiro and Masago, Akira and Shinya,

Hikari and Fukushima, Tetsuya and Sato, Kazunori, ACS Appl. Mater. Interfaces **15**, 43871-43879 (2023).
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2. Exploring finite-temperature electronic transport in CoSi alloys with transition metals (Cr, Mn, Fe, and Ni) using the KKR-CPA method
Nam, Ho Ngoc and Phung, Quan Manh and Suzuki, Katsuhiro and Shinya, Hikari and Masago, Akira and Fukushima, Tetsuya and Sato, Kazunori, J. Mater. Chem. A **12**, 451-459 (2024).
DOI:10.1039/D3TA06259G

HOSHI, Takeo [C class; 3800 (B), 500 (C)] (103)
— *HPC-based fusion of quantum simulation, experiment analysis and data-driven science*

1. A fast and efficient computation method for reflective diffraction simulations
S. Kudo, Y. Yamamoto, T. Hoshi Computer Physics Communications 296, 109029 (2024).
DOI:10.1016/j.cpc.2023.109029

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

HOSONO, Nobuhiko [C class; 3200 (B), 450 (C)] (295)
— *All-Atom Molecular Dynamics Simulation Study of Polymer Dynamics in Nanoporous Materials*

HOTTA, Takashi [C class; 3200 (B), 0 (C)] (233)
— *Research of Three-Channel Kondo Effect Emerging from Tb and Tm Ions*

HUKUSHIMA, Koji [C class; 1200 (B), 100 (C)] ()
— *Molecular dynamics study of Chromatin molecular model*

IDO, Kota [C class; 8200 (B), 850 (C)] (223)
— *Many-body topological phases in frustrated magnets*
— *Many-body topological phases in strongly correlated electron systems*

1. Update of HΦ: Newly added functions and methods in versions 2 and 3
Kota Ido, Mitsuaki Kawamura, Yuichi Motoyama, Kazuyoshi Yoshimi, Youhei Yamaji, Synge Todo, Naoki Kawashima, Takahiro Misawa Comput. Phys. Commun. **298**, 109093 (2024).
DOI:10.1016/j.cpc.2024.109093

2. Data Analysis of Ab initio Effective Hamiltonians in Iron-Based Superconductors — Construction of Predictors for Superconducting Critical Temperature
Kota Ido, Yuichi Motoyama, Kazuyoshi Yoshimi, Takahiro Misawa J. Phys. Soc. Jpn. **92**, 064702 (2023).
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3. Interface tool from Wannier90 to RESPACK: wan2respack
Kensuke Kurita, Takahiro Misawa, Kazuyoshi Yoshimi, Kota Ido, Takashi Koretsune Comput. Phys. Commun. 292, 108854 (2023).
DOI:10.1016/j.cpc.2023.108854

Data Repository
Update of HΦ: Newly added functions and methods in versions 2 and 3
https://isspns-gitlab.issp.u-tokyo.ac.jp/hphi-dev/hphi-paper2023

Interface tool from Wannier90 to RESPACK wan2respack

https://isspns-gitlab.issp.u-tokyo.ac.jp/kido902/wan2respack_paper

IITAKA, Toshiaki [C class; 2600 (B), 500 (C)] (123)
— *Extension of finite temperature calculation with random-phase sates to general variational wave functions*
— *Miscible-Immiscible Transition of Hydrous Silicate Melt*

IKEDA, Hiroaki [B class; 500 (B), 100 (C)] ()
— *Ab initio calculations of spin currents and chirality in chiral materials*

IKUHARA, Yuichi [C class; 6400 (B), 0 (C)] (87)
— *Exploring stable interface atomic structures and properties by first-principles calculations*
— *Structural analysis and property prediction of grain-boundary segregation by first-principles calculations*

IMADA, Masatoshi [E class; 14000 (B), 1500 (C)] (220)
— *Long-time simulation for strongly-correlated quantum systems*

1. Quantum criticality of bandwidth-controlled Mott transition
   Kensaku Takai, Youhei Yamaji, Fakher F. Assaad, Masatoshi Imada Phys. Rev. Res. **5**, 033186 (2023).
   DOI:10.1103/PhysRevResearch.5.033186

2. Superconductivity studied by solving ab initio low-energy effective Hamiltonians for carrier doped CaCuO2, Bi2Sr2CuO6, Bi2Sr2CaCu2O8, and HgBa2CuO4
   Michael Tobias Schmid, Jean-Baptiste More, Ryui Kaneko, Youhei Yamaji, Masatoshi Imada Phys. Rev. X **13**, 041036 (2023).
   DOI:10.1103/PhysRevX.13.041036

INAGAKI, Kouji [B class; 200 (B), 100 (C)] (206)
— *Analyses of diamond surface processes by machine-learing based potentials*

INAOKA, Takeshi [B class; 400 (B), 90 (C)] (193)
— *Search and realization of novel electronic properties of surfaces and interfaces and of nanostructures*

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— *Photoinduced entanglement generation dynamics in electron-phonon systems*

ISHII, Fumiyuki [C class; 9200 (B), 900 (C)] (62)
— *Development and applications of first-principles computational methods using Berry phase of Bloch wavefunctions*
— *First-principles calculation of van der Waals magnet*

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ISOBE, Masaharu [B class; 500 (B), 100 (C)] (337)
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— *Theoretical study of isoelectronic doping effects in iron-based superconductors*

JIE, Sun [C class; 1600 (B), 250 (C)] ()
— *The study of transport properties in two-dimensional materials on substrates using large-scale simulation methods based on machine learning*

JOUTSUKA, Tatsuya [C class; 1000 (B), 0 (C)] (166)
— *Reaction Analysis in Solid Catalysts by DFT Calculations and Informatics*

KADARISMAN, Hana [B class; 300 (B), 60 (C)] ()
— *First-principles calculation of diamond materials*

KAGAWA, Fumitaka [C class; 0 (B), 500 (C)] (247)
— *Numerical calculation of emergent electric field induced by current-driven non-collinear magnetic structure*

KAGESHIMA, Hiroyuki [C class; 2200 (B), 400 (C)] (130)
— *Study on physical properties of structural elementary excitations at solid surfaces and interfaces*

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— *Band engineering and electron correlation effects in artificially stacked systems*

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— *Equilibrium/nonequilibrium electrochemistry of disordered solid-state interfaces*

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— *Multiscale simulations for complex flows*

KAWAMURA, Hikaru [C class; 1800 (B), 0 (C)] ()
— *Novel order in frustrated magnets*

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— *Lattice thermal conductivity calculation of iridium oxide* $Ca_5Ir_3O_{12}$

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— *Tensor-Network Study of Classical Random Spin Systems*

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— *Efficient sampling simulation of the soft modes significantly contribute to protein properties*

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

KOBAYASHI, Nobuhiko [C class; 3400 (B), 450 (C)] (109)
— *Quantum transport theory by large scale first-principles electron transport calculations*

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— *Molecular dynamics simulation of nanocarbon stacking structure*

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— *Analyzing Ferromagnetic Order in Multi-Component Fermionic Systems using DMFT*
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LI, Hao [C class; 3800 (B), 0 (C)] (210)
— *Design of Effective Electrocatalysts by Theory and Ab Initio Computations*

MAEHIRA, Takahiro [B class; 400 (B), 100 (C)] (189)
— *Electronic Structure and Fermi surface of ReO_3*

MAKINO, Takayuki [B class; 400 (B), 90 (C)] (251)
— *Construction of ab-initio tight-binding Hamiltonian and determination of dielectric functions of rare-earth monoxides having insulating ground states*

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MATSUKAWA, Hiroshi [C class; 3600 (B), 450 (C)] ()
— *Physics of Friction*

MATSUSHITA, Katsuyoshi [C class; 1000 (B), 0 (C)] (319)
— *Division Plane Inference for Cell Division based on Computatinal Physics*
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— *Electronic structure of wide-gap semiconductors based on first-principles calculations: from power devices to quantum devices*
— *Proposal for Free Devices Based on First-Principles Calculations: From Material Exploration to Device Fabrication*

1. Atomic scale localization of KohnSham wavefunction at SiO_2/4HSiC interface under electric field, deviating from envelope function by effective mass approximation
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— *Molecular Dynamics of Polymer Chain under Deformation*

MICHISHITA, Yoshihiro [B class; 300 (B), 90 (C)] (352)
— *Machine-Learning-Assisted Exploration of Appropriate Transformation and Projections*

MINAMI, Susumu [B class; 800 (B), 170 (C)] (170)
— *First-principles study of magnetic thermoelectric effect in topological magnets*
— *First-principles study of stable interfacial structure analysis and magnetic tunnel conductance in topological magnets*

MISAWA, Masaaki [B class; 400 (B), 0 (C)] (199)
— *Phonon properties based on nanoscale structures in two-dimensional materials*

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— *Comprehensive ab initio investigation of high-Tc materials using database*

1. Compensated Ferrimagnets with Colossal Spin Splitting in Organic Compounds
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https://isspns-gitlab.issp.u-tokyo.ac.jp/k-yoshimi/tmttfpf6-pdep

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MITARAI, Yoko [B,D class; 1000 (B), 0 (C)] (165)
— *Phase equilibrium of high entropy alloys and shape memory alloys*

MIZUKAMI, Wataru [C class; 5000 (B), 900 (C)] (274)
— *Quantum-classical hybrid simulations for sensor materials based on quantum state tomography*

1. Comparative study on compact quantum circuits of hybrid quantum-classical algorithms for quantum impurity models
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— *Theoretical study on photoinduced nonequilibrium electron states in spin-orbit coupling systems and strongly correlated electron systems*

1. Theory of collective excitations in the quadruple-Q magnetic hedgehog lattices
Rintaro Eto, and Masahito Mochizuki Physical Review Letters 132, 226705 (2024).
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MOCHIZUKI, Yasuhide [C class; 5200 (B), 500 (C)] (94)
— *Quasi-harmonic approximated and molecular dynamic calculations for phonon-induced negative-thermal-expansion materials*

1. Mechanism of Negative Thermal Expansion in Monoclinic Cu2P2O7 from First Principles
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2. Thermal Properties of the Element and Binary Oxides toward Negative Thermal Expansion: A First-Principles Lattice-Dynamics Study
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3. Superlattice MAX phases with A-layers reconstructed into 0D-clusters, 1D-chains, and 2D-lattices
M. Khazaei, S. Bae, R. Khaledialidusti, A. Ranjbar, H.-P. Komsa, S. Khazaei, M. Bagheri, V. Wang, Y. Mochizuki, M. Kawamura, G. Cuniberti, S. M. Allaei, K. Ohno, H. Hosono, and H. Raebiger J. Phys. Chem. C **127**, 14906 (2023).
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MORI, Hatsumi [C,D class; 5600 (B), 0 (C)] (98)
— *First-principles NEB calculations of proton tautomeric conduction pathways*
— *First-principles NEB calculations of proton tautomeric conduction pathways (II)*
— *First-principles NEB calculations of proton tautomeric conduction pathways(I)*

MORI, RYO [B class; 400 (B), 70 (C)] ()
— *Investigation of spin and electronic structures in surface/interface of topological insulator thin films*

MORIKAWA, Yoshitada [E class; 14000 (B), 2400 (C)] (56)
— *Theoretical study on dynamical processes in heterogeneous catalysis using density functional theory and machine learning methods*

1. The quantitative study of methane adsorption on the Pt(997) step surface as the initial process for reforming reactions
Y. H. Choi, S. E. M. Putra, Y. Shiozawa, S. Tanaka, K. Mukai, I. Hamada, Y. Morikawa, J. Yoshinobu Surf. Sci. **732**, 122284 (2023).
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2. Electronic and optical properties of the hydrogen boride sheet from the many-body perturbation theory
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3. Machine learning molecular dynamics simulation of CO-driven formation of Cu clusters on the Cu(111) surface
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4. First-principles Microkinetic Study of NO Reduction on Cu Catalysts
M. R. Al Fauzan, T. N. Pham, H. H. Halim, Y. Hamamoto, K. Inagaki, I. Hamada, and Y. Morikawa J. Phys. Chem. C, **127**, 19451 (2023).
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5. DFT investigation of the oxygen reduction reaction over nitrogen (N) doped graphdiyne as an electrocatalyst: the importance of pre-adsorbed OH* and the solvation effect
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6. Machine-learned search for the stable structures of silicene on Ag(111)
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7. Stability of Pd_xO_y Particles Supported on Strontium Titanate Perovskite under Three-Way Catalyst Operating Conditions: Implications for Sintering Resistance
T. N. Pham, B. A. Choi Tan, Y. Hamamoto, K. Inagaki, I. Hamada, and Y. Morikawa ACS Catal., **14**, 1443 (2024).
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8. Origin of the Surface Facet Dependence in the Oxidative Etching of the Diamond (111) and (100) Surfaces from First-Principles Calculations
J. I. G. Enriquez, T. Yamasaki, M. Michiuchi, K. Inagaki, M. Geshi, I. Hamada, Y. Morikawa J. Phys. Chem. C, **128**, 6294 (2024).
DOI:10.1021/acs.jpcc.3c08378

MORITA, Katsuhiro [B class; 300 (B), 0 (C)] (354)
— *Finite temperature calculations of quantum spin systems*

MORITA, Satoshi [B class; 600 (B), 100 (C)] (331)
— *Study of critical phenomena by the bond-weighted tensor renormalization group method*

1. Ashkin-Teller phase transition and multicritical behavior in a classical monomer-dimer model
Satoshi Morita, Hyun-Yong Lee, Kedar Damle, and Naoki Kawashima, Phys. Rev. Research **5**, 043061 (2023).
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MOTOME, Yukitoshi [C,D class; 30400 (B), 1950 (C)] (215)
— *Large-scale analysis of scrambling rate by tensor quantum reservoir probing*
— *Numerical study of spin-charge coupled dynamics by machine learning potentials*
— *Theoretical study of strongly correlated topological phenomena and its application to machine learning*

1. Spin nematics meet spin liquids: Exotic quantum phases in the spin-1 bilinear-biquadratic model with Kitaev interactions
R. Pohle, N. Shannon, and Y. Motome Phys. Rev. B **107**, L140403 (2023).
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2. Ground-State Phase Diagram of the KitaevHeisenberg Model on a Three-dimensional Hyperhoneycomb Lattice
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3. Berry curvature contributions of kagome-lattice fragments in amorphous FeSn thin films
K. Fujiwara, Y. Kato, H. Abe, S. Noguchi, J. Shiogai, Y. Niwa, H. Kumigashira, Y. Motome, and A. Tsukazaki Nat. Commun. **14**, 3399 (2023).
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4. Thermally-robust spatiotemporal parallel reservoir computing by frequency filtering in frustrated magnets
K. Kobayashi and Y. Motome Sci. Rep. **13**, 15123 (2023).
DOI:10.1038/s41598-023-41757-3

5. Emergent electric field from magnetic resonances in a one-dimensional chiral magnet
K. Shimizu, S. Okumura, Y. Kato, and Y. Motome Phys. Rev. B **108**, 134436 (2023).
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6. Metallic ruthenium ilmenites: First-principles study of $MgRuO_3$ and $CdRuO_3$
S.-H. Jang and Y. Motome AIP Advances **14**, 015229 (2024).
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8. Unveiling the orbital-selective electronic band reconstruction through the structural phase transition in $TaTe_2$
N. Mitsuishi, Y. Sugita, T. Akiba, Y. Takahashi, M. Sakano, K. Horiba, H. Kumigashira, H. Takahashi, S. Ishiwata, Y. Motome, and K. Ishizaka Phys. Rev. Research **6**, 013155 (2024).
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9. Quantum reservoir probing of quantum information scrambling
K. Kobayashi and Y. Motome submitted to Phys. Rev. Applied

10. Possible Realization of Kitaev Spin Liquids in van der Waals Heterostructures of α-$RuCl_3$ and CrX_3 (X=Cl and I)
submitted to Phys. Rev. B

11. Spin Seebeck Effect as a Probe for Majorana Fermions in Kitaev Spin Liquids
Y. Kato, J. Nasu, M. Sato, T. Okubo, T. Misawa, and Y. Motome submitted to Phys. Rev. X

12. Magnetic field effects on the Kitaev model coupled to environment
K. Fukui, Y. Kato, and Y. Motome submitted to Phys. Rev. B

13. Quantum reservoir probing of quantum phase transitions
K. Kobayashi and Y. Motome submitted to Nature Commun.

14. Topological transitions by magnetization rotation in kagome monolayers of ferromagnetic Weyl semimetal Co-based shandite
K. Nakazawa, Y. Kato, and Y. Motome, preprint (arXiv:2402.16273) submitted to Phys. Rev. B

15. Exploring rare-earth Kitaev magnets by massive-scale computational analysis
S.-H. Jang and Y. Motome submitted to Communications Materials

16. Spin-Orbit Coupled Insulators and Metals on the Verge of Kitaev Spin Liquids in Ilmenite Heterostructures
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17. Eight-color chiral spin liquid in the S=1 bilinear-biquadratic model with Kitaev interactions
R. Pohle, N. Shannon, and Y. Motome submitted to Phys. Rev. B

MURASHIMA, Takahiro [C class; 3000 (B), 400 (C)] (298)
— *Nonequilibrium dynamics of multicyclic chains under elongational flow*

NADA, Hiroki [B,C class; 400 (B), 500 (C)] (322, 323)
— *A Large-Scale Metadynamics Simulation Study on the Binding Conformations of Ionic Polymers at a Geometrically Rough Surface of Calcium Carbonate Crystal*
— *A Large-Scale Molecular Dynamics Simulation Study on the Shape of an Ice Crystal Grown from Water Including Air Molecules*

1. Observation of hydrogen-ordered cubic ice thin films on the surface of ice Ic nanocrystals upon coarsening

A. Kouchi, T. Yamazaki, H. Katsuno, H. Nada, T. Hama, Y. Kimura Chem. Phys., **572** (2023) 111966.
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2. Anisotropy in spinodal-like dynamics of unknown water at ice V-water interface
H. Niinomi, T. Yamazaki, H. Nada, T. Hama, A. Kouchi, T. Oshikiri, M. Nakagawa, Y. Kimura Sci. Rep., **13** (2023) 16227.
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3. In situ cryogenic transmission electron microscopy observation on the formation of hydrogen-ordered hexagonal ices and its astrophysical implications
T. Yamazaki, A. Kouchi, K. Murata, H. Katsuno, H. Nada, T. Hama, Y. Kimura Monthly Notices of the Royal Astronomical Society, **527** (2024) 2858.
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H. Niinomi, T. Yamazaki, H. Nada, T. Hama, A. Kouchi, T. Oshikiri, M. Nakagawa, Y. Kimura J. Phys. Chem. Lett., **15** (2024) 659.
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5. Unknown crystal-like phases formed in an imidazolium ionic liquid: a metadynamics simulation study
H. Nada, Submitted to J. Chem. Phys.

NAKAGAWA, Naoko [C class; 4200 (B), 500 (C)] (37)
— *Steady metastable states contained in heat conducting phase coexistence*

NAKAMURA, Kazuma [C,D class; 4600 (B), 0 (C)] (45)
— *Ab initio calculations for optical property of transition-metal compound interface*
— *Construction of thermal conductivity and plasma frequency database from first principles*
— *Construction of thermal conductivity database from first principles*

1. Superconductivity of barium with highest transition temperatures in metallic materials at ambient pressure
M. Mito, H. Tsuji, T. Tajiri, K. Nakamura, Y. Tang, Z. Horita Sci. Rep. **14**,965 (2024).
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2. Ab initio calculation for electronic structure and optical property of tungsten carbide in a TiCN-based cermet for solar thermal applications
S. Hayakawa, T. Chono, K. Watanabe, S. Kawano, K. Nakamura, K. Miyazaki Sci. Rep. **13**, 9407 (2023).
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3. Insulating Nature of Iridium Oxide Ca5Ir3O12 Probed by Synchrotron-Radiation-Based Infrared Spectroscopy
H. Hanate, S. Kawano, M. Hayashida, K. Nakamura, Y. Ikemoto, T. Moriwaki, T. Hasegawa, S. Tsutsui, K. Matsuhira J. Phys. Soc. Jpn **92**, 064705 (2023).
DOI:10.7566/JPSJ.92.064705

NAKANO, Hiroki [C class; 3800 (B), 450 (C)] (287)
— *Numerical study on low-energy states of quantum spin systems*

1. Large-Scale Numerical-Diagonalization Study of the Shastry-Sutherland Model
H. Nakano and T. Sakai, JPS Conf. Proc.38, 011166 (2023).

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2. Translational symmetry broken magnetization plateau of the S=1 antiferromagnetic Heisenberg chain with competing anisotropies
T. Sakai, K. Okamoto, K. Okunishi, M. Hashimoto, T. Houda, R. Furuchi, H. Nakano, Phys. Rev. B 108, 174435 (2023).
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NAKANO, Hiroyoshi [C class; 7800 (B), 850 (C)] (264)
— *Analysis of microphase separation in active particle systems with self-propulsion*
— *Phase separation of active Brownian particles with Levy walks*

1. Universal properties of repulsive self-propelled particles and attractive driven particles
H. Nakano, K. Adachi Phys. Rev. Research **6**, 013074 (2024).
DOI:10.1103/PhysRevResearch.6.013074

NAKAYAMA, Akira [C class; 3000 (B), 400 (C)] (117)
— *DFT-MD and NNP-MD simulations for metal-oxide catalysis*

NASU, Joji [C class; 4200 (B), 550 (C)] (226)
— *Creation and manipulation of Majorana zero mode in quantum spin liquids*
— *Real-time dynamics of vison excitations in Kitaev spin liquids*

1. Field-driven spatiotemporal manipulation of Majorana zero modes in a Kitaev spin liquid
C. Harada, A. Ono, and J. Nasu, Phys. Rev. B **108**, L241118 (2023).
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2. Flavor-wave theory with quasiparticle damping at finite temperatures: Application to chiral edge modes in the Kitaev model
S. Koyama and J. Nasu, Phys. Rev. B **108**, 235162 (2023).
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3. Field-direction Dependence of Majorana-mediated Spin Transport
H. Taguchi, A. Koga, Y. Murakami, J. Nasu, and H. Tsuchiura, JPS Conf. Proc. **38**, 011152 (2023).
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NIKI, Kaori [C class; 1600 (B), 500 (C)] (147)
— *Electronic state analysis on molecular thin film surface*

1. Adsorbed CO2-Mediated CO2 Photoconversion Cycle into Solar Fuel at the O Vacancy Site of Zirconium Oxide
K. Hara, M. Nozaki, R. Hirayama, R. Ishii, K. Niki, and Y. Izumi J. Phys. Chem. C 2023, 127, 4, 1776 (2023).
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NISHIDATE, Kazume [C class; 800 (B), 0 (C)] (176)
— *Theoretical study of the reactivity of H_2O molecule on the double-perovskite*

1. Surface electronic structure and photo activity of double perovskite Ba2PrBiO6: First-principles investigations
K. Nishidate et al. Surfaces and Interfaces **24**, 103914 (2024).
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NISHIGUCHI, Kazutaka [B class; 400 (B), 90 (C)] (249)
— *Theoretical study of thermoelectric properties in Heusler compounds using weak-coupling approaches*

NISHIKAWA, Yoshihiko [C class; 3800 (B), 0 (C)] (292)
— *Phase transitions in a classical chiral magnet with a clock anisotropy*

NOGUCHI, Hiroshi [C class; 3200 (B), 450 (C)] (294)
— *structure formation of biomembrane*

NOGUCHI, Yoshifumi [C class; 6400 (B), 750 (C)] (80)
— *Development of second-order GW electron-hole interaction kernel*
— *Self-interaction corrections in GW approximation*

1. Significant contributions of second-order exchange terms in GW electron-hole interaction kernel for charge-transfer excitations
   Yamada and Yoshifumi Noguchi, J. Chem. Phys. **159**, 234105 (2023).
   DOI:10.1063/5.0178723

NOMURA, Yusuke [E class; 14500 (B), 1500 (C)] (219)
— *Development and application of tensor neural network methods*

NOZAWA, Kazuki [C class; 1800 (B), 200 (C)] (151)
— *First-principles study of surface atomic structure and chemical properties of intermetallic compounds*

1. First-principles Study of Adsorption of Atomic Oxygen on PdZn(111) Surface
   K. Iwamura, Y. Otani, Y. Takahashi, Y. Ishii, and K. Nozawa Materials Transactions, accepted

OBATA, Masao [B class; 600 (B), 140 (C)] (178)
— *Analysis of magnetic materials with anisotropic crystal structures*
— *First-principles investigation on magnetic shape memory alloy*

1. Computational acceleration on density functional approach code using GPU
   C. Pardede, M. Obata, R. Majumder, I. Pardede, and T. Oda Proceedings of the 34th IUPAP Conference on Computational Physics (CCP2023), accepted

OCHI, Masayuki [C class; 8400 (B), 0 (C)] (76)
— *Development of a first-principles calculation software for a many-body wave function theory*
— *Improvement of accuracy and software development for the first-principles wave function theory*

1. Pair correlations in the two-orbital Hubbard ladder: Implications for superconductivity in the bilayer nickelate $La_3Ni_2O_7$
   T. Kaneko, H. Sakakibara, M. Ochi, and K. Kuroki Phys. Rev. B **109**, 045154 (2024).
   DOI:10.1103/PhysRevB.109.045154

2. Possible High Tc Superconductivity in $La_3Ni_2O_7$ under High Pressure through Manifestation of a Nearly Half-Filled Bilayer Hubbard Model
   H. Sakakibara, N. Kitamine, M. Ochi, and K. Kuroki Phys. Rev. Lett. **132**, 106002 (2024).
   DOI:10.1103/PhysRevLett.132.106002

ODA, Tatsuki [C class; 5600 (B), 850 (C)] (84)
— *Analyses on electronic structure and magnetic anisotropy in high-performance spintronics magnetic materials and parallelization development/application in quasi-particle self-consistent GW code*
— *Analyses on electronic/magnetic structures in high-performance spintronics magnetic materials and parallelization development/application in quasi-particle self-consistent GW code*

1. Migration of the Twin Boundary in a Modulated Martensite Phase of Magnetic Shape Memory

Alloy Ni2MnGa
Rinku Majumder, Masao Obata, Chandro Pardede, Jakub Lutinec, Ladislav Kalvoda, and Tatsuki Oda, accepted for the proceedings of CCP2023 (34th IUPAP Conference on Computational Physics).

2. Computational acceleration on density functional approach code using GPU
Chandro Pardede, Masao Obata, Rinku Majumder, Indra Pardede, and Tatsuki Oda, accepted for the proceedings of CCP2023 (34th IUPAP Conference on Computational Physics).

3. Parallelization in the code of quasi-particle self-consistent GW and electronic structure in the magnetic shape memory alloy Ni2MnGa
Ko Hyodo, Masao Obata, Jakub Lutinec, Ladislav Kalvoda, Takao Kotani, and Tatsuki Oda, accepted for the proceedings of CCP2023 (34th IUPAP Conference on Computational Physics).

OHKUBO, Yuji [B class; 800 (B), 70 (C)] (174)
— Calculation of chemical shift of X-ray photoelectron binding energy of functional groups generated on fluoropolymer surface
— Calculation of chemical shift of X-ray photoelectron binding energy of hydrogen-containing functional groups generated on fluoropolymer surface

1. Identification of chemical species on plasma-treated polytetrafluoroethylene surface by ab-initio calculations of core-energy-level shift in X-ray photoelectron spectra
Misa Nishino, Kouji Inagaki, Yoshitada Morikawa, Kazuya Yamamura, Yuji Ohkubo Applied Surface Science, 655, 159369 (2024).
DOI:10.1016/j.apsusc.2024.159369

OHMURA, Satoshi [C class; 2400 (B), 0 (C)] (136)
— Nanoscale properties and CO_2 fixation of cement-based materials : ab initio molecular dynamics simulations

1. Quantum lattice model solver $H\Phi$
D. Murayama, S. Ohmura, R. Kodama and N. Ozaki, J. Appl. Phys. **134**, 095902 (2023).
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2. 分子動力学法による結晶状態と非晶質状態の 11 トバモライトの局所力学特性
I. Kanemasu, S. Ohmura, N. Takeda, セメント・コンクリート論文集、**77**, 9, (2023).
DOI:10.14250/cement.77.9

3. Molecular dynamics study of uniaxial tensile and compressive behavior of crystalline and amorphous tobermorite
I. Kanemasu and S. Ohtaka, Springer Proceedings in Physics for CCP 2023. accepted

OHNISHI, Masato [C,E class; 16600 (B), 1500 (C)] (54)
— Construction of anharmonic phonon database with first-principles calculations
— Data-drive materials development using anharmonic phonon database

1. Thermoelectric power of a single van der Waals interface between carbon nanotubes
H. Hamasaki, Y. Li, M. Ohnishi, J. Shiomi, K. Yanagi, and K. Hirahara ACS Nano 18, 612 (2024).
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2. Thermoelectric figure-of-merit of metastable crystalline ST12 germanium allotrope
H. Meng, M. Ohnishi, Meng An, and J. Shiomi Materials Today Physics 38, 101270 (2023).
DOI:10.1016/j.mtphys.2023.101270

OHNO, Kaoru [C class; 5600 (B), 500 (C)] (91)
— *Improvement and application of all-electron mixed basis program*

1. Electron-capture decay rate of ^{7}Be encapsulated in C_{70} fullerene cage
   Tsutomu Ohtsuki, Riichi Kuwahara, and Kaoru Ohno, Phys. Rev. C **108**, L011301 (2023).
   DOI:10.1103/PhysRevC.108.L011301

2. Electronic and optical properties of C_{60}/Ti_2CT_2 and $C_{60}/Ti_3C_2T_2$ (T = F, OH, or O) Heterostructures
   Zahra Hajiahmadi, Mohammad Khazaei, Ahmad Ranjbar, Alireza Mostafaei, Sergii Chertopalov, Thomas D. Khne, Gianaurelio Cuniberti, Hamid Hosano, Hannes Raebiger, and Kaoru Ohno, Comp. Mat. Sci. **228**, 112364 (2023).
   DOI:10.1016/j.commatsci.2023.112364

3. Superlattice MAX phases with A-layers reconstructed into 0D-clusters, 1D-chains, and 2D-lattices
   Mohammad Khazaei, Soungmin Bae, Rasoul Khaledialidusti, Ahmad Ranjbar, Hannu-Pekka Komsa, Somayeh Khazaei, Mohammad Bagheri, Yasuhide Mochizuki, Mitsuaki Kawamura, Gianaurelio Cuniberti, Mehdi Vaez Alaei, Kaoru Ohno, Hideo Hosono, and Hannes Raebiger, J. Phys. Chem. C **127**, 14906-14913 (2023).
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4. Electron-capture decay rate of ^{7}Be in cluster and crystal forms of beryllium: A first-principles study
   Riichi Kuwahara, Kaoru Ohno, and Tsutomu Ohtsuki, Phys. Rev. C **109**, 024609 (2024).
   DOI:10.1103/PhysRevC.109.024609

OHSAWA, Kazuhito [C class; 1200 (B), 0 (C)] (162)
— *Study of interaction between radiation damage and interstitial atom*

OHTO, Tatsuhiko [C class; 3200 (B), 0 (C)] (121)
— *First-principles calculations for molecular junctions*

1. Durable high-entropy non-noble metal anodes for neutral seawater electrolysis
   Fumiya Shiokawa, Aimi Asilah Haji Tajuddin, Tatsuhiko Ohto, Yue Yu, Takeshi Fujita, Hisanori Tanimoto, Zeyu Xi, Samuel Jeong, and Yoshikazu Ito journalChem. Eng. J. 479, 147862 (2024).
   DOI:10.1016/j.cej.2023.147862

OHTSUKI, Tomi [C class; 5200 (B), 300 (C)] (284)
— *The Anderson transitions in quasi-periodic systems*

1. Anisotropic Topological Anderson Transitions in Chiral Symmetry Classe
   Z. Xiao, K. Kawabata, X. Luo, T. Ohtsuki, R. Shindou Physical Review Letters **131**, 056301 (2023).
   DOI:10.1103/PhysRevLett.131.056301

2. Singular-value statistics of non-Hermitian random matrices and open quantum systems
   K. Kawabata, Z. Xiao, T. Ohtsuki, R. Shindou PRX Quantum **4**, 040312 (2023).
   DOI:10.1103/PRXQuantum.4.040312

3. Critical behavior of the Anderson transition in higher-dimensional Bogoliubovde Gennes symmetry classes
   T. Wang, Z. Pan, K. Slevin, T. Ohtsuki Physical Review B **108**, 144208 (2023).
   DOI:10.1103/PhysRevB.108.144208

4. Irrelevant corrections at the quantum Hall transition
   K. Slevin, T. Ohtsuki physica status solidi (RRL)Rapid Research Letters **17**, 2300080 (2023).

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5. Machine learning wave functions to identify fractal phases
T. Cadez, B. Dietz, D. Rosa, A. Andreanov, K. Slevin, T. Ohtsuki Physical Review B **108**, 184202 (2023).
DOI:10.1103/PhysRevB.108.184202

6. A Stochastic Method to Compute the L2 Localisation Landscape
M. Kakoi and K. Slevin Journal of the Physical Society of Japan, **92**, 054707 (2023).
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7. Time evolution of coherent wave propagation and spin relaxation in spin-orbit-coupled systems
M. Kakoi and K. Slevin Physical Review A, **109**, 033303 (2024).
DOI:10.1103/PhysRevA.109.033303

OKITSU, Kouhei [B class; 200 (B), 50 (C)] ()
— *Verification of the hypothesis concerning 'too much R-factor' of protein crystal structure analysis*

OKUBO, Masashi [B class; 500 (B), 100 (C)] ()
— *Theoretical calculation of intercalation-type electrode materials for aqueous proton rechargeable batteries*

OKUBO, Tsuyoshi [C class; 8400 (B), 850 (C)] (262, 371)
— *Study on finite temperature properties of frustrated magnets*
— *Tensor network study of quantum spin models on the honeycomb lattice.*

1. Possibility of a topological phase transition in two-dimensional RP^3 model
T. Okubo and N. Kawashima J. Phys. Soc. Jpn. **92**, 114701 (2023).
DOI:10.7566/Jpsj.92.114701

2. Spin Seebeck Effect as a Probe for Majorana Fermions in Kitaev Spin Liquids
Y. Kato, J. Nasu, M. Sato, T. Okubo, T. Misawa, and Y. Motome arXiv:2401.13175
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3. Quantum phase transition between spin liquid and spin nematics in spin-1 Kitaev honeycomb model
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SAKAI, Toru [C class; 5600 (B), 700 (C)] (268, 270)
— *Novel Magnetization PLateau of the Spin Ladder System*
— *Spin Nematic Phase of 2D Ferromagnetic Dimer Systems*

1. Translational symmetry broken magnetization plateau of the S=1 antiferromagnetic Heisenberg chain with competing anisotropies
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SASAKI, Takehiko [C class; 1600 (B), 250 (C)] (154)
— *Study on structures and reactions of platinum nanoparticles*

SATO, Ryuhei [C class; 1200 (B), 0 (C)] (311)
— *The Mechanism Study of Superionic Conduction Induced by Complex Ion Rotation Using Persistent Diagram*

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SEINO, Kaori [C class; 2000 (B), 250 (C)] (140)
— *First-principles study of defects in GaN*

SEKI, Yuya [B class; 400 (B), 100 (C)] (346)
— *Analysis of Ising model in statistical-mechanical informatics*

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— *Change in the electronic structure of atomic layered, organic and magnetic materials by doping*
— *Construction of model Hamiltonian to interpret experimental results of topological* $Pr_2Ir_2O_7$

1. Pitched π-stacking crystal structure and two-dimensional electronic structure of acenaphtho[1,2-k]fluoranthene analogues with various substituents
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— *Thermal effects on quantum frustrated magnetisms*
— *Thermal effects on quantum frustrated magnets*

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— *Molecular Simulation of Soft Materials using All-Atom and Coarse-Grained Force Field*

1. Fluorescence Turn-on of Tetraphenylethylene Derivative by Transfer from Cyclodextrin to Liposomes, HeLa Cells, and E. coli
   Kosuke Masuda, Riku Omokawa, Riku Kawasaki, Yuta Mise, Yousuke Ooyama, Shogo Harada,

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SHINOHARA, Yasushi [C class; 2400 (B), 0 (C)] (134)
— *First-principles simulations for optical absorption of dielectrics by multi-pulse laser fields*

SHIOMI, Junichiro [C class; 8000 (B), 800 (C)] (72)
— *Analysis of thermal transport in disordered systems*
— *Large-scale simulations based on machine learning for thermal transport in twisted layered materials*

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SUGINO, Osamu [C class; 8400 (B), 900 (C)] (71)
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SUWA, Hidemaro [C class; 3800 (B), 500 (C)] (229)
— *Novel magnetic phases emerging from spin-charge-lattice couplings*

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SUZUKI, Takafumi [C class; 2800 (B), 400 (C)] (299)
— *Dynamical properties of the extended Kitaev-Gamma model on a honeycomb lattice 2*

SUZUKI, Takehito [B class; 200 (B), 30 (C)] (358)
— *Classification of slow and fast earthquakes based on fluid pressure and porosity*
— *Understanding of the difference of magnitude-frequency relation between the fast and slow earthquakes based on a microscopic viewpoint*

SUZUKI, Yuji [C class; 2200 (B), 0 (C)] (141)
— *Development of Stretchable Electret Materials for Energy Harvesting with the Aid of Machine Learning*

TADA, Kohei [B class; 500 (B), 100 (C)] (182)
— *Theoretical investigation for systemataising surface diradical*

1. Model calculations for the prediction of the diradical character of physisorbed molecules: p-benzyne/MgO and p-benzyne/SrO
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— *Ionic conduction mechanism of superionic conductor $RbAg_4I_5$*

TAKAHASHI, Osamu [B class; 200 (B), 100 (C)] ()
— *Electronic structure of aqueous functional group materials*

TAKAYAMA, Akari [B class; 600 (B), 0 (C)] (332)
— *Topological phase transition in Sb/Bi heterostructure studied by TRHEPD*

TAKEMORI, Nayuta [C class; 600 (B), 250 (C)] (325)
— *Comparison of superconducting properties in quasicrystals and approximant crystals*

TAKETSUGU, Tetsuya [C class; 3800 (B), 450 (C)] (104)
— *Ab initio study on the structure and functions of nanomaterials*

TAMURA, Ryo [B class; 300 (B), 100 (C)] (350)
— *Development of prediction method for phase diagrams by machine learning*

TANAKA, Katsuhiro [B class; 400 (B), 70 (C)] (195)
— *First-principles study on designing magnetic tunnel junctions and calculating tunneling conductance*

TANAKA, Shu [B class; 400 (B), 100 (C)] (343)
— *Study on algorithms for Ising machines*

1. Dynamical process of a bit-width reduced Ising model with simulated annealing
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— *First-principles calculations of exchange coupling constants dependent on magnetic short-range order*

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— *Ab-initio research on nano particles, and surfaces and grain boundaries of magnetic materials*

TEN-NO, Seiichiro [C class; 7800 (B), 850 (C)] (74)
— *First-principles analysis of artificial photosynthesis using perovskite semiconductor photocatalysts*
— *Theoretical study of visible-light-driven semiconductor photocatalysts using first-principles calculations*

TERAO, Takamichi [B class; 700 (B), 150 (C)] (324)
— *Structural formation of non-spherical colloidal particles*

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TODO, Synge [C class; 5200 (B), 500 (C)] (278)
— *Simulation of quantum many-body systems by tensor network and sampling*

TOHYAMA, Takami [C class; 3600 (B), 0 (C)] (230)
— *Phtoinduced transient absorption spectrum in one-dimensional Mott insulator with strong dimer correlation*

1. Controlling inversion and time-reversal symmetries by subcycle pulses in the one-dimensional extended Hubbard model
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— *Numerical Study of the One-Dimensional Quantum Spin Systems*

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— *Ab initio path integral molecular dynamics investigations of the hydrous phases in the Earth's interior*

TSUJI, Yuta [B,C class; 1700 (B), 400 (C)] (145)
— *First-principles theoretical catalytic studies for C1 chemistry*
— *Theoretical study of oxygen-evolution reactions by first-principles calculations*

1. Frontier Orbital Views of Stacked Aromaticity
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TSUKAHARA, Noriyuki [B class; 200 (B), 70 (C)] (208)
— *DFT calculations of the metal-organic film and atoms/molecules captured by the film on metal surfaces*

TSUNEYUKI, Shinji [C class; 6000 (B), 0 (C)] (92)
— *Structural exploration and prediction of dielectric properties of molecular materials*

1. Evolutionary search for superconducting phases in the lanthanum-nitrogen-hydrogen system with universal neural network potential
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UCHIDA, Kazuyuki [C class; 400 (B), 0 (C)] (198)
— *First-principles Study on Superstructures of Si(111)-r7xr3-In Surface (PART II)*

UCHIDA, Takashi [B class; 200 (B), 80 (C)] (355)
— *Multiple-Q orders in two-dimensional Hubbard models*

UEHARA, MASATOMO [B class; 600 (B), 150 (C)] ()
— *Prediction of Transition Temperatures for Superconductors with Imperfect Crystal Structures Using Transition Learning*
— *Superconductor transition temperature prediction by deep learning and phonon density of states estimation by model analysis*

UEMURA, Naoki [C class; 2800 (B), 0 (C)] (127)
— *Analysis of mechanical properties of alloy materials using first-principles and molecular dynamics calculations*

1. First-principles study of generalized stacking fault energy in MgZnY alloy with long-period stacking-ordered structure
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USUI, Hidetomo [B class; 800 (B), 170 (C)] (169)
— *FIrst principles study on band structure of high entropy superconductors*

WAKABAYASHI, Daisuke [B class; 300 (B), 0 (C)] (204)
— *Compression behavior of xenon in silica melt*

WATANABE, Hiroshi [E class; 9500 (B), 1200 (C)] (261)
— *Dynamic properties of coarse-grained modeled red blood cells*

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— *Theoretical study of BCS-BEC crossover in solid-state materials*

WATANABE, Satoshi [C class; 8800 (B), 850 (C)] (65)
— *Analyses on local properties at complex structures such as surfaces, interfaces and defects via machine-learning potentials*
— *Analyses on local properties at complex structures via ab-initio-based methods*

1. Prediction of Born effective charges using neural network to study ion migration under electric fields: applications to crystalline and amorphous Li_3PO_4
   K. Shimizu, R. Otsuka, M. Hara, E. Minamitani, and S. Watanabe Sci. Technol. Adv. Mater. Methods **3**, 2253135 (2023).
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   E. Minamitani, I. Obayashi, K. Shimizu, and S. Watanabe J. Chem. Phys. **159**, 084101 (2023).
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4. ニューラルネットワークを用いた電場中でのイオン挙動計算手法の開発：アモルファスリン酸リチウム中でのイオン伝導への応用
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   安藤 康伸, 清水 康司, 渡邉 聡分子シミュレーション学会誌””アンサンブル **26**, 40 (2024).

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   M. Motoyama, K. Shimizu, T. Kimura, T. Yamamoto, S. Watanabe, and Y. Iriyama ACS Central Science, submitted.

8. *Enthralling anodic protection by molybdate on high-entropy alloy based electrocatalyst for sustainable seawater oxidation*
   S. Khatun, K. Shimizu, S. Pal, S. Nandi, S. Watanabe, and P. Roy Small, submitted.

9. *Enhanced ionic conductivity through crystallization of glass-Li_3PS_4 by machine learning molecular dynamics simulations*
   K. Shimizu, P. Bahuguna, S. Mori, A. Hayashi, and S. Watanabe J. Phys. Chem. C, submitted.

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Data Repository
Neural network model for Born effective charges
https://github.com/shimizu00000/born-effective -charge-nn.git

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— *Analysis of novel rechargeable battery materials using first-principles calculations and neural network force field*

1. High-Voltage Electrochemical Properties of Lithium-Rich Spinel Oxides
K. Kawai, T. Sudayama, D. Asakura, J. Kikkawa, E. Watanabe, M. Okubo, A. Yamada J. Phys. Chem. C **127**, 12428 (2023).
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— *Analyses of the superconductivity and magnetic states in Hubbard models and their applicatoins to strongly correlated electron systems.*

YAMADA, Masahiko [C class; 2000 (B), 400 (C)] (3004)
— *Parallelization and application of matrix product renormalization group*

YAMAGUCHI, Naoya [C class; 1400 (B), 500 (C)] (153)
— *Development of First-principles Codes for Evaluation of Physical Properties Through Local Berry Phases*

1. First-principles study of anomalous Nernst effect in Cr-doped Bi_2Se_3
R. Syariati, V. Saraswati, H. Sawahata, N. Yamaguchi, and F. Ishii Jpn. J. Appl. Phys. **63**, 01SP26 (2024).
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— *Development of variational-wave-function spectroscopy for quantum materials*

1. Quantum criticality of bandwidth-controlled Mott transition
K. Takai, Y. Yamaji, F. F. Assaad, and M. Imada, Phys. Rev. Research **5**, 033186 (2023).
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YAMAMOTO, Go [C class; 5200 (B), 700 (C)] (273)
— *Decreasing Topological Defects Sensitivity in Multi-Walled Carbon Nanotubes Through Interwall Coupling*
— *Machine learning-assisted high-throughput molecular dynamics simulation of high-performance CNT yarn structure*

YAMASHITA, Tomoki [C class; 4200 (B), 500 (C)] (101)
— *Crystal structure prediction of Li-ion solid electrolyte materials*

YAMAUCHI, Kunihiko [C class; 4000 (B), 0 (C)] (108)
— *First-principles calculation of anomalous Hall effect in antiferromagnets*

1. Ab initio prediction of anomalous Hall effect in antiferromagnetic CaCrO3
   Thi Phuong Thao Nguyen and Kunihiko Yamauchi, Phys. Rev. B **107**, 155126 (2023).
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2. Hydrogen-induced insulating state accompanied by interlayer charge ordering in SmNiO3
   Kunihiko Yamauchi and Ikutaro Hamada, Phys. Rev. B 108, 045108 (2023).
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3. GoodenoughKanamoriAnderson Rules in 2D Magnet: A Chemical Trend in MCl2 with M = V, Mn, and Ni
   Thi Phuong Thao Nguyen and Kunihiko Yamauchi, J. Phys. Soc. Jpn. 93, 034710 (2024).
   DOI:10.7566/JPSJ.93.034710

4. Antiferromagnetic topological insulator with selectively gapped Dirac cones
   A. Honma, D. Takane, S. Souma, K. Yamauchi, Y. Wang, K. Nakayama, K. Sugawara, M. Kitamura, K. Horiba, H. Kumigashira, K. Tanaka, T. K. Kim, C. Cacho, T. Oguchi, T. Takahashi, Yoichi Ando, and T. Sato Nat. Commun. 14, 7396 (2023).
   DOI:10.1038/s41467-023-42782-6

5. Observation of a giant band splitting in altermagnetic MnTe
   T. Osumi, S. Souma, T. Aoyama, K. Yamauchi, A. Honma, K. Nakayama, T. Takahashi, K. Ohgushi, and T. Sato Phys. Rev. B **109**, 115102 (2024).
   DOI:10.1103/PhysRevB.109.115102

YANAGISAWA, Susumu [C class; 6200 (B), 0 (C)] (89)
— *First-principles bandstructure calculation with electron-phonon interactions in organic semiconductor crystals*

1. Proving weak electronic interaction between molecules and substrate: a study of pentacene monolayer on graphite
   Y. Hasegawa, T. Yamaguchi, M. Meissner, T. Ueba, F. Bossolotti, S. Ideta, K. Tanaka, S. Yanagisawa, and S. Kera arXiv preprint arXiv:2304.14734 (2023).
   DOI:10.48550/arXiv.2304.14734

YANAGISAWA, Takashi [B class; 700 (B), 160 (C)] (239)
— *Numerical study of the mechanism of high-temperature superconductivity in strongly correlated electron systems*
— *Research on the mechanism of high-temperature superconductivity in strongly correlated electron systems*

1. From Resistance Minimum to Kondo Physics
   T. Yanagisawa New Physics: Sae Mulli 73, 1098 (2023).
   DOI:10.3938/NPSM.73.1098

2. Inhomogeneous charge distribution and coexistence with superconductivity in the two-dimensional Hubbard model
   T. Yanagisawa preprint

YASUDA, Chitoshi [C class; 1800 (B), 0 (C)] (309)
— *Frustration and randomness in the honeycomb-lattice spin systems*

YASUHARA, Sou [B,C class; 3200 (B), 0 (C)] (119, 120)
— *Investigation on a mechanism of Ferroelectricity in a wurtzite-type LiGaO2*
— *Stable Structure Exploration of K2NdNb5O15 and Phase Transition Mechanism Analysis Based on First-Principles Calculations*

YOKO, Akira [C class; 1400 (B), 350 (C)] (156)
— *First-principles calculations of sub-3 nm metal oxide particles*

○ A class

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

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

FUJISAWA, Shuji [A class; 100 (B), 50 (C)] ()
Structure optimization of nanocellulose using DFT calculations

FUKUDA, Tuneo [A class; 100 (B), 50 (C)] ()
First-principles Study of the Phase Diagram of Si(111)-In surface structures

INUI, Koji [A class; 100 (B), 50 (C)] ()
Inverse design of Hamiltonians with target properties using automatic differentiation

KAIJU, Hideo [A class; 100 (B), 50 (C)] ()
Electronic structure analysis of spin devices using first-principles calculation
— *Electronic structure analysis of lattice-matched magnetic tunnel junctions using first-principles calculation*

KATOW, Hiroki [A class; 100 (B), 50 (C)] (390)
Development of First Principles methods for Light-Matter Interaction

KUSANO, Akane [A class; 100 (B), 50 (C)] ()
Fundamental Materials Informatics Research on Binary Systems of Materials

LI, Yanjun [A class; 100 (B), 50 (C)] ()
Study of TiO2 surface catalysis

MOTOTAKE, Yoh-ichi [A class; 100 (B), 50 (C)] ()
Ab initio molecular dynamics study of inorganic polymer

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

NAKAGAWA, Takeshi [A class; 100 (B), 50 (C)] ()
Structural analysis of single layer borophene on Ni surfaces

SAKURAI, Hiroshi [A class; 100 (B), 50 (C)] ()
Development of method for reconstruction of momentum density with a sparse modeling

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

TANAKA, Katsuhiro [A class; 100 (B), 50 (C)] (195, 417)
Exploring physical properties of noncollinear magnets from first-principles

TATENO, Michio [A class; 100 (B), 50 (C)] ()
Impact of pore morphology on compressive yielding in sticky spheres

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

UEMURA, Naoki [A class; 100 (B), 50 (C)] (127, 420)
A benchmark test using VASP for alloy materials

WANG, Yinqiao [A class; 100 (B), 50 (C)] ()
Hyperuniform glass

YAMAMOTO, Sayoko [A class; 100 (B), 50 (C)] ()
Theoretical study of water splitting reaction by oxides

YASUHARA, Sou [A class; 100 (B), 50 (C)] (119, 120, 424)
Investigation of substitution for a wurtzite-type ferroelectric material LiGaO2

YOKOMORI, So [A class; 100 (B), 50 (C)] ()
Elucidation of electronic structure modulation effects of solid solution and element substitution in single-component molecular conductors

YUAN, Jiaxing [A class; 100 (B), 50 (C)] ()
Hydrodynamic Simulations of Soft Matter

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

□ SCCMS Projects

FUKUSHIMA, Tetsuya [4000 (B), 400 (C)] (361)
— *Creating of magnetic material maps by KKR Green ' s function method*

1. First-principles Calculation of Magnetocrystalline Anisotropy of Y(Co,Fe,Ni,Cu)5 Based on Full-potential KKR Green ' s Function Method
   H. Okumura, T. Fukushima, H. Akai, and M. Ogura Solid State Communications **373-374**, 115257 (2023).
   DOI:10.1016/j.ssc.2023.115257

2. Computational Materials Design of High-Entropy Alloys Based on Full Potential Korringa-Kohn-Rostoker Coherent Potential Approximation and Machine Learning Techniques
   K. Sato, G. Hayashi, K. Ogushi, S. Okabe, K. Suzuki, T. Terai, and T. Fukushima Materials Transactions **64**, 2174 (2023).
   DOI:10.2320/matertrans.MT-MG2022012

3. Insight into Scattering Mechanisms and Transport Properties of AgCuS for Flexible Thermoelectric Applications
   H. N. Nam, Q. M. Phung, K. Suzuki, A. Masago, H. Shinya, T. Fukushima, and K. Sato ACS Applied Materials & Interfaces **15**, 43871 (2023).
   DOI:10.1021/acsami.3c09437

4. Theoretical Study on the Origin of Anomalous Temperature-dependent Electric Resistivity of Ferromagnetic Semiconductor
   H. Shinya, T. Fukushima, K. Sato, S. Ohya, and H. Katayama-Yoshida APL Materials **11**, 111114 (2023).
   DOI:10.1063/5.0165352

5. Exploring finite-temperature electronic transport in CoSi alloys with transition metals (Cr, Mn, Fe, and Ni) using the KKR-CPA method
   H. N. Nam, Q. M. Phung, K. Suzuki, H. Shinya, A. Masago, T. Fukushima, and K. Sato Journal of Materials Chemistry A **12**, 451 (2024).
   DOI:10.1039/D3TA06259G

MATUBAYASHI, Nobuyuki [2000 (B), 200 (C)] (366)
— *Systematic evaluation of solubility of polypeptides in solvents by free energy calculation method using all-atom model*

1. Free-energy decomposition of salt effects on the solubilities of small molecules and the role of excluded-volume effects
   S. Hervø-Hansen, D. Lin, K. Kasahara, and N. Matubayasi, Chem. Sci. **15**, 477 (2024).
   DOI:10.1039/d3sc04617f

MIYAKE, Takashi [2000 (B), 100 (C)] (363)
— *First-principles study of magnetic materials*

1. Towards understanding structure-property relationships in materials with interpretable deep learning
   Tien-Sinh Vu, Ming-Quyet Ha, Duong-Nguyen Nguyen, Hieu-Chi Dam, Viet-Cuong Nguyen, Yukihiro Abe, Truyen Tran, Huan Tran, Hiori Kino, Takashi Miyake and Koji Tsuda npj Comp. Materials **9**, 215 (2023).
   DOI:10.1038/s41524-023-01163-9

MORIWAKE, Hiroki [4000 (B), 400 (C)] ()
— *Computational Exploring of Novel high permittivity Materials*
— *Data-driven Exploration of High Dielectric Constant Materials*

OGATA, Shigenobu [2000 (B), 200 (C)] (364)
— *Atomistic analysis of hydrogen impact on mechanical properties of structural material and database construction*

OHKUBO, Tadakatsu [5000 (B), 500 (C)] (369)
— *Phonon-calculation method for magnetic random alloys*

1. Clarification of origin of positive excess volume of PdFe binary alloys by using first-principles calculations and HAXPES
   M. Watanabe, Y. Takagi, T. Tanaka, Y. Gohda, M. Adachi, M. Uchikoshi, T. Nakamura, M. Takata, and H. Fukuyama, Acta Mater. **267**, 119718 (2024).
   DOI:10.1016/j.actamat.2024.119718

2. Strain-induced specific orbital control in a Heusler-alloy-based interfacial multiferroics
   J. Okabayashi, T. Usami, A.M. Yatmeidhy, Y. Murakami, Y. Shiratsuchi, R. Nakatani, Y. Gohda, and K. Hamaya, NPG Asia Mater. **16**, 3 (2024).
   DOI:10.1038/s41427-023-00524-6

3. Unidirectional Nano-Modulated Binding and Electron Scattering in Epitaxial Borophene
   S. Kamal, I. Seo, P. Bampoulis, M. Jugovac, C.A. Brondin, T. Menteş, I. Šarić-Janković, A. Matetskiy, P. Moras, P. Sheverdyaeva, T. Michely, A. Locatelli, Y. Gohda, M. Kralj, M. Petrović, ACS Appl. Mater. Interfaces 15, 57890 (2023).
   DOI:10.1021/acsami.3c14884

4. Metastable Co3Mn/Fe/Pb(Mg1/3Nb2/3)O3-PbTiO3 multiferroic heterostructures
   Y. Murakami, T. Usami, R. Watarai, Y. Shiratsuchi, T. Kanashima, R. Nakatani, Y. Gohda and K. Hamaya, J. Appl. Phys. 134, 224101 (2023).
   DOI:10.1063/5.0180644

5. Unveiling the Origin of Large Coercivity in (Nd, Dy)-Fe-B Sintered Magnets
   X. Tang, J.N. Li, H. Sepehri-Amin, A. Bolyachkin, A. Martin-Cid, S. Kobayashi, Y. Kotani, M. Suzuki, A. Terasawa, Y. Gohda, T. Ohkubo, T. Nakamura, and K. Hono, NPG Asia Mater. 15, 50 (2023).
   DOI:10.1038/s41427-023-00498-5

6. Strain-induced magnetic anisotropy in Heusler alloys studied from first principles
   A.M. Yatmeidhy and Y. Gohda, Appl. Phys. Express 16, 053001 (2023).
   DOI:10.35848/1882-0786/accfe1

7. Subphase exploration for SmFe12-based permanent magnets by Gibbs energies obtained with first-principles cluster-expansion method
   S. Enomoto, S. Kou, T. Abe, and Y. Gohda, J. Alloys Compd. 950, 169849 (2023).
   DOI:10.1016/j.jallcom.2023.169849

SHIMAZAKI, Tomomi [2000 (B), 200 (C)] (368)
— *Theoretical study on proton transfer in fuel cell material based on first-principles method with nuclear quantum effect*

SHITARA, Kazuki [4000 (B), 400 (C)] (365)
— *Computational Exploring of Novel Ferroelectric Materials*
— *Computational and Data-driven Exploration of Ferroelectric Materials*

TEN-NO, Seiichiro [2000 (B), 200 (C)] (74)
— *Theoretical study of visible-light hydrogen-evolution semiconductor photocatalysts using first-principles calculations*

□ Doctor Theses

1. **AMANO, Tomohito**
   First-principles and machine learning study of anharmonic vibration and dielectric properties of materials
   The University of Tokyo, 2024-03

2. **Amran Mahfudh Yatmeidhy**
   First-principles study of multiferroic composite with strain transfer
   Tokyo Institute of Technology, 2023-09

3. **AOMURA, Kosuke**
   Molecular mechanism of strain-induced crystallization in polymer gels
   The University of Tokyo, 2024-03

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   Improvement of numerical algorithm for quantum dimer models
   The University of Tokyo, 2023-09

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   All-day passive radiative cooling and water harvesting by hierarchical polymer films
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   Elucidation of the Photothermal Conversion Mechanism for Tungsten Carbide
   Kyushu Institute of Technology, 2024-03

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   Graph neural network prediction of hopping motion induced by a cavity in deeply supercooled binary hard disk systems
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37. **OHMOTO, Mizuho**
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49. **SHOJI, Makoto**
Structural analysis of B/Al(111) using electron and positron diffraction
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Cyber-physical loop with dynamic Monte Carlo simulation and application for optimization of photocatalitic performance of $SrTiO_3$.
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Data assimilation model for first-principles and experimental data on the bandgap of perovskite metal oxides.
Nara Institute of Science and Technology, 2024-03

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Theoretical analysis of SEI film formation process in cyclic phosphate electrolytes
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Structure and Stability of Oxidized PdZn (111) Surface: density functional theory study
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