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

AKAI, Hisazumi [B class; 1300 (B), 90 (C)] (24)
— *Finite temperature magnetic properties of permanent magnet materials*
— *First-principles calculation of magnetocrystalline anisotropy of permanent magnet materials*

1. First-principles investigation of $Nd(Fe,M)_{12}$ (M = K–Br) and $Nd(Fe,Cr,Co,Ni,Ge,As)_{12}$: Possible enhancers of Curie temperature for $NdFe_{12}$ magnetic compounds
   T. Fukazawa, H. Akai, Y. Harashima, and T. Miyake, Acta.Mater. **226**, 117597 (2022).
   DOI:10.1016/j.actamat.2021.117597

2. Direct observation of magnetic Friedel oscillation at Fe(001) surface
   T. Mitsui, S. Sakai, S. Li, T. Ueno, T. Watanuki, Y. Kobayashi, R. Masuda, M. Seto, and H. Akai Hyperfine Interactions **242**,37 (2021).
   DOI:10.1007/s10751-021-01772-0

3. Atomistic theory of thermally activated magnetization processes in $Nd_2Fe_{14}B$ permanent magnet Seiji Miyashita, Masamichi Nishino, Yuta Toga, Taichi Hinokihara, Ismail Uysal, Takashi Miyake, Hisazumi Akai, Satoshi Hirosawa, and Akimasa Sakumaa Sci. Tech. Adv. Mater. **22**,658 (2021).
   DOI:10.1080/14686996.2021.1942197

4. Data assimilation method for experimental and first-principles data: Finite-temperature magnetization of $(Nd, Pr, La, Ce)_2(Fe, Co, Ni)_{14}B$
   Y. Harashima, K. Tamai, S. Doi, M. Matsumoto, H. Akai, N. Kawashima, M. Itho, N. Sakuma, K. Kato, T. Shoji, and T. Miyake, Phys. Rev. Mater. **5**, 013806 (2021).
   DOI:10.1103/PhysRevMaterials.5.013806

5. Spin-wave dispersion and exchange stiffness in $Nd_2Fe_{14}B$ and $RFe_{11}Ti$ (R=Y, Nd, Sm) from first-principles calculations
   Fukazawa, H. Akai, Y. Harashima, and T. Miyake, Phys. Rev. B **103**, 024418 (2021).
   DOI:10.1103/PhysRevB.103.024418

AKASHI, Ryosuke [B class; 600 (B), 100 (C)] (141)
— *Development of the first-principles method for calculating Tc based on density functional theory for superconductors*

AOYAMA, Kazushi [B class; 1000 (B), 120 (C)] (276)
— *Effect of magnetic anisotropy on spin textures in pyrochlore antiferromagnets*
— *Stability of the hedgehog-lattice topological spin texture in breathing-pyrochlore antiferromagnets*

1. Emergent skyrmion-based chiral order in zero-field Heisenberg antiferromagnets on the breathing kagome lattice
   K. Aoyama and H. Kawamura, Phys. Rev. B **105**, (2022) L100407.
   DOI:10.1103/PhysRevB.105.L100407

2. Effects of spin-lattice coupling and a magnetic field in classical Heisenberg antiferromagnets on the breathing pyrochlore lattice
   K. Aoyama, M. Gen, and H. Kawamura, Phys. Rev. B **104**, (2021) 184411.
   DOI:10.1103/PhysRevB.104.184411

3. Spin Dynamics Simulation of the Z_2-vortex Fluctuations
   Yo. P. Mizuta, K. Aoyama, K. Tomiyasu, M. Matuura, and H. Kawamura, J. Phys. Soc. Jpn. **91**, (2022) 035001 SHORT NOTES.
   DOI:10.7566/JPSJ.91.035001

ARAI, Munehito [C class; 7600 (B), 0 (C)] (220)
— *Rational design of novel proteins for medical and industrial applications*
— *Theoretical Design of Novel Artificial Proteins to Inhibit Viral Infection*

ARAI, Toyoko [C class; 1400 (B), 500 (C)] (117)
— *RSDFT calculation of atomic displacement captured by energy dissipation channel of noncontact atomic force microscope*

ARIMA, Kenta [B class; 600 (B), 110 (C)] (288)
— *First-principles simulation of graphene nanoribbon and investigation of reactivity as machining catalyst*
— *Investigations of electronic structures and reactivity of graphene nanoribbons with different widths*

1. Atomic-scale insights into the origin of rectangular lattice in nanographene probed by scanning tunneling microscopy
   J. Li, S. Li, T. Higashi, K. Kawai, K. Inagaki, K. Yamamura, and K. Arima, Phys. Rev. B **103**, 245433 (2021).
   DOI:10.1103/PhysRevB.103.245433

ARUGA, Tetsuya [B class; 300 (B), 80 (C)] (166)
— *Interaction between magnetic metal phthalocyanine molecules and bi-layer metal films*

ASANO, Yuta [E class; 23500 (B), 2550 (C)] (206)
— *Effects of cavitation on soundwaves*
— *Molecular Dynamics Simulation of Complex Fluids*

1. Effects of polymers on the cavitating flow around a cylinder: A Large-scale molecular dynamics analysis
   Y. Asano, H. Watanabe, and H. Noguchi, J. Chem. Phys. **155**, 014905 (2021).
   DOI:10.1063/5.0056988

2. Effects of gas-liquid phase transitions on soundwave propagation: A molecular dynamics study
   Y. Asano, H. Watanabe, and H. Noguchi, Phys. Rev. Fluids, (2022) in press.

BUI, VANPHO [C class; 2200 (B), 350 (C)] (110)
— *Study on removal mechanism of single crystalline Si planarized by catalyst referred etching in pure*

water

EGAMI, Yoshiyuki [C class; 8600 (B), 1000 (C)] (64)
— *Development and application of first-principles method for electron-transport calculations of large-scale interface structures*
— *First-principles study on electron-transport through semiconductor interface structures*

FUCHIZAKI, Kazuhiro [C class; 3000 (B), 0 (C)] (256)
— *Kinetics of phase transition and polyamorphism*
1. Thermodynamics of polyamorphism
   K. Fuchizaki Mem. Fac. Sci. Ehime Univ. **24**, 43 (2022).

FUJII, Susumu [C class; 2600 (B), 0 (C)] (260)
— *Nanoscale phonon transport across ceramics interfaces*
1. Structure and lattice thermal conductivity of grain boundaries in silicon by using machine learning potential and molecular dynamics
   S. Fujii and A. Seko, Comput. Mater. Sci. **204**, 111137 (2022).
   DOI:10.1016/j.commatsci.2021.111137

FUJIMOTO, Satoshi [B class; 600 (B), 90 (C)] (196)
— *Topological nematic phase transition in Kitaev spin liquid*

FUJIMOTO, Yoshitaka [C class; 600 (B), 0 (C)] (145)
— *Physical properties of layered graphene*
1. Electronic states and modulation doping of hexagonal boron-nitride trilayer
   T. Haga, Y. Matsuura, Y. Fujimoto and S. Saito, Physical Review Materials **5**, 094003 (2021).

2. Stability of Hydrogen Boride Sheets in Water
   K. I. Rojas, N. T. Cuong, H. Nishino, R. Ishibiki, S. Ito, M. Miyauchi, Y. Fujimoto, S. Tominaka, S. Okada, H. Hosono, N. Arboleda, T. Kondo, Y. Morikawa, and I. Hamada, Communications Materials **2**, 1 (2021).

3. Chemistry and Physics of Carbon Nanotube Structures
   Y. Fujimoto, Handbook of Carbon Nanotubes, pp.1-19, edited by J. Abraham, S. Thomas, and N. Kalarikkal (Springer Nature 2021).

4. Detection of environmentally toxic molecules using carbon nanotubes: A first principles theoretical study
   Y. Fujimoto and S. Saito, Journal of The Electrochemical Society, **169**, 037512 (2022).

5. Theoretical study on quantum transport of carbon nanotubes for detecting toxic molecules: The role of dopants
   Y. Fujimoto, Journal of Electrochemical Science and Engineering, Accepted.

FUJINO, Tomoko [D class; 2500 (B), 0 (C)] (194)
— *Estimation of Coulomb repulsion in charge transfer salts of EDXT oligomers*
1. Conjugation length effect on the conducting behavior of single-crystalline oligo(3,4-ethylenedioxythiophene) (nEDOT) radical cation salts
   R. Kameyama, T. Fujino, S. Dekura, and H. Mori, Chem. Phys. Phys. Chem, 2022, 24, 91309134.
   DOI:10.1039/D2CP00250G

2. Band-filling Effects in Single-crystalline Oligomer Models for Doped PEDOT: 3,4-Ethylenedioxythiophene (EDOT) Dimer Salt with Hydrogen-bonded Infinite Sulfate Anion Chains
R. Kameyama, T. Fujino, S. Dekura, S. Imajo, T. Miyamoto, H. Okamoto, and H. Mori, submitted to J. Mat. Chem. C, accepted.

FUJISHIRO, Hiroki [C class; 2600 (B), 0 (C)] ()
— *Strained Band-Structure Engineering for Antimonide-Based Terahertz Transistors*

FUKUDA, Jun-ichi [B class; 900 (B), 0 (C)] (280)
— *Calculation of ordered structures, dynamics and optical properties of soft materials*
1. Liquid Crystalline Half-Skyrmions and Their Optical Properties
Jun-ichi Fukuda, Andriy Nych, Uliana Ognysta, Slobodan Žumer, and Igor Muševič, Annalen der Physik **534**, 2100336 (2022).
DOI:10.1002/andp.202100336

FUKUDA, Masahiro [B class; 400 (B), 70 (C)] (156)
— *AB type 2D materials search by high-throughput DFT calculations*
1. A structure map for AB_2 type 2D materials using high-throughput DFT calculations
Masahiro Fukuda, Jingning Zhang, Yung-Ting Lee, and Taisuke Ozaki, Mater. Adv., **2**, 4392 (2021).
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FUKUDA, Tuneo [C class; 800 (B), 0 (C)] (139)
— *Molecular dynamics simulation of substitution reaction on metal surface*

FUKUMOTO, Yoshiyuki [B class; 700 (B), 0 (C)] (289, 290)
— *Numerical studies on excitation spectra of Heisenberg antiferromagnets on the triangular and kagome lattices*
— *Towards a unified understanding of thermodynamic properties in S=1/2 spherical kagome systems $W_{72}V_{30}$ and $Mo_{72}V_{30}$*

GOHDA, Yoshihiro [C class; 5200 (B), 800 (C)] (79)
— *Maximization of interface magnetoelectric coupling with Bayesian optimization*
1. Role of ferroelectricity, delocalization, and occupancy of d states in the electrical control of interface-induced magnetization
R. Costa-Amaral and Y. Gohda, Phys. Rev. Appl. **15**, 064014 (2021).
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2. Giant converse magnetoelectric effect in a multiferroic heterostructure with polycrystalline Co_2FeSi
S. Fujii, T. Usami, Y. Shiratsuchi, A.M. Kerrigan, A.M. Yatmeidhy, S. Yamada, T. Kanashima, R. Nakatani, V.K. Lazarov, T. Oguchi, Y. Gohda, and K. Hamaya, NPG Asia Mater., in press.

3. Intrinsic superconductivity of two-monolayer-thick indium film
T. Ogino, I. Seo, H. Tajiri, M. Nakatake, S. Takakura, Y. Sato, Y. Hasegawa, Y. Gohda, K. Nakatsuji, and H. Hirayama, submitted to Phys. Rev. Lett.

4. Origin of anisotropic magnetoresistance tunable with electric field in Co2FeSi/BaTiO3 multiferroic inetrfaces
S. Tsuna, R. Costa-Amaral, and Y. Gohda, submitted to Phys. Rev. Mater.

GOHLKE, Matthias [C class; 4400 (B), 600 (C)] (233)

— *Ground state and dynamical properties of the J_1J_2K-Heisenberg model on the square lattice*

HAGITA, Katsumi [C class; 3600 (B), 0 (C)] (254)
— *DPD simulations of cross-linked networks to study topological effect using MP-SRP method*

1. Viscosity Overshoot in Biaxial Elongational Flow: Coarse-Grained Molecular Dynamics Simulation of RingLinear Polymer Mixtures
   T. Murashima, K. Hagita and T. Kawakatsu, Macromolecules **54**, 7210–7225 (2021).
   DOI:10.1021/acs.macromol.1c00267

2. Molecular Dynamics Simulations of Ring Shapes on a Ring Fraction in Ring-Linear Polymer Blends
   K. Hagita and T. Murashima, Macromolecules **54**, 8043–8051 (2021).
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3. Role of chain crossing prohibition on chain penetration in ring-linear blends through dissipative particle dynamics simulations
   K. Hagita, T. Murashima, H. Shiba, N. Iwaoka, and T. Kawakatsu, Comput. Mater. Sci. **203**, 111104 (2022).
   DOI:10.1016/j.commatsci.2021.111104

HAMAGUCHI, Satoshi [C class; 8800 (B), 1050 (C)] (62)
— *Analysis of Surface Reactions in Atomic Layer Etching Processes*

HAMAMOTO, Yuji [C class; 1600 (B), 0 (C)] (123)
— *Global search for the structures of two-dimensional materials by Gaussian process regression*

HARADA, KENJI [C class; 2200 (B), 0 (C)] (263)
— *Data analysis method using a tensor network representation*

HARASHIMA, Yosuke [C class; 1000 (B), 0 (C)] (134)
— *Critical concentration of metal-insulator transition in doped semiconductors and Coulomb gap*
— *Critical exponent of metal-insulator transition in doped semiconductors and spin ordering*

1. Analysis of Kohn-Sham Eigenfunctions Using a Convolutional Neural Network in Simulations of the Metal-Insulator Transition in Doped Semiconductors
   Y. Harashima, T. Mano, K. Slevin, and T. Ohtsuki, J. Phys. Soc. Jpn. **90**, 094001 (2021).
   DOI:10.7566/JPSJ.90.094001

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— *Electrochemical reaction analysis using density functional calculation + implicit solvation model 3*

1. Thermodynamic Analysis of Li-Intercalated Graphite by First- Principles Calculations with Vibrational and Configurational Contributions
   J. Haruyama, S. Takagi, K. Shimoda, I. Watanabe, K. Sodeyama, T. Ikeshoji, and M. Otani, J. Chem. Phys. C **125**, 27891 (2021).
   DOI:10.1021/acs.jpcc.1c08992

HASHIMOTO, Tamotsu [C class; 3000 (B), 600 (C)] (253)
— *Molecular dynamics simulation of $BaTiO_3$ nano structure*

HATANO, Naomichi [B class; 400 (B), 70 (C)] ()
— *Novel Spectral Clustering Method of Directed Networks*

HATSUGAI, Yasuhiro [C class; 3200 (B), 600 (C)] (251)

— *Topological phases and science of bulk-edge correspondence by numerical methods*

1. Chiral edge modes in evolutionary game theory: A kagome network of rock-paper-scissors cycles
   T. Yoshida, T. Mizoguchi, and Y. Hatsugai, Phys. Rev. E 104, 025003 (2021).
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2. Bulk-edge correspondence in the adiabatic heuristic principle
   K. Kudo, Y. Kuno, and Y. Hatsugai, Phys. Rev. B **104**, L241113 (2021).
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3. Adiabatic Continuity of the Spinful Quantum Hall States
   K. Kudo and Y. Hatsugai, arXiv:2201.07893
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HATTORI, Ken [B class; 300 (B), 60 (C)] ()

— *Atomic structure and electronic states for silicide films*

HAYAMI, Satoru [C class; 3400 (B), 650 (C)] (191)

— *Searching for meron crystal in itinerant magnets*

1. Essential role of anisotropic magnetic dipole in anomalous Hall effect
   S. Hayami and H. Kusunose, Phys. Rev. B **103**, L180407 (2021).
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2. Skyrmion crystals in centrosymmetric itinerant magnets without horizontal mirror plane
   R. Yambe and S. Hayami, Sci. Rep. **11**, 11184 (2021).
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3. Field-Direction Sensitive Skyrmion Crystals in Cubic Chiral Systems: Implication to 4f-Electron Compound EuPtSi
   S. Hayami and R. Yambe, J. Phys. Soc. Jpn. **90**, 073705 (2021).
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4. In-plane magnetic field-induced skyrmion crystal in frustrated magnets with easy-plane anisotropy
   S. Hayami, Phys. Rev. B **103**, 224418 (2021).
   DOI:10.1103/PhysRevB.103.224418

5. Spin-orbital-momentum locking under odd-parity magnetic quadrupole ordering
   S. Hayami and H. Kusunose, Phys. Rev. B **104**, 045117 (2021).
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6. Multipole classification in 122 magnetic point groups for unified understanding of multiferroic responses and transport phenomena
   M. Yatsushiro, H. Kusunose, and S. Hayami Phys. Rev. B **104**, 054412 (2021).
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7. Meron-antimeron crystals in noncentrosymmetric itinerant magnets on a triangular lattice
   S. Hayami and R. Yambe, Phys. Rev. B **104**, 094425 (2021).
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8. Charge density waves in multiple-Q spin states
   S. Hayami and Y. Motome, Phys. Rev. B **104**, 144404 (2021).
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9. Nonreciprocal magnon excitations by the Dzyaloshinskii-Moriya interaction on the basis of bond magnetic toroidal multipoles

T. Matsumoto and S. Hayami, Phys. Rev. B **104**, 134420 (2021).
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10. Temperature-driven transition from skyrmion to bubble crystals in centrosymmetric itinerant magnets
S. Hayami, New J. Phys. **23**, 113032 (2021).
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11. Phase Shift in Skyrmion Crystals
S. Hayami, T. Okubo, and Y. Motome, Nat. Commun. **12**, 6927 (2021).
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12. Locking of skyrmion cores on a centrosymmetric discrete lattice: Onsite versus offsite
S. Hayami and R. Yambe, Phys. Rev. Research **3**, 043158 (2021).
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13. Spin excitation spectra in helimagnetic states: Proper-screw, cycloid, vortex-crystal, and hedgehog lattices
Y. Kato, S. Hayami, and Y. Motome Phys. Rev. B **104**, 224405 (2021).
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14. Essential model parameters for nonreciprocal magnons in multisublattice systems
S. Hayami and T. Matsumoto, Phys. Rev. B **105**, 014404 (2022).
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15. Skyrmion crystal and spiral phases in centrosymmetric bilayer magnets with staggered Dzyaloshinskii-Moriya interaction
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16. Mechanism of antisymmetric spin polarization in centrosymmetric multiple-Q magnets based on effective chiral bilinear and biquadratic spin cross products
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17. Multiple Skyrmion Crystal Phases by Itinerant Frustration in Centrosymmetric Tetragonal Magnets
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S. Hayami, J. Magn. Magn. Mater. **553**, 169220 (2022).
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19. Helicity locking of a square skyrmion crystal in a centrosymmetric lattice system without vertical mirror symmetry
S. Hayami and R. Yambe, Phys. Rev. B **105**, 104428 (2022).
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HIDA, Kazuo [B class; 400 (B), 70 (C)] (309)
— *Numerical Study of One Dimensional Frustrated Quantum Spin Systems*

1. Infinite Series of Ferrimagnetic Phases Emergent from the Gapless Spin Liquid Phase of Mixed Diamond Chains

Kazuo Hida, J. Phys. Soc. Jpn. **90**, 054701 (2021).
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2. First Order Transitions Between the Gapped Spin-Liquid and Ferrimagnetic Phases in (1/2,1/2,1) Mixed Diamond Chains with Bond Alternation
Kazuo Hida, J. Phys. Soc. Jpn. **91**, 024706 (2022).
DOI:10.7566/JPSJ.91.024706

HIGUCHI, Yuji [C class; 4600 (B), 750 (C)] (230)
— *Structure and mechanical properties of crystalline polymers absorbing water molecules*

1. Hydrophobic immiscibility controls self-sorting or co-assembly of peptide amphiphiles
R. Wakabayashi, R. Imatani, M. Katsuya, Y. Higuchi, H. Noguchi, N. Kamiya, and M. Goto, Chem. Commun. **58**, 585 (2021).
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— *Exploration of exotic surface sites for catalyst informatics*

1. Surface activation by electron scavenger metal nanorod adsorption on TiH2, TiC, TiN, and Ti2O3
Yoyo Hinuma, Shinya Mine, Takashi Toyao, Zen Maeno and Ken-ichi Shimizu, Phys. Chem. Chem. Phys. 23, 16577 (2021).

2. Factors determining surface oxygen vacancy formation energy in ternary spinel structure oxides with zinc
Yoyo Hinuma, Shinya Mine, Takashi Toyao, Takashi Kamachi and Ken-ichi Shimizu, Phys. Chem. Chem. Phys. 23, 23768 (2021).

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— *Calculation of Infrared and Raman spectra by molecular dynamics simulation using machine learning*
— *Validation of a Machine Learning Method for Predicting Vibration Spectra*

HIRAYAMA, Naomi [C class; 1800 (B), 0 (C)] ()
— *Development of inter-atomic potentials of Fe-based amorphous alloys and MD simulation of crystallization process*

HIYAMA, Miyabi [C class; 3200 (B), 800 (C)] (249)
— *Theoretical analysis of absorption and fluorescence spectra for firefly bioluminescence related molecules*

1. Absorption Spectra for Firefly Bioluminescence Substrate Analog: TokeOni in Various pH Solutions
H. Ogawa, R. Ono, Y. Noguchi, N. Kitada, R. Saito-Moriya, S. A. Maki, H. Akiyama, H. Itabashi, and M. Hiyama, Photochem. Photobiol. **97**, 1016 (2021).
DOI:10.1111/php.13458

HOSHI, Takeo [C class; 5200 (B), 0 (C)] (344)
— *HPC-based fusion of experiment analysis, simulation and data-driven science*

1. Data-driven sensitivity analysis in a total-reflection high-energy positron diffraction (TRHEPD)
Takeo Hoshi, Daishiro Sakata, Shotaro Oie, Izumi Mochizuki, Satoru Tanaka, Toshio Hyodo, and Koji Hukushima, Comput. Phys. Commun. 271, 108186 (2022).
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2. Performance prediction of massively parallel computation by Bayesian inference
Hisashi Kohashi, Harumichi Iwamoto, Takeshi Fukaya, Yusaku Yamamoto, and Takeo Hoshi

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4. Data-analysis software framework 2DMAT and its application to experimental measurements for two-dimensional material structures
Yuichi Motoyama, Kazuyoshi Yoshimi, Harumichi Iwamoto, Hayato Ichinose, and Takeo Hoshi, arXiv:2204.04484
DOI:10.48550/arXiv.2204.04484

HOTTA, Chisa [B class; 1000 (B), 80 (C)] (278)
— *Development and application of methods to calculate thermodynamic properties in low dimensional magnets*

1. Dimensional reduction in quantum spin-1/2 system on a 1/7-depleted triangular lattice
R. Makuta and C. Hotta, Phys. Rev. B **104**, 224415 (2021).
DOI:10.1103/PhysRevB.104.224415

HOTTA, Takashi [C class; 5000 (B), 0 (C)] (188)
— *Research of multi-channel Kondo effect emerging from heavy rare-earth ions*

1. Three-Channel Kondo Effect Emerging from Ho Ions
Takashi Hotta, J. Phys. Soc. Jpn. **90**, 113701 (2021).
DOI:10.7566/JPSJ.90.113701

IDO, Kota [B,C class; 4700 (B), 390 (C)] (232)
— *Development of COMPutation ARchive of Exact Diagonalization(COMPARED)*
— *Neural network quantum states for excited states in strongly correlated electron systems*

1. Unconventional dual 1D2D quantum spin liquid revealed by ab initio studies on organic solids family
Kota Ido, Kazuyoshi Yoshimi, Takahiro Misawa, Masatoshi Imada, npj Quantum Materials 7, 48 (2022).
DOI:10.1038/s41535-022-00452-8

Data Repository
COMPARED
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IITAKA, Toshiaki [C class; 2000 (B), 0 (C)] (115)
— *Structure and Property of Basalt Melt and Glass*

1. A comparative study on pressure-induced structural transformations in a basaltic glass and melt from Ab initio molecular dynamics calculations
S. Q. Feng, A. Majumdar, H. Y. Kuang, Y. M. Pan, T. Iitaka, and J. S. Tse Phys. Chem. Miner. 48, 41 (2021).
DOI:10.1007/s00269-021-01165-3

IKEDA, Hiroaki [B class; 400 (B), 70 (C)] ()
— *Electronic structure calculations in quantum liquid crystals*

IKEDA, Tatsuhiko [B class; 600 (B), 40 (C)] (198)
— *Numerical study of nonequilibrium phases in periodically driven systems with dissipation*

1. Criticality and rigidity of dissipative discrete time crystals in solids
   K. Chinzei and T.N. Ikeda, Phys. Rev. Research **4**, 023025 (2022).
   DOI:10.1103/PhysRevResearch.4.023025

IKUHARA, Yuichi [C class; 2000 (B), 0 (C)] (113)
— *Determining grain-boundary stable atomic structure by first-principle calculations*
— *First principles calculations for proving stable grain-boundary structures in perovskite oxides*

1. Oxygen Atom Ordering on SiO2/4H-SiC 0001 Polar Interfaces formed by Wet Oxidation
   M. Saito, H. Li, K. Inoue, H. Matsuhata, Y. Ikuhara, Acta Mater. **221**, 117360 (2021).
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2. Arrangement of polyhedral units for [0001]-symmetrical tilt grain boundaries in zinc oxide
   K. Inoue, J.Y. Roh, K. Kawahara, M. Saito, M. Kotani, Y. Ikuhara, Acta Mater. **212** 116864 (2021).
   DOI:10.1016/j.actamat.2021.116864

IMADA, Masatoshi [E class; 28500 (B), 3000 (C)] (174)
— *Quantum Spin Liquids on Pyrochlore Lattice*
— *Studies on Effects of Non-Local Coulomb Interaction for High Termperature Superconductivity*

1. Unconventional dual 1D-2D quantum spin liquid revealed by ab initio studies on organic solids family
   Kota Ido, Kazuyoshi Yoshimi, Takahiro Misawa, and Masatoshi Imada, npj Quantum Mater. **7**, 48 (2022).
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— *Numerical study of heat transport through a mesoscopic device*
— *Theoretical study of spin Hall magnetoresistance by the quantum Monte Carlo method*

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MISAWA, Masaaki [B class; 500 (B), 0 (C)] (149)
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1. 第一原理計算と機械学習による固体材料における衝撃圧縮特性の分子動力学解析
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— *Simulations of quantum-classical-hybrid algorithms for sensor materials with considering noise*

1. Variational quantum simulation for periodic materials
   Nobuyuki Yoshioka, Takeshi Sato, Yuya O. Nakagawa, Yu-ya Ohnishi, and Wataru Mizukami, Phys. Rev. Research 4, 013052 (2022).
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— *Numerical study on the tolerance of Majorana-based qubits in topological superconductors*

1. Manipulation of Majorana Kramers Qubit and its Tolerance in Time-Reversal-Invariant Topological Superconductor
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   Y. Tanaka, T. Sanno, T. Mizushima, and S. Fujimoto, submitted

MOCHIZUKI, Masahito [B,C,D class; 12100 (B), 0 (C)] (180, 181)

— *Novel dynamics of magnetic skyrmion crystal phases due to extra degrees of freedom*

— *Numerical studies on the photoinduced phenomena of magnetic skyrmion lattices in metallic magnets*

— *Theoretical study on the spin-wave excitations of multiple-Q magnetic hedgehogs*

1. Dynamical switching of magnetic topology in microwave-driven itinerant magnet
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   DOI:10.1103/PhysRevB.104.104425

2. Low-energy excitations of skyrmion crystals in a centrosymmetric Kondo-lattice magnet: Decoupled spin-charge excitations and nonreciprocity
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3. Dynamical phase transitions in the photodriven charge-ordered Dirac-electron system
   Y. Tanaka and M. Mochizuki, arXiv:2203.04542
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MOMIDA, Hiroyoshi [C class; 2600 (B), 400 (C)] (102)

— *Structure stability and electronic structures of point defects in wide-gap oxide materials*

1. Tavorite-like orthorhombic $A_x\mathrm{VPO_4F}$ (A = Li, Na) for novel high-voltage cathodes in rechargeable batteries
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— *Quantum Simulations on Dynamical Heterogeneous Catalysts*

1. Theoretical study on adsorption and reaction of polymeric formic acid on the Cu(111) surface
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MORITA, Satoshi [B class; 600 (B), 90 (C)] (295)
— *Improvement of tensor network renormalization for high-dimensional systems*

1. Symmetry-protected topological phases and competing orders in a spin-1/2 XXZ ladder with a four-spin interaction
Takuhiro Ogino, Shunsuke Furukawa, Ryui Kaneko, Satoshi Morita, and Naoki Kawashima, Phys. Rev. B **104**, 075135 (2021).
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— *Development of multiscale simulation technique for liquids and solids*

1. Viscosity Overshoot in Biaxial Elongational Flow: Coarse-Grained Molecular Dynamics Simulation of Ring-Linear Polymer Mixtures
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— *Elucidation of pathways for the crystallization of ionic liquids by large-scale metadynamics simulation*

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— *Ab initio calcualtion for reflectivity for SrVO3/SrTiO3 CaCuO2/SrTiO3, and Ca5Ir3O12*
— *Ab initio derivation of effective low-energy models for SrVO3/SrTiO3 and CaCuO2/SrTiO3 multi-*

layer system

1. Ab initio derivation of low-energy Hamiltonians for systems with strong spin-orbit interaction: Application to $Ca_5Ir_3O_{12}$
   M. Charlebois, J. B. Moree, K. Nakamura, Y. Nomura, T. Tadano, Y. Yoshimoto, Y. Yamaji, T. Hasegawa, K. Matsuhira, and M. Imada, Phys. Rev. B **104**, 075153 (2021).
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— *First-principles electronic structure calculation of double-perovskite photocatalyst*

NISHIGUCHI, Kazutaka [B class; 400 (B), 0 (C)] (314)
— *Theoretical study of thermoelectric properties in doped Fe_2VAl: A weak-coupling approach*

1. Possibility of N-type Doping in $CaAl_2Si_2$-type Zintl Phase Compound $CaZn_2X_2$ (X = As, P)
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OBATA, Masao [B class; 700 (B), 120 (C)] (136)
— *Analysis of ferroelectric-ferromagnetic interface and magnetic material with an anisotropic crystal structure*
— *Analysis of insulator-ferromagnetic interface and magnetic material with an anisotropic crystal structure*

1. Effect of electron localization in theoretical design of Ni-Mn-Ga based magnetic shape memory alloys
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— *Magnetocaloric Effect of Transition-Metal Alloys*

1. Tavorite-type orthorhombic A_xVPO$_4$F (A = Li, Na) for novel high-voltage cathodes in rechargeable batteries
   Huu Duc Luong, Van An Dinh, Hiroyoshi Momida, Tamio Oguchi, J. Alloys Compd. **875**, 159963 (2021).

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— *Clarification of atomistic mechanism application of process design for adhesion interface between metal and plasma-treated fluoropolymers using first principles calculation*

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   Y. Motoyama, R. Tamura, K. Yoshimi, K. Terayama, T. Ueno, and K. Tsuda, submitted.

TANAKA, Shu [B class; 400 (B), 70 (C)] (307)
— *Development of Algorithms for Ising Machines Based on Statistical Mechanics*

1. Exact bounds for dynamical critical exponents of transverse-field Ising chains with a correlated disorder
   T. Shirai and S. Tanaka, Ann. Phys. (N. Y.) **435**, 168483 (2021).
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2. Continuous black-box optimization with an Ising machine and random subspace coding
   S. Izawa, K. Kitai, S. Tanaka, R. Tamura, and K. Tsuda, Physical Review Research, **4** (2022) 023062.
   DOI:10.1103/PhysRevResearch.4.023062

3. Structural analysis based on unsupervised learning: Search for a characteristic low-dimensional space by local structures in atomistic simulations
   R. Tamura, M. Matsuda, J. Lin, Y. Futamura, T. Sakurai, and T. Miyazaki, Phys. Rev. B **105**, 075107 (2022).
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4. Bayesian optimization package: PHYSBO
   Y. Motoyama, R. Tamura, K. Yoshimi, K. Terayama, T. Ueno, and K. Tsuda, submitted.

TANAMOTO, Tetsufumi [B class; 200 (B), 60 (C)] (321)
— *Analysis of transport properties of spin-qubit based on FinFET*

TATETSU, Yasutomi [C class; 2600 (B), 350 (C)] (103)
— *Theoretical analyses for surfaces and grain boundaries with magnetic elements from first-principles calculations*

1. Inter-element miscibility driven stabilization of ordered pseudo-binary alloy

K. Matsumoto, R. Sato, Y. Tatetsu, R. Takahata, S. Yamazoe, M. Yamauchi, Y. Inagaki, Y. Horibe, M. Kudo, T. Toriyama, M. Auchi, M. Haruta, H. Kurata, and T. Teranishi, Nat. Commun., **13**, 1047 (2022).
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TERAO, Takamichi [B class; 700 (B), 90 (C)] (283)
— *Structural formation of patchy particles*

1. Eigenvalue analysis of the three-dimensional tight-binding model with non-Hermitian disorder
   T. Terao, Phys. Rev. B **103**, 224201 (2021).

TERASAWA, Asako [B class; 400 (B), 80 (C)] ()
— *First-principles analysis of structure and exchange coupling constants of subphases and interface in Nd-based permanent magnets*

TEZUKA, Masaki [C class; 4400 (B), 0 (C)] (242)
— *Scrambling and effect of dissipation in quantum many-body systems*

TODO, Synge [C class; 6000 (B), 900 (C)] (222)
— *Topological order and quantum operation in quantum many-body systems*

1. Bond-weighted tensor renormalization group
   D. Adachi, T. Okubo, and S. Todo, Phys. Rev. B **105**, L060402 (2022).
   DOI:10.1103/PhysRevB.105.L060402

TOHYAMA, Takami [C class; 3000 (B), 700 (C)] (193)
— *Analysis of string excitations in the optical conductivity of doped Mott insulators*

1. Resonating dimer-monomer liquid state in a magnetization plateau of a spin-12 kagome-strip Heisenberg chain
   K. Morita, S. Sota, and T. Tohyama, Commun. Phys. **2**, 161 (2021).
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2. Coexistence of strong and weak Majorana zero modes in an anisotropic XY spin chain with second-neighbor interactions
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   DOI:10.1103/PhysRevB.104.205123

4. Magnetic phase diagrams of the spin-12 Heisenberg model on a kagome-strip chain: Emergence of a Haldane phase
   K. Morita, S. Sota, and T. Tohyama, Phys. Rev. B **104**, 224417 (2021).
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TOKUMOTO, Yuki [B class; 400 (B), 70 (C)] (150)
— *Defect formation energy and band structure of Pb-based topological insulators*

TONEGAWA, Takashi [B class; 600 (B), 0 (C)] (296)
— *Numerical Study of the One-Dimensional Quantum Spin Systems with Spatial Structures*

TOYODA, Masayuki [B class; 500 (B), 0 (C)] (148)
— *Thickness-dependent electronic structure of exfoliated boron monosulfide*

TSUMURAYA, Takao [C class; 1000 (B), 550 (C)] (124)
— *Origins of phase stabilities and physical properties in Mg based alloys: A first-principles study*

1. Origin of phase stability in Fe with long-period stacking order as an intermediate phase in cyclic γ-ϵ martensitic transformation
Takao Tsumuraya and Ikumu Watanabe and Takahiro Sawaguchi Phys. Rev. Research 3, 033215 (2021).
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TSUNEYUKI, Shinji [C class; 6000 (B), 900 (C)] (70)
— *Elucidation of mechanism and theoretical prediction of super-functional materials using high-density hydrogen*

1. Superionic Conductivity Combined CB9H10 − Rotation and Li-ion Concerted Motion in LiCB9H10: An Ab Initio and Neural-Net Potential Molecular Dynamics Study
Ryuhei Sato, Shigeyuki Takagi, Tamio Ikeshoji, Toyota Sato, Takashi Honda, Toshiya Otomo, Shin-ichi Orimo, Shinji Tsuneyuki, submitted to J. Phys. Chem. Lett.

TSURUTA, Kenji [C class; 600 (B), 550 (C)] (130)
— *Ab-initio and artificial neural-network molecular-dynamics calculations for molecule-modified nanointerfaces*

UCHIDA, Takashi [B class; 300 (B), 90 (C)] (316)
— *Multiple spin density waves in inversion-symmetric two-dimensional Hubbard models*
— *Spontaneous formation of multiple-Q orders in inversion-symmetric Hubbard models*

UMEMOTO, Koichiro [C class; 2200 (B), 650 (C)] ()
— *Order-disorder transitions in post-post-perovskite phases in Mg-Si-O system*

WAKABAYASHI, Daisuke [B class; 400 (B), 0 (C)] (312)
— *Large-scale molecular-dynamics simulation of silica melt and glass under high pressure with ANN potentials by active learning*

WATANABE, Haruki [B class; 500 (B), 100 (C)] ()
— *Comprehensive material search based on symmetry indicators*

WATANABE, Hiroshi [B,C class; 5300 (B), 430 (C)] (229)
— *Analysis of the phase boundary under the steady-state heat conduction*

— *Development of an Efficient Phase Diagram Exploration Method Using Gaussian Process Regression*

WATANABE, Hiroshi [B class; 400 (B), 70 (C)] (200)
— *Study of cuprate high-temperature superconductors using 4-band d-p model*

1. Unified description of cuprate superconductors using a four-band *d-p* model
   H. Watanabe, T. Shirakawa, K. Seki, H. Sakakibara, T. Kotani, H. Ikeda, S. Yunoki, Phys. Rev. Research **3**, 033157 (2021).
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WATANABE, Satoshi [C class; 10800 (B), 1150 (C)] (47)
— *Analyses related to atomic structures and atom dynamics at complex structures such as surfaces, interfaces and defects*

1. ニューラルネットワークポテンシャルによる金–リチウム合金化過程の解析
   清水康司, E. F. Arguelles, 李文文, 安藤康伸, 南谷英美, 渡邉聡表面と真空 **64**, 369 (2021).
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2. 窒化物半導体におけるフォノン関連物性の解析のための 機械学習ポテンシャルの開発
   渡邉聡, 清水康司, 南谷英美日本結晶成長学会誌 **48**, 48-4-05 (2021).

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   K. Nishio, S. Ichinokura, A. Nakanishi, K. Shimizu, Y. Kobayashi, N. Nakamura, D. Imazeki, R. Shimizu, T. Hirahara, S. Watanabe, and T. Hitosugi, Nano Lett. **21**, 10086 (2021).
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4. Neural network potential study of point defect properties in multiple charge states: GaN with nitrogen vacancy
   K. Shimizu, Y. Dou, E. F. Arguelles, T. Moriya, E. Minamitani, and S. Watanabe, arXiv.2203.16789
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YAMADA, Atsuo [C class; 6200 (B), 900 (C)] (69)
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1. Soft X-ray Emission Studies on Hydrate-Melt Electrolytes
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   DOI:10.1021/acs.chemmater.1c03328

YAMADA, Atsushi [C class; 600 (B), 400 (C)] (195)
— *Studies of the superconductivity and magnetic states in the strongly correlated electron systems based on Hubbard models.*

YAMADA, Masahiko [C class; 6000 (B), 650 (C)] (223, 224)
— *Glass transition in the disordered Kitaev model*
— *Heat capacity and magnetic susceptibility of the SU(N) Heisenberg models*

YAMAGUCHI, Naoya [B class; 900 (B), 110 (C)] (131)
— *First-principles Calculations of Magnetic Insulators Under Uniform Electric Fields*

— *First-principles Calculations of Spin-to-charge Conversion Materials Utilizing Organic Molecules*

1. First-principles LCPAO Approach to Insulators Under Finite Electric Fields
   N. Yamaguchi and F. Ishii, submitted to Comp. Phys. Commun.

2. First-principles calculation of anomalous Hall and Nernst conductivity by local Berry phase
   H. Sawahata, N. Yamaguchi, S. Minami and F. Ishii, submitted to Phys. Rev. B

YAMAJI, Youhei [E class; 14500 (B), 2150 (C)] (177)

— *Numerical studies of Mott transitions in quantum spin liquid candidates*

1. Ab initio derivation of low-energy Hamiltonians for systems with strong spin-orbit interaction: Application to $Ca_5Ir_3O_{12}$
   Maxime Charlebois, Jean-Baptiste More, Kazuma Nakamura, Yusuke Nomura, Terumasa Tadano, Yoshihide Yoshimoto, Youhei Yamaji, Takumi Hasegawa, Kazuyuki Matsuhira, Masatoshi Imada, Phys. Rev. B **104**, 075153 (2021).
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YAMASHITA, Tomoki [C class; 5200 (B), 800 (C)] (76)

— *Development of crystal structure prediction methods using machine learning*

1. CrySPY: a crystal structure prediction tool accelerated by machine learning
   T. Yamashita, S. Kanehira, N. Sato, H. Kino, H. Sawahata, T. Sato, F. Utsuno, K. Tsuda, T. Miyake, and T. Oguchi, Sci. Technol. Adv. Mater. Meth. **1**, 87 (2021).
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YAMAUCHI, Kunihiko [C class; 5000 (B), 800 (C)] (80)

— *First-principles design of topological interfaces toward next-generation spintronics application*

1. Electric-field tuning of the magnetic properties of bilayer VI3: A first-principles study
   Thi Phuong Thao Nguyen, Kunihiko Yamauchi, Tamio Oguchi, Danila Amoroso, and Silvia Picozzi, Phys. Rev. B **104**, 014414 (2021).
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2. First-principles Study on Piezoelectricity and Spontaneous Polarization in Bi(Fe,Co)O3
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4. Spin-Polarized Band Structure at MoTe2=Bi2Se3 Interface Designed from First Principles
   Kunihiko Yamauchi, Ryoma Shimazu1, and Tamio Oguchi, J. Phys. Soc. Jpn. **91**, 044705 (2022).
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YANAGISAWA, Susumu [C class; 5800 (B), 650 (C)] ()
— *First-principles band structure calculation of organic crystals at finite-temperature*
— *First-principles investigation on the electronic properties of polymer organic semiconductors*

YANAGISAWA, Takashi [B class; 300 (B), 30 (C)] (202)
— *New quantum phenomena in strongly correlated many-body electron systems*
1. Ground-state phase diagram of the three-band d-p model
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2. Enhancement of superconductivity due to kinetic energy effect in the strongly correlated phase in the two-dimensional Hubbard model
   T. Yanagisawa: Phys. Lett. A 403, 127382 (2021).

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— *Numerical study of spin systems on the honeycomb lattice*

YASUDA, Yusuke [B class; 300 (B), 30 (C)] (317)
— *Molecular Dynamics Simulations of Reversiblly Cross-linked Rubbers*

YOKO, Akira [B,C class; 3000 (B), 580 (C)] (95)
— *Hydrogen formation by reaction of water on reduced CeO_2 (100) surface*
— *Interaction between metallic atom and instable CeO2 (100) facet*
1. Atomistic Origin of High-Concentration Ce3+ in 100-Faceted Cr-Doped CeO2 Nanocrystals
   X. Hao, A. Yoko, K. Inoue, Y. Xu, M. Saito, C. Chen, G. Seong, T. Tomai, S. Takami, A.L. Shluger, B. Xu, T. Adschiri, Y. Ikuhara, Acta Materialia. **203**, 116473 (2021).
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YOSHIDA, Tsuneya [C class; 5200 (B), 0 (C)] (185)
— *Exotic phenomena induced by strong correlations and non-Hermitian topology*
1. Surface exceptional points in a topological Kondo insulator
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2. Chiral edge modes in evolutionary game theory: A kagome network of rock-paper-scissors cycles
   T. Yoshida, T. Mizoguchi, and Y. Hatsugai, Phys. Rev. E 104, 025003 (2021).
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3. Topological d-wave superconductivity in two dimensions
   Y. Yanase, A. Daido, K. Takasan, and T. Yoshida, Physica E: Low-dimensional Systems and

Nanostructures, 140, 115143 (2022).
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YOSHIMOTO, Yuta [C class; 2600 (B), 0 (C)] (259)
— *Next-generation integrated engineering for developing polymer materials*

○ 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), 40 (C)] ()
— *Band calculation of topological insulator systems*

FUJINO, Tomoko [A class; 100 (B), 40 (C)] (194, 351)
— *Electronic states of electron-rich oligomer-based conductors*

GONOME, Hiroki [A class; 100 (B), 40 (C)] ()
— *Study of the principle of photothermal conversion by ab initio calculations*

ISHITANI, Yoshihiro [A class; 100 (B), 40 (C)] ()
— *Phonon-property analysis for phonon control in electronic/photonic devices by wide-bandgap semiconductors*

IWASE, Fumitatsu [A class; 100 (B), 40 (C)] ()
— *The ground state of cairo-fractal lattice*

KITAGAWA, Kentaro [A class; 100 (B), 40 (C)] ()
— *Screening test for crystal nucleation of flux method*

KOTA, Yohei [A class; 100 (B), 40 (C)] ()
— *First-principles calculation of physical properties in various magnetic materials*

MASAKI, Yusuke [A class; 100 (B), 50 (C)] (367)
— *Microscopic calculations of fractional vortices in topological superfluids*

MITARAI, Yoko [A class; 100 (B), 40 (C)] ()
— *Phase stability of high-entropy alloys*

NISHIGUCHI, Kazutaka [A class; 100 (B), 50 (C)] (314, 373)
— *First-principles study of thermoelectric and magnetic properties in doped Fe_2VAl*

OKUBO, Masashi [A class; 100 (B), 50 (C)] (157, 377)
— *Development of all-solid-state capacitors using sulfide-based solid electrolytes*

OYA, Yutaka [A class; 100 (B), 40 (C)] ()
— *Molecular dynamics simulation of matrix resin for composite materials*

SATO, Shunsuke [A class; 100 (B), 40 (C)] ()
— *Theoretical investigation on THz-field induced electron dynamics in graphene*

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1. Reassessment of vibration spectra in alkali phosphate crystals
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TSUKAHARA, Noriyuki [A class; 100 (B), 40 (C)] ()
— *Adsorption states of an organic halogen molecule on semiconductor and metal surfaces*

UCHIDA, Ken [A class; 100 (B), 40 (C)] ()
— *Calculation of thermal conductivity of Hexagonal Tungsten Bronze*

WAKABAYASHI, Daisuke [A class; 100 (B), 50 (C)] (312, 387)
— *Large-scale molecular-dynamics simulation of silica melt under high pressure with ANN potentials*

□ SCCMS Projects

FUJITA, Takatoshi [4000 (B), 0 (C)] (329)
— *Large-Scale GW/BSE electronic structure calculations for metal-organic hybrid materials*
— *Developments of non-linear optical response theory based on electronic structure calculations and their applications to nano and biological systems*

1. Fragment-Based Excited-State Calculations Using the GW Approximation and the Bethe–Salpeter Equation
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FUKUSHIMA, Tetsuya [4000 (B), 700 (C)] (334)
— *Development of high-throughput calculation tools and evaluation of magnetic properties in hard magnetic materials*
— *High-throughput calculation of magnetic anisotropy energy in permanent magnet materials*

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   A. Masago, H. Shinya, T. Fukushima, K. Sato, and H. Katayama-Yoshida, Appl. Phys. Exp. **14**, 091007 (2021).
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GOHDA, Yoshihiro [2000 (B), 200 (C)] (79)
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2. Giant converse magnetoelectric effect in a multiferroic heterostructure with polycrystalline Co_2FeSi
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3. Intrinsic superconductivity of two-monolayer-thick indium film
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   S. Tsuna, R. Costa-Amaral, and Y. Gohda, submitted to Phys. Rev. Mater.

IMADA, Masatoshi [10000 (B), 1400 (C)] (174)
— *Integrated analyses on spectroscopic experiments and ab initio electronic structure calculations for mechanisms of unconventional superconductors*
— *Analysis on Superconducting Mechanism of Cuprate Superconductors*

1. Unconventional dual 1D-2D quantum spin liquid revealed by ab initio studies on organic solids

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Maxime Charlebois, Jean-Baptiste Morée, Kazuma Nakamura, Yusuke Nomura, Terumasa Tadano, Yoshihide Yoshimoto, Youhei Yamaji, Takumi Hasegawa, Kazuyuki Matsuhira, and Masatoshi Imada, Phys. Rev. B **104**, 075153 (2021).
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5. Dirac-type nodal spin liquid revealed by refined quantum many-body solver using neural-network wave function, correlation ratio, and level spectroscopy
Yusuke Nomura and Masatoshi Imada, Phys. Rev. X **11**, 031034 (2021).
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Marcin Raczkowski, Fakher F. Assaad, Masatoshi Imada Phys. Rev. B **103**, 462 (2021).
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MIYAKE, Takashi [600 (B), 0 (C)] (338)
— *Development of high-performance permanent magnets by large-scale simulation and data-driven approach*

1. Evolutionary search for cobalt-rich compounds in yttrium-cobalt-boron system
Takahiro Ishikawa, Taro Fukazawa, Guangzong Xing, Terumasa Tadano and Takashi Miyake, Phys. Rev. Mater. **5**, 054408 (2021).
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2. Ordered and disordered phases in $CaCu_5$-type derived structures: Dumbbell cluster modeling with first-principles calculations
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