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; 1200 (B), 150 (C)] (141, 142)
— *Magnetic properties of rare earth magnetic materials with structural disorder*

1. 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. Materials **5**, 013806 (2021).
   DOI:10.1103/PhysRevMaterials.5.013806

2. Spin-wave dispersion and exchange stiffness in $Nd_2Fe_{14}B$ and $R Fe_{11}Ti$ (R=Y, Nd, Sm) from first-principles calculations
   T. Fukazawa, H. Akai, Y. Harashima, and T. Miyake Phys. Rev. B **103**, 024418 (2021).
   DOI:0.1103/PhysRevB.103.024418

3. Magnetic Friedel Oscillation at Fe(001) Surface: Direct Observation by Atomic-Layer-Resolved Synchrotron Radiation ^{57}Fe Mössbauer Spectroscopy
   T. Mitsui, S. Sakai, S. Li, T. Ueno, T. Watanuki, Y. Kobayashi, R. Masuda, M. Seto, and H. Akai Phys. Rev. Lett. **125**,236806 (2020).
   DOI:10.1103/PhysRevLett.125.236806

4. First-principles calculations of finite temperature electronic structures and transport properties of Heusler alloy Co_2MnSi
   H. Shinya, S. Kou, T. Fukushima, A. Masago, K. Sato, H. Katayama-Yoshida, and H. Akai Appl. Phys. Lett. **117**,042402 (2020).
   DOI:10.1063/5.0017862

5. Element- and orbital-selective magnetic coherent rotation at the first-order phase transition of a hard uniaxial ferrimagnet
   Sh. Yamamoto, D. I. Gorbunov, H. Akai, H. Yasumura, Y. Kotani, T. Nakamura, T. Kato, N. V. Mushnikov, A. V. Andreev, H. Nojiri, and J. Wosnitza Phys. Rev. B **101**,174430 (2020).
   DOI:10.1103/PhysRevB.101.174430

6. Calculating Curie temperatures for rare-earth permanent magnets: Ab initio inspection of localized magnetic moments in d-electron ferromagnetism
   M. Matsumoto and H. Akai Phys. Rev. B **101**, 1444402 (2020).

DOI:10.1103/PhysRevB.101.144402

AKASHI, Ryosuke [C class; 4000 (B), 750 (C)] (93)
— *First principles exploration of the metastable phases of hydrides and their superconductivity*
— *First principles exploration of the metastable phases of hydrides and their superconductivity II*

1. AtomREM: Non-empirical seeker of the minimum energy escape paths on many-dimensional potential landscapes without coarse graining
   Y. S. Nagornov and R. Akashi Comput. Phys. Commun. **254** (2020) 107260.

2. Effect of spin fluctuations on superconductivity in V and Nb: A first-principles study
   K. Tsutsumi, Y. Hizume, M. Kawamura, R. Akashi, and S. Tsuneyuki, Phys. Rev. B **102** (2020) 214515.

AKERA, Hiroshi [C class; 4000 (B), 650 (C)] (95)
— *Generation of spin and pseudospin polarizations in atomic-layer inplane heterostructures and stacked structures*

AOYAMA, Kazushi [B class; 1000 (B), 200 (C)] (280)
— *Spin transport near a phase transition in magnets*
— *Transport properties of multiple-q states in frustrated magnets*

1. Hedgehog-lattice spin texture in classical Heisenberg antiferromagnets on the breathing pyrochlore lattice
   K. Aoyama and H. Kawamura Phys. Rev. B **103** (2021) 014406.

ARAI, Munehito [C class; 4400 (B), 350 (C)] (252)
— *Computational rational design of novel proteins for industrial and pharmaceutical applications*
— *Protein design toward the development of therapeutic drugs for COVID-19*

ARAI, Toyoko [C class; 1800 (B), 400 (C)] (130)
— *DFT calculation of atomic displacement captured by energy dissipation channel of noncontact atomic force microscope*

ARIMA, Kenta [B class; 600 (B), 150 (C)] (171)
— *Analysis of electronic structures around the Fermi level of graphene nanoribbons with different widths*
— *Origin of specific dot patters on small graphene sheets observed by STM*

ARUGA, Tetsuya [B class; 200 (B), 0 (C)] ()
— *Interaction among phthalocyanine molecules adsorbed on metal surfaces*

ASANO, Yuta [E class; 22500 (B), 4000 (C)] (36)
— *Molecular dynamics simulation of cavitation in complex fluids*

1. Molecular Dynamics Simulation of Soundwave Propagation in a Simple Fluid
   Y. Asano, H. Watanabe, and H. Noguchi, J. Chem. Phys. 153, 124504 (2020).
   DOI:10.1063/5.0024150

2. Rotational Dynamics of Water at the Phospholipid Bilayer Depending on the Head Groups Studied by Molecular Dynamics Simulations
   Y. Higuchi, Y. Asano, T. Kuwahara, and M. Hishida, Langmuir **37**, 5329 (2021).
   DOI:10.1021/acs.langmuir.1c00417

3. 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, 14905 (2021).
DOI:10.1063/5.0056988

BUI, VANPHO [C class; 1000 (B), 100 (C)] (152)
— *Study on removal mechanism in catalyst referred etching of single crystalline Si with pure water*
— *Study on removal mechanism of single crystalline Si planarized by catalyst referred etching in pure water*

EGAMI, Yoshiyuki [C class; 7200 (B), 1100 (C)] (63)
— *Development and application of algorithms for large-scale first-principles electron-transport simulation*
— *Development and application of first-principles algorithms for for long-range electron transport simulation*

1. Calculation of the Green's function in the scattering region for first-principles electron-transport simulations
   Y. Egami, S. Tsukamoto, and T. Ono, Phys. Rev. Res. **3**, 013038 (2021).
   DOI:10.1103/PhysRevResearch.3.013038

FUCHIZAKI, Kazuhiro [C class; 1800 (B), 250 (C)] (271)
— *Kinetics of phase transition and polyamorphism*

1. A unique multianvil 6–6 assembly for a cubic-type multianvil apparatus
   K. Fuchizaki, T. Wada, H. Naruta, A. Suzuki, and K. Irino Rev. Sci. Instrum. **92**, 025117 (2021).
   DOI:10.1063/5.0039306

2. Application of nonequilibrium relaxation scheme to machine learning for detecting a phase transition
   K. Fuchizaki, K. Nakamura, and D. Hiroi, J. Phys. Soc. Jpn. in press.

3. The microscopic transition process from high-density to low-density amorphous state of SnI_4
   K. Fuchizaki, A. Ohmura, H. Naruta, and T. Nishioka, submitted to J. Phys.: Condens. Matter.

FUJII, Susumu [B class; 600 (B), 0 (C)] (303)
— *Systematic Investigation on Phonon Transport at Nanoscale Interfaces*

FUJIMOTO, Satoshi [D class; 6000 (B), 1000 (C)] (236)
— *O(N) solution to the disordered Kitaev model using the large-scale parallel computing*

1. Anderson-Kitaev spin liquid
   Masahiko G. Yamada, npj Quantum Mater **5**, 82 (2020).
   DOI:10.1038/s41535-020-00285-3

FUJIMOTO, Yoshitaka [C class; 1000 (B), 0 (C)] (154)
— *Doping and molecular adsorption of graphene*

1. Stacking and curvature-dependent behaviors of electronic transport and molecular adsorptions of graphene: A comparative study of bilayer graphene and carbon nanotube
   Y. Fujimoto and S. Saito, Applied Surface Science Advances **1**, 100028 (2020).

2. Carbon annealed HPHT-Hexagonal boron nitride: Exploring defect levels using 2D materials combined through van der Waals interface
   M. Onodera, M. Isayama, T. Taniguchi, K. Watanabe, S. Masubuchi, R. Moriya, T. Haga, Y. Fujimoto, S. Saito and T. Machida, Carbon **167**, 785 (2020).

3. First-Principles Materials Design for Graphene-based Sensor Devices

Y. Fujimoto, Sustainable Materials for Next Generation Energy Devices, p.343 (Elsevier 2021).

4. Quantum transport, electronic properties and molecular adsorption in graphene
   Y. Fujimoto, Modern Physics Letters B **35**, 2130001 (2021).

5. Electronic states and modulation doping of hexagonal boron-nitride trilayer
   T. Haga, Y. Matsuura, Y. Fujimoto and S. Saito, Physical Review Materials, submitted.

6. Stability of Hydrogen Boride Sheets in Water
   K. I. Rojas, N. T. Cuong, H. Nishino et al., Communications Materials, submitted.

FUJISHIRO, Hiroki [C class; 2200 (B), 0 (C)] (128)
— *Strained Band-Structure Engineering for Antimonide-Based Terahertz Transistors*

FUKUDA, Jun-ichi [B class; 800 (B), 0 (C)] (289)
— *Calculation of ordered structures dynamics and optical properties of soft materials*

1. Lattice orientation of cholesteric blue phases in contact with surfaces enforcing unidirectional planar anchoring
   J. Fukuda and S. Žumer, Physical Review Research **2** (2020) 033407/1-11.

FUKUDA, Masahiro [B class; 300 (B), 100 (C)] (182)
— *Analysis of local quantities of electron field in material surface*

FUKUMOTO, Yoshiyuki [B class; 500 (B), 0 (C)] (309)
— *Effects of exchange randomness on magnetic properties of a spherical-kagome spin-system W72V30*
— *Exact diagonalization calculations of density of states and dynamical structure factor for the spherical-kagome spin-system $W_{72}V_{30}$*

FUKUSHIMA, Tetsuya [B,C class; 1700 (B), 300 (C)] (132)
— *Construction of magnetic materials database by KKR Green's function method*
— *Highthroughput screening calculations by KKR Green's function method*

1. Hole-mediated ferromagnetism in a high-magnetic moment material, Gd-doped GaN
   A. Masago, H. Shinya, T. Fukushima, K. Sato, and H. Katayama-Yoshida, J. Phys.: Condens. Matter **32**, 485803 (2020).
   DOI:10.1088%2F1361-648x%2Fabac8e

2. First-principles calculations of finite temperature electronic structures and transport properties of Heusler alloy Co_2MnSi
   H. Shinya, S. Kou, T. Fukushima, A. Masago, K. Sato, H. Katayama-Yoshida, and H. Akai, Appl. Phys. Lett. **117**, 042402 (2020).
   DOI:10.1063/5.0017862

GOHDA, Yoshihiro [C class; 2800 (B), 550 (C)] (112)
— *Theoretical analysis of influences of phonons on magnetism*

1. First-principles determination of intergranular atomic arrangements and magnetic properties in rare-earth permanent magnets
   Y. Gohda, Sci. Technol. Adv. Mater. **22**, 113 (2021).
   DOI:10.1080/14686996.2021.1877092

2. Prediction of the Curie temperature considering the dependence of the phonon free energy on magnetic states
   T. Tanaka and Y. Gohda, npj Comput. Mater. **6**, 184 (2020).

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3. Effective quantum-well width of confined electrons in ultrathin Ag(111) films on Si(111)7x7 substrates
K. Sugawara, I. Seo, S. Yamazaki, K. Nakatsuji, Y. Gohda, and H. Hirayama, Surf. Sci. 704, 121745 (2020).
DOI:10.1016/j.susc.2020.121745

4. First-principles study of magnetism-dependent phonons governed by exchange ligand field
T. Tanaka and Y. Gohda, J. Phys. Soc. Jpn. **89**, 093705 (2020).
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5. First-principles Calculations on High-temperature Desorption Loss from Iridium
I. Seo, S. Yokota, Y. Imai, and Y. Gohda, Comput. Mater. Sci. **184**, 109897 (2020).
DOI:10.1016/j.commatsci.2020.109897

6. First-principles study on magnetism of a crystalline grain-boundary phase in Nd–Fe–B permanent magnets
Y. Ainai, S. Kou, Y. Tatetsu, and Y. Gohda Jpn. J. Appl. Phys. **59**, 060904 (2020).
DOI:10.35848/1347-4065/ab9402

7. First-principles study of the adsorption of 3d transition metals on BaO- and TiO2-terminated cubic-phase BaTiO3(001) surfaces
R. Costa-Amaral and Y. Gohda, J. Chem. Phys. **152**, 204701 (2020).
DOI:10.1063/5.0008130

GOHLKE, Matthias [C class; 1800 (B), 400 (C)] (268)
— *Numerical study of spin-nematic order in the $S = 1/2$ J_1J_2K-Heisenberg model on the square lattice*

HAGITA, Katsumi [D class; 6500 (B), 0 (C)] (239)
— *Confirmation of stress-overshoot phenomena under biaxial elongational flow of ring-linear mixtures*

1. Effect of Chain-Penetration on Ring Shape for Mixtures of Rings and Linear Polymers.
K. Hagita, T. Murashima, Polymer, 2021, 218, 123493.

2. Multi-Ring Configurations and Penetration of Linear Chains through Rings on Bonded Rings and Poly-Catenanes in Linear Chain Matrices.
K. Hagita, T. Murashima, Polymer, 2021, 223, 123705.

3. Multi-Interval Trajectory Recording for Efficient Analyses of Time Correlations.
K. Hagita, T. Murashima J. Phys. Soc. Jpn. 89, 024002 (2020).

HAMADA, Ikutaro [C class; 2800 (B), 0 (C)] (122)
— *First-principles study of molecule/metal interfaces*

1. Manipulable Metal Catalyst for Nanographene Synthesis
A. Shiotari, I. Hamada, T. Nakae, S. Mori, T. Okujima, H. Uno, H. Sakaguchi, Y. Hamamoto, Y. Morikawa, and Y. Sugimoto Nano Lett. **11** (2020) 8339.

HAMAGUCHI, Satoshi [C class; 6000 (B), 1150 (C)] (68)
— *Analyses of Surface Reactions in Atomic Layer Etching Processes*

1. Self-limiting processes in thermal atomic layer etching of nickel by hexafluoroacetylacetone
A. H. Basher, I. Hamada, and S. Hamaguchi, Jpn. J. Appl. Phys. 59, 090905 (2020).

HAMAMOTO, Yuji [C class; 2800 (B), 0 (C)] (120)
— *van der Waals density functional study of Cu phthalocyanine adsorbed on the Au(110) surface*
— *van der Waals density functional study of Cu phtyalocyanine adsorbed on the Au(110) surface*

1. Identifying Atomic-Level Correlation Between Geometric and Electronic Structure at a Metal-Organic Interface
   H. Koshida, H. Okuyama, S. Hatta, T. Aruga, Y. Hamamoto, I. Hamada, and Y. Morikawa, J. Phys. Chem. C **124**, 17696 (2020).
   DOI:10.1021/acs.jpcc.0c04678

HARADA, KENJI [C class; 1600 (B), 500 (C)] (270)
— *Development of entanglement optimization method*

HARASHIMA, Yosuke [C class; 800 (B), 0 (C)] (170)
— *First-principles study on complexes of impurity and dislocation in GaN p-n diodes*
— *leakage current on power semiconductor devices and an electronic structure on a threading dislocation*

1. Screw dislocation that converts p-type GaN to n-type: Microscopic study on Mg condensation and leakage current in p-n diodes
   T. Nakano, Y. Harashima, K. Chokawa, K. Shiraishi, A. Oshiyama, Y. Kangawa, S. Usami, N. Mayama, K. Toda, A. Tanaka, Y. Honda, and H. Amano, Appl. Phys. Lett. **117**, 012105 (2020).
   DOI:10.1063/5.0010664

HARUYAMA, Jun [C class; 6000 (B), 1100 (C)] (71)
— *Electrochemical reaction analysis using density functional calculation + implicit solvation model 2*
— *Electrochemical reaction analysis using density functional calculation + implicit solvation model 2-2*

HASHIMOTO, Tamotsu [C class; 800 (B), 150 (C)] (284)
— *Molecular dynamics simulation of liquid $BaTiO_3$*

1. Structure of Amorphous $BaTiO_3$ by Molecular Dynamics Simulations Using a Shell Model
   T. Hashimoto and H. Moriwake, J. Phys. Soc. Jpn **90**, 044604 (2021).
   DOI:10.7566/JPSJ.90.044604

HATSUGAI, Yasuhiro [C class; 3600 (B), 700 (C)] (262)
— *Numerical study of bulk-edge correspondence and topological phases: From quantum to classical mechanics*

1. Adiabatic heuristic principle on a torus and generalized Streda formula
   Koji Kudo and Yasuhiro Hatsugai, Phys. Rev. B **102**, 125108 (2020).
   DOI:10.1103/PhysRevB.102.125108

2. Chiral edge modes in game theory: a kagome network of rock-paper-scissors
   Tsuneya Yoshida, Tomonari Mizoguchi, Yasuhiro Hostage, arXiv:2012.05562.

3. Fate of fractional quantum Hall states in open quantum systems: Characterization of correlated topological states for the full Liouvillian
   Tsuneya Yoshida, Koji Kudo, Hosho Katsura, and Yasuhiro Hatsugai, Phys. Rev. Research **2**, 033428 (2020).
   DOI:10.1103/PhysRevResearch.2.033428

4. Mirror skin effect and its electric circuit simulation
   Tsuneya Yoshida, Tomonari Mizoguchi, and Yasuhiro Hatsugai, Phys. Rev. Research **2**, 022062(R) (2020).
   DOI:10.1103/PhysRevResearch.2.022062

5. Higher-order topological phases in a spring-mass model on a breathing kagome lattice
Hiromasa Wakao, Tsuneya Yoshida, Hiromu Araki, Tomonari Mizoguchi, and Yasuhiro Hatsugai, Phys. Rev. B 101, 094107 (2020).

6. Detecting Bulk Topology of Quadrupolar Phase from Quench Dynamics
Tomonari Mizoguchi, Yoshihito Kuno, and Yasuhiro Hatsugai Phys. Rev. Lett. **126**, 016802 (2021).
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7. Machine Learning of Mirror Skin Effects in the Presence of Disorder
Hiromu Araki, Tsuneya Yoshida, and Yasuhiro Hatsugai J. Phys. Soc. Jpn. **90**, 053703 (2021).
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8. Square-root topological phase with time-reversal and particle-hole symmetry
Tsuneya Yoshida, Tomonari Mizoguchi, Yoshihito Kuno, Yasuhiro Hatsugai arXiv: 2103.11305.

9. Bulk-edge correspondence of classical diffusion phenomena
Tsuneya Yoshida Yasuhiro Hatsugai Scientific Reports **11**, 888 (2021)
DOI:10.1038/s41598-020-80180-w

HATTORI, Ken [B class; 500 (B), 100 (C)] (174)
— *Atomic structure and electronic states for silicide films*

HAYAMI, Satoru [C class; 5000 (B), 900 (C)] (202)
— *Search for multiple-Q magnetic orders in systems with bond-dependent anisotropic interactions*
— *Search for square-lattice skyrmion crystal in itinerant electron systems*

1. Magnetic hedgehog lattices in noncentrosymmetric metals
S. Okumura, S. Hayami, Y. Kato, and Y. Motome Phys. Rev. B **101**, 144416 (2020).
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2. Spontaneous antisymmetric spin splitting in noncollinear antiferromagnets without spin-orbit coupling
S. Hayami, Y. Yanagi, and H. Kusunose Phys. Rev. B **101**, 220403(R) (2020).
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3. Nonreciprocal magnons due to symmetric anisotropic exchange interaction in honeycomb antiferromagnets
T. Matsumoto and S. Hayami, Phys. Rev. B **101**, 224419 (2020).
DOI:10.1103/PhysRevB.101.224419

4. Multiple-Q magnetism by anisotropic bilinear-biquadratic interactions in momentum space
S. Hayami, J. Magn. Magn. Mater. **513**, 167181 (2020).
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5. Anomalous Hall effect in κ-type organic antiferromagnets
M. Naka, S. Hayami, H. Kusunose, Y. Yanagi, Y. Motome, and H. Seo Phys. Rev. B **102**, 075112 (2020).
DOI:10.1103/PhysRevB.102.075112

6. Degeneracy Lifting of Neel, Bloch, and Anti-Skyrmion Crystals in Centrosymmetric Tetragonal Systems
S. Hayami and R. Yambe, J. Phys. Soc. Jpn. **89**, 103702 (2020).
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7. Complete Multipole Basis Set for Single-Centered Electron Systems
H. Kusunose, R. Oiwa, and S. Hayami J. Phys. Soc. Jpn. **89**, 104704 (2020).
DOI:10.7566/JPSJ.89.104704

8. Bottom-up design of spin-split and reshaped electronic band structures in spin-orbit-coupling free antiferromagnets: Procedure on the basis of augmented multipoles
S. Hayami, Y. Yanagi, and H. Kusunose Phys. Rev. B **102**, 144441 (2020).
DOI:10.1103/PhysRevB.102.144441

9. Imaging the coupling between itinerant electrons and localised moments in the centrosymmetric skyrmion magnet GdRu2Si2
Y. Yasui, C. J. Butler, N. D. Khanh, S. Hayami, T. Nomoto, T. Hanaguri, Y. Motome, R. Arita, T.-h. Arima, Y. Tokura, and S. Seki Nat. Commun. **11**, 5925 (2020).
DOI:10.1038/s41467-020-19751-4

10. NQR and NMR spectra in odd-parity multipole material CeCoSi
M. Yatsushiro and S. Hayami Phys. Rev. B **102**, 195147 (2020).
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11. Square skyrmion crystal in centrosymmetric itinerant magnets
S. Hayami and Y. Motome, Phys. Rev. B **103**, 0244439 (2021).
DOI:10.1103/PhysRevB.103.024439

12. Noncoplanar multiple-Q spin textures by itinerant frustration: Effects of single-ion anisotropy and bond-dependent anisotropy
S. Hayami and Y. Motome, Phys. Rev. B **103**, 054422 (2021).
DOI:10.1103/PhysRevB.103.054422

13. Modeling a nanometric skyrmion lattice using anisotropic exchange interactions in a centrosymmetric host
M. Hirschberger, S. Hayami, and Y. Tokura New J. Phys. **23**, 023039 (2021).
DOI:10.1088/1367-2630/abdef9

14. Spin-texture-driven electrical transport in multi-Q antiferromagnets
S. Seo, S. Hayami, Y. Su, S. M. Thomas, F. Ronning, E. D. Bauer, J. D. Thompson, S.-Z. Lin and P. F. S. Rosa Commun. Phys. **4**, 58 (2021).
DOI:10.1038/s42005-021-00558-8

HIDA, Kazuo [B class; 500 (B), 150 (C)] (300)
— *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
K. Hida, arXiv:2102.02116, J. Phys. Soc. Jpn. in press.

HIGUCHI, Yuji [C class; 5400 (B), 850 (C)] (242)
— *Large deformation process of amphiphilic molecular aggregate*
— *Self-assemble process of amphiphilic molecules by coarse-grained molecular dynamics simulation*

1. Coarse-grained molecular dynamics simulations of void generation and growth processes in the fracture of the lamellar structure of polyethylene
Y. Higuchi, Phys. Rev. E **103**, 042502 (2021).
DOI:10.1103/PhysRevE.103.042502

2. Rotational Dynamics of Water at the Phospholipid Bilayer Depending on the Head Groups Studied by Molecular Dynamics Simulations
Y. Higuchi, Y. Asano, T. Kuwahara, and M. Hishida, Langmuir **37**, 5329 (2021).
DOI:10.1021/acs.langmuir.1c00417

3. 高分子材料の破壊に関する粗視化シミュレーション
樋口祐次, 分子シミュレーション学会誌「アンサンブル」 **22**, 216-221 (2020).

HINUMA, Yoyo [B class; 800 (B), 0 (C)] (168, 169)
— *Calculation of multication oxide surface properties for catalyst informatics*
— *Search of accessible surfaces for catalyst informatics*

1. Changes in Surface Oxygen Vacancy Formation Energy at Metal/Oxide Perimeter Sites: A Systematic Study on Metal Nanoparticles Deposited on an In2O3(111) Support
Yoyo Hinuma, Takashi Toyao, Nobutsugu Hamamoto, Motoshi Takao, Ken-ichi Shimizu, and Takashi Kamachi, J. Phys. Chem. C 2020, 124, 27621
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2. Surface Oxygen Vacancy Formation Energy Calculations in 34 Orientations of beta-Ga2O3 and theta-Al2O3
Yoyo Hinuma, Takashi Kamachi, Nobutsugu Hamamoto, Motoshi Takao, Takashi Toyao, and Ken-ichi Shimizu, J. Phys. Chem. C 2020, 124, 10509
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HIRATSUKA, Masaki [B class; 400 (B), 100 (C)] ()
— *Estimation of Infrared and Raman spectra using ab initio calculation and machine learning*

HIYAMA, Miyabi [B class; 500 (B), 50 (C)] (308)
— *Theoretical analysis for photo absorption- and emission spectra for firefly bioluminescence related molecules*
— *Theoretical study for caged compound and its conjugate acid/bases*

1. Theoretical Study of the Wavelength Selection for the photocleavage of Coumarin-caged D-luciferin
J. Usukura, M. Hiyama, M. Kurata, Y. Hazama, X-P. Qiu, F. M. Winnik, H. Akiyama, and N. Koga, Photochem. Photobiol. (2020) 96, 805-814

2. Quantum-Mechanical Hydration Plays Critical Role in the Stability of Firefly Oxyluciferin Isomers: State-of-the-art Calculations of the Excited States
Y. Noguchi, M. Hiyama, M. Shiga, H. Akiyama, O. Sugino, J. Chem. Phys. (2020) 153, 201103

HORI, Yuta [B,C class; 3700 (B), 0 (C)] (98)
— *The analysis of the hydrogen-bonding structures in proton-conduction organic crystals*
— *The analysis of the local structures and molecular dynamics in proton-conduction acid-base composites*

HOSHI, Takeo [C class; 4600 (B), 850 (C)] (82, 346)
— *Fusion of computational material science and data-driven science with massively parallel computation*
— *Fusion of computational material science and data-driven science with parallel computation*

1. Development of data-analysis software for total-reflection high-energy positron diffraction (TRHEPD)

K. Tanaka, T. Hoshi, I. Mochizuki, T. Hanada, A. Ichimiya, T. Hyodo, Acta. Phys. Pol. A 137, 188-192 (2020).

2. Two-stage data-analysis method for total-reflection high-energy positron diffraction (TRHEPD)
K. Tanaka, I. Mochizuki, T. Hanada, A. Ichimiya, T. Hyodo, T. Hoshi, JJAP Conf. Series, in press; Preprint: https://arxiv.org/abs/2002.12165

3. Revisiting the Charge-Transfer States at Pentacene/C60 Interfaces with the GW/Bethe–Salpeter Equation Approach
   Takatoshi Fujita, Yoshifumi Noguchi, Takeo Hoshi, Materials 13, 2728/1-15 (2020).

4. An a posteriori verification method for generalized Hermitian eigenvalue problems in large-scale electronic state calculations
   Takeo Hoshi, Takeshi Ogita, Katsuhisa Ozaki, Takeshi Terao J. Comp. Appl. Math. 376, 112830/1-13 (2020).

5. Recent progress in large-scale electronic state calculations and data-driven sciences
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TANAKA, Shu [B class; 400 (B), 100 (C)] (310)
Building Algorithms for Ising Machines

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TANAMOTO, Tetsufumi [B class; 200 (B), 50 (C)] (321)
— *All to all connections in two dimensional qubit array with two-body interactions aiming at quantum annealing machine*

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   T. Tanamoto, M. Ueda, arXiv:1910.05649

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TATENO, Michio [B class; 700 (B), 0 (C)] (293, 295)
— *Coarsening mechanism in mass-conserved reaction diffusion systems*
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TATETSU, Yasutomi [C class; 4600 (B), 850 (C)] (81)
— *First-principles study on grain boundaries in Ga-doped permanent magnets*
— *First-principles study on grain boundaries with multiple subphases in permanent magnets*

1. First-principles study on magnetism of a crystalline grain-boundary phase in Nd–Fe–B permanent magnets
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TERAO, Takamichi [B class; 600 (B), 150 (C)] (290)
— *Molecular simulation of colloidal particles*

1. Wave propagation in double-negative acoustic metamaterial multilayers
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— *first-principles calculation of exchange coupling constants and investigation of interface magnetism for various phases and their interfaces of permanent magnets*

TODO, Synge [C class; 5200 (B), 1500 (C)] (238, 345)
— *Topological Order and Quantum Dynamics in Quantum Many-body Systems*

1. Anisotropic tensor renormalization group
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TOHYAMA, Takami [C class; 3800 (B), 550 (C)] (204)
— *Time-dependent DMRG study of spectral shape in the optical conductivity of Mott insulators*
— *Time-dependent DMRG study of spectral shape in the optical conductivity of two-dimensional Hubbard model*

1. Characterization of photoexcited states in the half-filled one-dimensional extended Hubbard model assisted by machine learning
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T. Sugimoto, K. Morita, and T. Tohyama, Phys. Rev. Research **2**, (2020) 023420.

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TONEGAWA, Takashi [B class; 700 (B), 0 (C)] (291)
— *Numerical Study of the One-Dimensional Quantum Spin Systems with Spatial Structures*

TSUNEYUKI, Shinji [C class; 6600 (B), 1100 (C)] (64)
— *Development of data assimilation method for crystal structure prediction and its application to hydrogen-containing compounds*
— *Prediction of hydrogen function by advanced calculation of solids containing hydrogen*

1. Effect of spin fluctuations on superconductivity in V and Nb: A first-principles study
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常行真司 まてりあ **60** (2021) 176.
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TSURUTA, Kenji [C class; 1200 (B), 700 (C)] (134)
— *Hybrid Ab-Initio/Machine-Learning Optimization of Nano Interfaces and Molecular Structures*

1. Characterization of the Σ5(210) / [001] Grain Boundary of Methyl-Ammonium Lead Triiodide Perovskite using Density Functional Theory
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UCHIDA, Takashi [B class; 200 (B), 100 (C)] (320)
— *Multiple helical spin density waves in inversion-symmetric itinerant magnets*
— *Multiple-Q states in two-dimensional itinerant magnets*

UMEMOTO, Koichiro [B,C class; 2300 (B), 450 (C)] (124, 126)
— *First principles study of effect of Al impurity on the post-post-perovskite transitions*
— *Order-disorder transition in ultrahigh-pressure phase of the Na-Mg-F system*

WATANABE, Haruki [B class; 800 (B), 200 (C)] ()
— *Comprehensive material search based on symmetry indicators*

WATANABE, Hiroshi [B class; 1000 (B), 150 (C)] (281)
— *Code Optimization using Machine Learning on Parallel Computer*
— *Molecular Dynamics Study of Crown Formation During the Splash*

WATANABE, Hiroshi [B class; 300 (B), 0 (C)] (218)
— *Study for stripe order and superconductivity in high-T_c cuprates by variational Monte Carlo method*

WATANABE, Satoshi [C class; 9200 (B), 1300 (C)] (56)
— *Analyses related to atomic structures and atom dynamics at complex structures such as surfaces interfaces and defects*

1. Straintronic effect for superconductivity enhancement in Li-intercalated bilayer MoS_2
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   N. H. Shimada, E. Minamitani, and S. Watanabe, J. Phys. Condensed Matter **32**, 435002 (2020).
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7. ニューラルネットワークを用いた原子間ポテンシャルの材料科学における応用事例
清水康司, 渡邉聡, 日本神経回路学会誌 **28**, 3 (2021).
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8. Tuning the Schottky Barrier Height at the Interfaces of Metals and Mixed Conductors
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YAMADA, Atsuo [C class; 2000 (B), 750 (C)] (123)
— *First principles analyses on novel materials for secondary batteries*

1. Theoretical analysis of electrode-dependent interfacial structures on hydrate-melt electrolytes
N. Takenaka, T. Inagaki, T. Shimada, Y. Yamada, A. Yamada J. Chem. Phys. **152**, 124706 (2020).
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YAMADA, Atsushi [C class; 0 (B), 200 (C)] (219)
— *Studies of the superconductivity and magnetic states in the strongly correlated electron systems using Hubbard models.*

YAMADA, Masahiko [B class; 300 (B), 50 (C)] (317)
— *Numerical simulation of the spin Seebeck effect in Kitaev spin liquids*

YAMAGUCHI, Naoya [B,C class; 1000 (B), 150 (C)] (150)
— *First-principles Analysis of Band Dispersion in Bulk Insulators/Semiconductors Under Finite Electric Fields by Using the LCPAO Method*
— *First-principles Calculation of Electric Field Effects in Spin-to-charge Conversion Materials*

1. Simple Model for Corrugation in Surface Alloys Based on First-Principles Calculations
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YAMAJI, Youhei [E class; 19000 (B), 3000 (C)] (187, 188)
— *Numerical studies of quantum spin liquid candidates by highly accurate ab initio effective hamiltonians*
— *Numerical studies of quantum spin liquids by quantum mutual information*

YAMASHITA, Tomoki [C class; 3000 (B), 600 (C)] (99)
— *Development of surface and interface structure prediction methods*

1. CrySPY: a crystal structure prediction tool accelerated by machine learning
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YAMAUCHI, Kunihiko [C class; 4400 (B), 650 (C)] (87)
— *First-principles electronic structure calculations of non-centrosymmetric antiferromagnets*

1. Impact of Inter-site Spin-Orbit Coupling on Perpendicular Magnetocrystalline Anisotropy in Cobalt-Based Thin Films
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YANAGISAWA, Susumu [C class; 4600 (B), 350 (C)] (91)
— *First-principles investigation on the electronic properties of polymer organic semiconductors*
— *First-principles theoretical study on the electronic structure and interface gap states of organic semiconductor polymers*

1. Quantitative analysis of the electrostatic and electronic polarization energies in molecularly mixed films of organic semiconductors
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YANAGISAWA, Takashi [B class; 600 (B), 150 (C)] (216)
— *Numerical study of strongly correlated electron systems*
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1. Phase diagram of cuprate high-temperature superconductors based on the optimization Monte Carlo method
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    T. Yanagisawa Prog. Theor. Exper. Phys. 2021 (2021) 033A01

YASUDA, Chitoshi [B class; 900 (B), 150 (C)] (282)
— *Magnetism in the multiple-spin exchange model on the honeycomb lattice*

YOKO, Akira [B,C class; 5100 (B), 650 (C)] (78)
— *First-principles calculation for low-temperature oxygen transfer in metal oxide*
— *First-principles calculation of oxygen storage capacity and structural distortion of metal doped cerium oxide*
— *Oxidative reaction of CH_4 on CeO_2 (100)*

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; 7200 (B), 0 (C)] (199)
— *Bulk-edge correspondence for non-Hermitian topological systems*
— *Correlation effects on non-Hermitian topological states*

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2. Fate of fractional quantum Hall states in open quantum systems: Characterization of correlated topological states for the full Liouvillian
   Tsuneya Yoshida, Koji Kudo, Hosho Katsura, and Yasuhiro Hatsugai, Phys. Rev. Research **2**, 033428 (2020).
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   Tsuneya Yoshida, Tomonari Mizoguchi, Yasuhiro Hatsugai, arXiv:2012.05562.

4. Real-space dynamical mean field theory study of non-Hermitian skin effect for correlated systems: Analysis based on pseudospectrum
   Tsuneya Yoshida, Phys. Rev. B **103**, 125145 (2021).
   DOI:10.1103/PhysRevB.103.125145

5. Bulk-edge correspondence of classical diffusion phenomena
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6. Exceptional points in the one-dimensional Hubbard model
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7. Square-root topological phase with time-reversal and particle-hole symmetry
   Tsuneya Yoshida, Tomonari Mizoguchi, Yoshihito Kuno, Yasuhiro Hatsugai arXiv: 2103.11305.

8. Machine Learning of Mirror Skin Effects in the Presence of Disorder
   Hiromu Araki, Tsuneya Yoshida, and Yasuhiro Hatsugai J. Phys. Soc. Jpn. **90**, 053703 (2021).
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YOSHIDOME, Takashi [C class; 800 (B), 450 (C)] (276, 277)
— *A Method for Analyzing Protein Dynamics: A Hybrid of Cryo-Electron Microscopy Experiment and Molecular Simulation*
— *A theoretical study for thermal unfolding of proteins with quite similar native structure*

1. F1-ATPase Rotation and Its Inhibition from the Viewpoint of Solvent Entropy
   T. Yoshidome, Chemical Physics Letters, **757**, 137886/1-6 (2020).

YOSHIOKA, Nobuyuki [B class; 500 (B), 50 (C)] (305)
— *Developing numerical tool for open quantum dynamics based on neural networks*

1. Neural-Network Quantum States for the Electronic Structure of Real Solids
   N. Yoshioka, W. Mizukami, and F. Nori, submitted to Communications Physics

2. Purifying Deep Boltzmann Machines for Thermal Quantum States
   Y. Nomura, N. Yoshioka, and F. Nori, submitted to Phys. Rev. Lett.

○ 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 calculation in metal-intercalated graphene*

ARUGA, Tetsuya [A class; 100 (B), 50 (C)] (351)
— *Electronic structure and interaction at the interface of π-electron organic molecules and metals*

CHIBA, Takahiro [A class; 100 (B), 50 (C)] ()
— *Band structure and spin texture of Bi-Te/ferromagnetic-metal interface*

GONOME, Hiroki [A class; 100 (B), 50 (C)] ()
— *Study of the principle of photothermal conversion by ab initio calculations*

HATANO, Naomichi [A class; 100 (B), 50 (C)] ()
— *Molecular Dynamics Calculation of Non-equilibrium Steady State in Systems with Temperature Gradient*

HATTORI,Ken [A class; 100 (B), 0 (C)] (174, 356)
— *Atomic structure and electronic states for silicide films*

ISHIBASHI, Shoji [A class; 100 (B), 50 (C)] (167, 361)
— *Prediction of properties of organic ferroelectrics and piezoelectrics by first-principles calculation*

ISHIKAWA, Ryo [A class; 100 (B), 50 (C)] ()
— *First-principles calculation on charged defects in α-Al_2O_3*

KOTA, Yohei [A class; 100 (B), 50 (C)] ()
— *Analysis of N-doping effect on electronic structure in antiferromagnetic Cr*

1. Mechanism of highly sensitive strain response in antiferromagneitc chromium
   Yohei Kota, Eiji Niwa, and Masayuki Naoe, Journal of Applied Physics **129**, 203901 (2021)
   DOI:10.1063/5.0045728

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

OHTO, Tatsuhiko [A class; 100 (B), 0 (C)] (127, 381)
— *First-principles transport calculations for molecular junctions*

SAKAI, Masatoshi [A class; 100 (B), 50 (C)] (217, 386)
— *Excess carrier dependent electronic state in organic charge order phase*

SATO, Taku [A class; 100 (B), 50 (C)] (387)
— *Magnetic excitations in the quantum pyrochlore magnet*

TANUMA, Yasunari [A class; 100 (B), 50 (C)] ()
— *Study on numerical analysis method of superconducting junctions with broken time reversal symmetry states*

TOKUMOTO, Yuki [A class; 100 (B), 50 (C)] ()
— *Exploring dopants to improve bulk-insulation of Pb-based topological insulators*

YAMASHITA, Tomoki [A class; 100 (B), 0 (C)] (99, 400)
— *Development of surface and interface structure prediction methods*

YAMATO, Takahisa [A class; 100 (B), 50 (C)] (325)
— *Non-uniform thermal transport properties in proteins*

1. Energy transfer across nonpolar and polar contacts in proteins: role of equilibrium fluctuations
P. Humanath, K. M. Reid, T. Yamato, and D. M. Leitner, J. Phys. Chem. B. **124**, 9852 (2020).
DOI:10.1021/acs.jpcb.0c08091

YOSHIZAWA, Kanako [A class; 100 (B), 50 (C)] ()
— *Performance measurement of Quantum ESPRESSO*

□ SCCMS Projects

FUJITA, Takatoshi [5500 (B), 0 (C)] (330)
— *Investigation of charge photogeneration process in organic thin film solar cells by large-scale GW/Bethe-Salpeter equation method*
— *Computational Investigation of Charge Photogeneration in Organic Solar Cells by Fragment-Based GW/BSE Method*

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   Kanazawa University, 2020-09

2. **ASAD, Md. Abdullah Al**
   First Principles Study on Water Intercalated Grain Boundary of Methyl Ammonium Lead Iodide Perovskite
   Okayama University, 2020-09

3. **FUKUI, Kiyu**
   Functional Renormalization Group Study on Kitaev Quantum Spin Liquid
   The University of Tokyo, 2021-03

4. **GUO, Jiang**
   Optimal design of spectrally selective photonic structures for thermal radiation applications
   The University of Tokyo, 2021-03

5. **HWANG, Jaekyun**
   Material Property Predictions and Discovery Using a Novel Descriptor "Elemental Fingerprints" with Neural Networks
   The University of Tokyo, 2021-03

6. **ISHIKAWA, Fumihiro**
   Exploration of Classical Integrable Systems Assisted by Neural Networks
   The University of Tokyo, 2021-03

7. **JANG, Seonghoon**
   Materials design of *f*-electron based Kitaev-type magnets
   The University of Tokyo, 2020-09

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   Topological invariants and adiabatic principle in correlated systems
   University of Tsukuba, 2021-03

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   Theoretical Study on Electric Field Control of Magnetism in 2D Materials
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    The University of Tokyo, 2020-09

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Theoretical near-field vibrational spectroscopy
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First-Principles calculations of spin-polarized cation vacancies in wide-gap semiconductors
Kanazawa University, 2021-03

16. **YASSIN, Abdulrahman Hikmat Basher**
Mechanisms of Thermal Atomic Layer Etching (ALE) for Metals
Osaka University, 2020-08

17. **YOSHIKAWA, Seiji**
A Noise-Robust Data Assimilation Method for Crystal Structure Predictions Using Powder Diffraction Intensity
The University of Tokyo, 2021-03

□ Master Theses

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   Numerical study of two-dimensional quantum dimer model
   The University of Tokyo, 2020-09

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   Classical ground states of the multiple-spin exchange model in a magnetic field on a honeycomb lattice
   University of the Ryukyus, 2021-03

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   Density Functional Theory Study of Surface States at Noble Metal Surfaces
   Osaka University, 2021-03

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   Theoretical approach for understanding group-III nitride device structures
   The University of Tokyo, 2020-09

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   First-principles Study of the Oxidative Etching Mechanism of the Diamond (100) Surface
   Osaka University, 2020-09

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   Non-uniform thermal transport in proteins
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   Numerical Study on the Magnetization Process of the Heisenberg Antiferromagnet on the Floret Pentagon Lattice
   University of Hyogo, 2021-3

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First-principles study of two photon absorption spectra in perovskite semiconductors
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Microscopic Origin of Stable High-Temperature Superconductivity in Multilayer Copper Oxides
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Material design of α-SrSi2 based on theoretical calculations snd structural and electronic properties of Mg2Si doped with Sb and Zn by synchrotron radiation analysis
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Nagoya University, 2021-03

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First-principles analyses of strain effects on properties of layered transition-metal dichalcogenides
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Monte Carlo study of the multiple-spin exchange model in a magnetic field on a honeycomb lattice
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Machine Learning Construction of Electron-Temperature-Dependent Interatomic Potential
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Theoretical study for ground-state properties of the Heisenberg antiferromagnet on the the Cairo Pentagon lattice
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Stability of TiAl-based multicomponent alloys from first principles
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30. **NISHINO, Koki**
Analyses of thermal transport properties of carbon-based materials using neural Network Potentials
The University of Tokyo, 2021-03

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Electronic state analysis of organic molecules in angle-resolved photoelectron spectroscopy
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First-principles study of diffusion and distribution of oxygen vacancies in metal oxides
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Dynamical Variational Monte Carlo Approaches for Excitation Spectra of Many-Body Fermions in Continuum Space
The University of Tokyo, 2021-03

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First-principles calculation of effects on PdZn surface by intermediates of methanol steam reforming
Kagoshima University, 2021-03

35. **SEO, Insung**
First-principles study on iridium loss at high temperatures
Tokyo Institute of Technology, 2020-9

36. **SHIMAZU Ryoma**
First-principles Calculation of Topological Insulator Hetero Structure with Spin Splitting Bands
Osaka University, 2021-03

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Theoretical study on control of topological spin textures based on spin moire picture
The University of Tokyo, 2021-03

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Local Atomic Structures and Magnetic Properties of Mn doped ZnSnAs2

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Rational design of the peptide inhibitor targeting the interaction of the KIX domain of the transcriptional coactivator CBP with transcriptional activators
The University of Tokyo, 2021-03

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Interaction of diamond and alkali metals and its application
Hokkaido University, 2021-03

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