

## **4 PUBLICATION LIST**

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## □ ISSP Joint Research Projects

**ADACHI, Takahiro** [ C class; 500 (B) ] (319)

— *Heat Transfer Characteristics of Condensate/Evaporate Film Flow along Vertical Plates with Microscopic Grooves*

**AKAGI, Kazuto** [ C class; 4500 (B) ] (99)

— *Exploration of structure motifs characterizing the metal oxides*

1. Interactions of hydrogen with amorphous hafnium oxide  
M. Kaviani et al.: Phys. Rev. B **95** (2017) 075117.
1. First-principles investigation of local structure deformation induced by x-ray irradiation in  $\kappa$ -(BEDT-TTF)<sub>2</sub>Cu[N(CN)<sub>2</sub>]Br  
L.J. Kang et al.: Phys. Rev. B **95** (2017) 214106.
1. Dopant Clustering in Oxygen-Deficient Rh<sup>3+</sup>:SrTiO<sub>3- $\delta$</sub>  Visible-Light Photocatalyst  
M. Lippmaa et al.: J. Am. Chem. Soc., submitted.

**AKAI, Hisazumi** [ B class; 1400 (B) ] (137,139)

— *Electronic structure of light rare earth permanent magnets*

1. Atomistic-model study of temperature-dependent domain walls in the neodymium permanent magnet Nd<sub>2</sub>Fe<sub>14</sub>B  
Masamichi Nishino, Yuta Toga, Seiji Miyashita, Hisazumi Akai, Akimasa Sakuma, and Satoshi Hirose: Phys. Rev. B **95**, 094429/17 (2017).
2. L-edge resonant magneto-optical Kerr effect of a buried Fe nanofilm  
Y. Kubota, M. Taguchi, H. Akai, Sh. Yamamoto, T. Someya, Y. Hirata, K. Takubo, M. Araki, M. Fujisawa, K. Yamamoto, Y. Yokoyama, S. Yamamoto, M. Tsunoda, H. Wadati, S. Shin, and I. Matsuda: Phys. Rev. B **96**, 134432/16 (2017).
3. Determination of the element-specific complex permittivity using a soft x-ray phase modulator  
Y. Kubota, Y. Hirata, J. Miyawaki, S. Yamamoto, H. Akai, R. Hobara, Sh. Yamamoto, K. Yamamoto, T. Someya, K. Takubo, Y. Yokoyama, M. Araki, M. Taguchi, Y. Harada, H. Wadati, M. Tsunoda, R. Kinjo, A. Kagamihata, T. Seike, M. Takeuchi, T. Tanaka, S. Shin, and I. Matsuda: Phys. Rev. B **96**, 214417/16 (2017).
4. Quantum Theory of Rare-Earth Magnets  
T. Miyake and H. Akai: J. Phys. Soc. Jpn **87**, 041009-110 (2018).
5. First-principles study of intersite magnetic couplings and Curie temperature in RFe<sub>12-x</sub>Cr<sub>x</sub> (R = Y, Nd, Sm)  
T. Fukazawa, H. Akai, Y. Harashima, and T. Miyake: J. Phys. Soc. Jpn **87**, 044706/15 (2018).
6. Maximum performance of permanent magnet materials  
H. Akai: Scripta Materialia (2018) in press.
7. First-principles calculation of transition-metal Seebeck coefficients

S. Kou and H. Akai: Solid State Commun. **296**, 15 (2018).

**AKASHI, Ryosuke** [ C class; 5500 (B) ] (85)

— *Exploration of hydrogen-1s metallic state and superconductivity in oxyhydride compounds*

1. Weak Phonon-mediated pairing in BiS<sub>2</sub> superconductor from first principles  
C. Morice, R. Akashi, T. Koretsune, S. S. Saxena, and R. Arita: Phys. Rev. B **95**, (2017) 180505(R).
2. Refined phase diagram of the H-S system with high-T<sub>c</sub> superconductivity  
I. Kruglov, R. Akashi, S. Yoshikawa, A. R. Oganov, and M. M. D. Esfahani: Phys. Rev. B **96**, (2017) 220101(R).

**AMAMOTO, Yoshifumi** [ B class; 600 (B) ] ( )

— *Polymer Fatigue Revealed by Molecular Dynamic Simulation*

**AOYAMA, Kazushi** [ B class; 1200 (B) ] (298)

— *Spin-lattice-coupling effects in pyrochlore antiferromagnets*

— *Theoretical study of dynamical spin correlations in frustrated magnets*

**ARAI, Munehito** [ B class; 1300 (B) ] (296)

— *Computational rational design of novel binding proteins*

— *Folding mechanisms of the bioactive proteins essential for regenerative medicine*

**ARAIDAI, Masaaki** [ C class; 4500 (B) ] (98)

— *Electronic States and Thermodynamic Stability of Two-Dimensional Crystals of Group IV Elements*

1. First-principles study on adsorption structure and electronic state of stanene on  $\alpha$ -alumina surface  
M. Araidai, M. Kurosawa, A. Ohta, K. Shiraiishi: Jpn. J. Appl. Phys. **56** (2017) 095701.

**ARAKAWA, Naoya** [ B class; 700 (B) ] (312)

— *Microscopic theory of magnon physics in a three-dimensional chiral magnet*

1. Magnon Dispersion and Specific Heat of Chiral Magnets on the Pyrochlore Lattice  
N. Arakawa: Journal of Physical Society of Japan, **86** (2017) 094705.
2. Weak localization of magnons in a disordered two-dimensional antiferromagnet  
N. Arakawa and J. Ohe: Phys. Rev. B **97** (2018) 020407(R).
3. Negative magnetothermal resistance in a disordered two-dimensional antiferromagnet  
N. Arakawa and J. Ohe: Phys. Rev. B **96** (2017) 214404.
4. Tunneling between chiral magnets: Spin current generation without external fields  
N. Arakawa: Phys. Rev. B **95** (2018) 235438.

**ARAKI, Takeaki** [ B class; 700 (B) ] (311)

— *Conformational changes of polyelectrolyte chains in solvent mixtures*

1. Colloidal suspensions in one-phase mixed solvents under shear flow  
A. Barbot and T. Araki: Soft Matter **13** (2017), 5911.

**ASAI, Yoshihiro** [ C class; 5500 (B) ] (83)

— *Theoretical and first principle studies of non-equilibrium transport properties of strongly correlated materials*

1. Resistive switching mechanism of GeTeSb<sub>2</sub>Te<sub>3</sub> interfacial phase change memory and topological properties of embedded two-dimensional states  
Hisao Nakamura, Ivan Rungger, Stefano Sanvito, Nobuki Inoue, Junji Tominaga and Yoshihiro Asai: Nanoscale **9** (2017) 9836.
2. Bandgap Engineering in OH- Functionalized Silicon Nanocrystals: Interplay between Surface Functionalization and Quantum Confinement  
Marius Bürkle Mickaël Lozač Calum McDonald Davide Mariotti Koji Matsubara Vladimir Švrček: Adv. Funct. Mater. **27** (2017) 1701898.

**EGAMI, Yoshiyuki** [ C class; 2000 (B) ] (131)— *Development and application of time-dependent electron-transport simulator based on first-principles method*

1. First-principles study on electron transport through BN-dimer embedded zigzag carbon nanotubes  
Y. Egami and H. Akera: *Physica E* **88** (2017) 212.
2. Controlling Rashba spin-orbit interaction in quantum wells by adding symmetric potential  
Y. Egami and H. Akera: *Appl. Phys. Express* **10** (2017) 063007.
3. ニッケルおよび無電解ニッケルの超精密切削加工におけるダイヤモンド工具の損耗機構  
宇田 豊, 名越 将大, 宇治宮 俊樹, 本田 素郎, 江上 喜幸, 田中 宏明, 古城 直道, 島田 尚一: *精密工学* 会誌 **83** (2017) 762.a
4. First-principles study on electron transport through Mn(dmit)<sub>2</sub> molecular junction depending on relative angle between ligands  
Y. Egami and M. Taniguchi: *Jpn. J. App. Phys.* **57** (2018) 021601.

**FUCHIZAKI, Kazuhiro** [ C class; 5500 (B) ] (252)— *Melting phenomena and polymorphism*

1. Pressure-induced structural change in liquid GeI<sub>4</sub>  
K. Fuchizaki, H. Nishimura, T. Hase, and H. Saitoh: *J. Phys.: Condens. Matter* **30** (2018) 045401.
2. An effective way to determine the melting curve  
K. Okamoto and K. Fuchizaki: *Molecular Simulation* **44** (2018) 384.

**FUJIKWA, Sachie** [ C class; 1000 (B) ] ()— *Study of band structure for InSbN based dilute nitride semiconductor by using first-principle simulation***FUJIMOTO, Yoshitaka** [ C class; 500 (B) ] (159)— *First-principles study of atomic structures, stabilities, and electronic properties of atomic-layered materials*

1. Formation and physical properties of h-BN atomic layers: A first-principles density-functional study  
Y. Fujimoto: *Nanomaterials and Nanotechnology* **2017**, 2676432 (2017).
2. First-principles theoretical investigation of graphene layers for sensor applications: A review  
Y. Fujimoto: *Nanomaterials and Nanotechnology* **7**, 1 (2017).
3. First-Principles Computational Analysis of Nanocomposite for Detecting Environmental Polluting Gas  
Y. Fujimoto: *New Polymer Nanocomposites for Environmental Remediation* (Elsevier 2018) Chapter 9, p.207.
4. Gas adsorption effects on the stabilities, electronic structures and scanning tunneling microscopy of graphene monolayers doped with B or N  
Y. Fujimoto and S. Saito: submitted.

**FUKUDA, Jun-Ichi** [ B class; 1900 (B) ] (283)— *Calculation of ordered structures and their optical properties of soft materials*

1. Spontaneous formation and dynamics of half-Skyrmions in a chiral liquid-crystal film  
A. Nych\*, J. Fukuda\*, U. Ognysta, S. Žumer and I. Mušević: *Nature Phys.* **13** (2017) 1215
2. Reflection spectra and near-field images of a liquid crystalline half-Skyrmion lattice  
J. Fukuda and S. Žumer: *Opt. Exp.* **26** (2018) 1174.
3. Numerical calculation of Kossel diagrams of cholesteric blue phases  
J. Fukuda, Y. Okumura and H. Kikuchi: *Proc. SPIE* **10555** (2018) 105550A

**FUKUI, Ken-Ichi** [ C class; 3000 (B) ] (274)— *Analysis on Structuring and Dynamics of Electrolyte Solutions Forming Electric Double Layer at Electrode Interfaces*

1. Computational investigations of electronic structure modifications of ferrocene-terminated self-assembled monolayers: Effects of electron donating/withdrawing functional groups attached on ferrocene moiety

Y. Yokota, S. Akiyama, Y. Kaneda, A. Imanishi, K. Inagaki, Y. Morikawa and K. Fukui: Phys. Chem. Chem. Phys., 19, 32751-32722 (2017).

2. Structural and dynamic properties of 1-butyl-3-methyl-imidazolium bis(trifluoromethanesulfonyl)imide / mica and graphite interfaces revealed by molecular dynamics simulation  
Y. Yokota, H. Miyamoto, A. Imanishi, K. Inagaki, Y. Morikawa, K. Fukui: Phys. Chem. Chem. Phys., 20, 6668-6676 (2017).

**FUKUMOTO, Yoshiyuki** [ B class; 600 (B) ] (313)

— *A series expansion study on the magnon spectrum of a kagome antiferromagnet in  $Cs_2Cu_3SnF_{12}$*

1. Impact of Dzyaloshinsky-Moriya Interactions and Tilts of the  $g$  Tensors on the Magnetization Process of a Spherical Kagomé Cluster in  $\{W_{72}V_{30}\}$   
Y. Fukumoto, Y. Yokoyama, and H. Nakano: submitted to J. Phys. Soc. Jpn. (arXiv:1803.06485).

**GOHDA, Yoshihiro** [ C class; 6000 (B) ] (77)

— *First-principles calculations of magnetic ultrathin films on surfaces*

1. Prediction of ferromagnetism in MnB and MnC on nonmagnetic transition-metal surfaces studied by first-principles calculations  
S. Nakamura and Y. Gohda: Phys. Rev. B **96**, 245416 (2017).
2. Electron Theory on Grain-Boundary Structures and Local Magnetic Properties of Neodymium Magnets  
Y. Gohda, Y. Tatetsu, and S. Tsuneyuki: Mater. Trans. **59**, 332 (2018).
3. ネオジム磁石の粒界構造と局所磁性の電子論  
合田 義弘、立津 慶幸、常行 真司: 日本金属学会誌 **81**, 26 (2017).

**HAGITA, Katsumi** [ E class; 18000 (B) ] (210)

— *Coarse grained MD simulation for fracture and reinforcement of polymer materials*

1. Thinning approximation for two-dimensional scattering patterns from coarse-grained polymer melts under shear flow  
K. Hagita, T. Murashima, H. Takano, and T. Kawakatsu, J. Phys. Soc. Jpn. **86** (2017) 124803.
2. 分子動力学シミュレーションによるフェノール樹脂の架橋構造モデリングと構造の解析  
首藤靖幸, 和泉篤士, 萩田克美, 中尾俊夫, 柴山充弘, ネットワークポリマー **38** (2017) 136-143.
3. 粗視化分子動力学シミュレーションによるフェノール樹脂架橋ネットワーク構造のモデリングと応力歪解析  
和泉篤士, 首藤靖幸, 萩田克美, 柴山充弘, ネットワークポリマー **38** (2017) 226-231.
4. Filler network model of filled rubber materials to estimate system size dependence of two-dimensional small-angle scattering patterns  
K. Hagita, T. Tominaga, T. Hatazoe, T. Sone, and H. Takano, J. Phys. Soc. Jpn. **87** (2018) 014802.
5. Large-scale reverse Monte Carlo analysis for the morphologies of silica nanoparticles in end-modified rubbers based on ultra-small-angle X-ray scattering data  
K. Hagita, T. Tominaga, and T. Sone, Polymer **135** (2018) 219-229.
6. ディープラーニングを用いたゴム中フィラー凝集構造の画像判別の特長評価  
萩田克美, 富永哲雄, 曾根卓男, 高橋一郎, Lee Chonho, 荻野正雄, 日本ゴム協会誌 **91** (2018.1) 3-8.
7. Molecular dynamics simulations of cross-linked phenolic resins using a united-atom model  
A. Izumi, Y. Shudo, K. Hagita, and M. Shibayama, Macromolecular Theory and Simulations (2018) in press. Super resolution for asymmetric resolution of FIB-SEM 3D imaging of silica nanoparticles in SBR K. Hagita, T. Higuchi, H. Jinnai, Scientific reports, **8** (2018) 5877.

**HAMADA, Ikutaro** [ C class; 4000 (B) ] (109)

— *van der Waals density functional theory study of molecular adsorption on solid surfaces*

**HAMAMOTO, Yuji** [ C class; 2500 (B) ] (122)

— *First principles study of Pt clusters adsorbed on graphene edges*

**HARADA, Kenji** [ C class; 6000 (B) ] (244)

— *Numerical study of non-equilibrium systems*

1. Entanglement branching operator  
K. Harada: Phys Rev B 97, 045124 (2018).

**HASHIMOTO, Tamotsu** [ C class; 4000 (B) ] (269)

— *Molecular dynamics simulation of ferroelectrics using a shell model III*

**HASHMI, Arqum** [ C class; 1000 (B) ] ()

— *Discovery of new 2D semiconductors*

**HATSUGAI, Yasuhiro** [ C class; 4500 (B) ] (264)

— *Numerical studies of bulk-edge correspondence in topological phases*

1. Many-Body Chern Numbers of  $\nu = \frac{1}{3}$  and  $\frac{1}{2}$  States on Various Lattices  
Hiromu Araki, Toshikaze Kariyado, Takahiro Fukui, Yasuhiro Hatsugai: Journal of the Physical Society of Japan, 86, 103701 (2017).
2. Entanglement Chern number for three-dimensional topological insulators: Characterization by Weyl points of entanglement Hamiltonians  
Hiromu Araki, Takahiro Fukui, and Yasuhiro Hatsugai: Phys. Rev. B 96, 165139/1-8 (2017).
3. Fractional Quantum Hall Effect in  $n = 0$  Landau Band of Graphene with Chern Number Matrix  
Journal of the Physical Society of Japan, to appear

**HATTORI, Kazumasa** [ C class; 2500 (B) ] (277)

— *XY model on a diamond lattice: effects of frustration*

**HATTORI, Ken** [ B,C class; 4600 (B) ] (89)

— *Model calculations in Si surfaces with adsorbates*

**HAYAMI, Satoru** [ C class; 2500 (B) ] (195)

— *Skyrmion crystal phase in itinerant magnets with spin-orbit coupling*

1. Effective bilinear-biquadratic model for noncoplanar ordering in itinerant magnets  
S. Hayami, R. Ozawa, and Y. Motome: Phys. Rev. B **95** (2017) 224424.
2. Shape of magnetic domain walls formed by coupling to mobile charges  
R. Ozawa, S. Hayami, K. Barros, and Y. Motome: Phys. Rev. B **96** (2017) 094417.
3. Manipulating magnetoelectric effect – Essence learned from  $\text{Co}_4\text{Nb}_2\text{O}_9$   
Y. Yanagi, S. Hayami, and H. Kusunose: Phys. Rev. B **97** (2018) 020404.
4. Emergent odd-parity multipoles and magnetoelectric effects on a diamond structure: implication to 5d transition metal oxides  $\text{AOsO}_4$  ( $A = \text{K, Rb, and Cs}$ )  
S. Hayami, H. Kusunose, and Y. Motome: Phys. Rev. B **97** (2018) 024414.
5. Microscopic Description of Electric and Magnetic Toroidal Multipoles in Hybrid Orbitals  
S. Hayami and H. Kusunose: J. Phys. Soc. Jpn. **87** (2018) 033709.
6. Néel- and Bloch-Type Magnetic Vortices in Rashba Metals  
S. Hayami and Y. Motome: submitted to Phys. Rev. Lett.

**HIDA, Kazuo** [ B class; 500 (B) ] (317)

— *Numerical Study of One Dimensional Frustrated Quantum Spin Systems*

1. Partial Ferrimagnetism in  $S=1/2$  Heisenberg Ladders with a Ferromagnetic Leg, an Antiferromagnetic Leg, and Antiferromagnetic Rungs  
K. Sekiguchi and K. Hida: J. Phys. Soc. Jpn. **86**, 084706 (2017)

**HIGUCHI, Yuji** [ C class; 4000 (B) ] (268)

— *Deformation and fracture dynamics of crystalline polymers by large-scale coarse-grained molecular dynamics simulation*

**HINOKIHARA, Taichi** [ C class; 4000 (B) ] (267)

— *Analysis of magnetization reversal process based on atomistic models*

1. Explorations of the effects of dipole-dipole interactions in Nd<sub>2</sub>Fe<sub>14</sub>B thin films based on a stochastic cutoff method with a novel efficient algorithm  
T. Hinokihara, M. Nishino, Y. Toga, and S. Miyashita: Phys. Rev. B **97** (2018) 104427.

**HINUMA, Yoyo** [ B class; 600 (B) ] (158)

— *Finding the ground state of prussian blue derivatives*

**HIRATSUKA, Masaki** [ B class; 600 (B) ] ( )

— *ab initio calculations to determine the phase equilibrium conditions of semicathrate hydrates*

**HIYAMA, Miyabi** [ B class; 700 (B) ] (310)

— *Theoretical study for excited states of bioluminescence related molecules*

1. Theoretical insights into the effect of pH values on oxidation processes in the emission of firefly luciferin in aqueous solution  
M. Hiyama, H. Akiyama and N. Koga: Luminescence: The Journal of Biological and Chemical Luminescence, **32** (2017) 1100.
2. Effect of dynamical fluctuations of hydration structures on the absorption spectra of oxyluciferin anions in aqueous solution  
M. Hiyama, M. Shiga, N. Koga, O. Sugino, H. Akiyama and Y. Noguchi: Phys. Chem. Chem. Phys. **19** (2017) 10028.

**HOSHI, Takeo** [ C,E class; 15500 (B) ] (45)

— *Large-scale device-material research by massively parallel electronic structure calculation and data science*

1. Efficient methods for computing integrals in electronic structure calculations  
Hisashi Kohashi, Kosuke Sugita, Masaaki Sugihara and Takeo Hoshi: JSIAM Letters 9, 81-84 (2017).
2. Solution of the k-th eigenvalue problem in large-scale electronic structure calculations  
Dongjin Lee, Takeo Hoshi, Tomohiro Sogabe, Yuto Miyatake, Shao-Liang Zhang, submitted; Preprint (<http://arxiv.org/abs/1710.05134>)

**HOSHINO, Shintaro** [ C class; 4000 (B) ] (191)

— *Quantum Monte Carlo approach to local electronic correlations in unconventional superconductors*

1. Spontaneous Orbital-Selective Mott Transitions and the Jahn-Teller Metal of A3C60  
S. Hoshino and P. Werner: Phys. Rev. Lett. 118, 177002 (2017)a
2. Fan-type spin structure in uni-axial chiral magnets  
Misako Shinozaki, Shintaro Hoshino, Yusuke Masaki, A N Bogdanov, A O Leonov, Junichiro Kishine, Yusuke Kato: arXiv:1705.07778 (2017)
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P. Werner, H.U.R. Strand, S. Hoshino, M. Eckstein: Phys. Rev. B 95, 195405 (2017)
4. Field-Induced Transitions in Anisotropic Kondo Lattice - Application to CeT<sub>2</sub>Al<sub>10</sub> -  
T. Kikuchi, S. Hoshino, N. Shibata, Y. Kuramoto: J. Phys. Soc. Jpn. 86, 094602 (2017)a
5. Theory of the magnetic skyrmion glass  
S. Hoshino and N. Nagaosa: Phys. Rev. B 97, 024413 (2018)
6. Enhanced pairing susceptibility in a photodoped two-orbital Hubbard model  
P. Werner, H.U.R. Strand, S. Hoshino, Y. Murakami, M. Eckstein: Phys. Rev. B 97, 165119 (2018)

**HOTTA, Takashi** [ C class; 4500 (B) ] (188)

— *Two-channel Kondo effect and multipole susceptibility*

1. Two-Channel Kondo Effect Emerging from Nd Ions  
Takashi Hotta: J. Phys. Soc. Jpn. **86** (2017) 083704/1-4.a
2. Local Nodal Cooper Pairs in Multiorbital Systems

Kazumasa Hattori, Takuya Nomoto, Takashi Hotta, and Hiroaki Ikeda: J. Phys. Soc. Jpn. **86** (2017) 113702/1-5.

3. Mean-field theory for multipole ordering in  $f$ -electron systems on the basis of a  $j$ - $j$  coupling scheme  
Ryosuke Yamamura and Takashi Hotta: Physica B **536C** (2018) 6-11.
4. Kondo effect in the seven-orbital Anderson model hybridized with  $\Gamma_8$  conduction electrons  
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5. Multipole interactions of  $\Gamma_3$  non-Kramers doublet systems on cubic lattices  
Katsunori Kubo and Takashi Hotta: To appear in J. Phys.: Conf. Ser.

**HUKUSHIMA, Koji** [ C class; 3500 (B) ] ( )

— *Statistical-mechanical study of phase transition and cooperative phenomena*

1. Real-space analysis of scanning tunneling microscopy topography datasets using sparse modeling approach  
MJ Miyama and K Hukushima: J. Phys. Soc. Jpn. **87** (2018) 044801/1-8.
2. Bayesian optimization for computationally extensive probability distributions  
R Tamura and K Hukushima: PloS one **13** (2018) e0193785.a
3. Typical approximation performance for maximum coverage problem  
S Takabe, T Maehara and K Hukushima: Phys. Rev. E **97** (2018) 022138/1-9.
4. An Exact Algorithm Exhibiting RSRSB/EasyHard Correspondence for the Maximum Independent Set Problem  
J Takahashi, S Takabe and K Hukushima: J. Phys. Soc. Jpn. **86** (2017) 073001/1-4.
5. Method for estimating spin-spin interactions from magnetization curves  
R Tamura and K Hukushima: Phys. Rev. B **95** (2017) 064407/1-8.

**IGARASHI, Ryo** [ C class; 1500 (B) ] ( )

— *Monte Carlo simulation using low-rank approximation to long-range interaction matrices*

**IKEDA, Hiroaki** [ B class; 1500 (B) ] (135)

— *Analysis of superconductivity based on a first-principles approach*

— *search for high-temperature superconductors based on a first-principles approach*

**IKUHARA, Yuichi** [ C class; 7000 (B) ] (71)

— *Random atomic structure and selective segregation behavior around defects in functional ceramic materials*

— *Study of atomic structure and properties in functional materials*

1. Direct Determination of Atomic Structure and Magnetic Coupling of Magnetite Twin Boundaries  
C. Chen, H. Li, T. Seki, D. Yin, G. Sanchez-Santolino, K. Inoue, N. Shibata, and Y. Ikuhara: ACS Nano, **12** (2018) 2662-2668.
2. Atomic-Scale Origin of the Quasi-One-Dimensional Metallic Conductivity in Strontium Niobates with Perovskite-Related Layered Structures  
C. Chen, D. Yin, K. Inoue, F. Lichtenberg, X. Ma, Y. Ikuhara, J. G. Bednorz: ACS Nano, **11** (2007) 12519-12525.

**IMADA, Masatoshi** [ D,E class; 50500 (B) ] (205)

— *Development of neural network method with deep learning as a solver for many-body quantum systems*

— *Nonequilibrium superconductivity emerging from synergistic effects of light and phonons in strongly correlated systems*

— *Numerical Studies on Magnetic Anisotropy and Quantum Anomalous Hall Effect in Perovskite Transition Metal Oxide SrRuO<sub>3</sub>*

1. Quantum spin liquid signatures in Kitaev-like frustrated magnets  
Matthias Gohlke, Gideon Wachtel, Youhei Yamaji, Frank Pollmann, and Yong Baek Kim: Phys. Rev. B. **97** (2018) 075126
2. Finite-Temperature Signatures of Spin Liquids in Frustrated Hubbard Model  
Takahiro Misawa and Youhei Yamaji: J. Phys. Soc. Jpn. **87** (2018) 023707.



3. Competition among various charge-inhomogeneous states and d-wave superconducting state in Hubbard models on square lattices  
Kota Ido, Takahiro Ohgoe, and Masatoshi Imada: Phys. Rev. B. **97** (2017) 045138.
4. Competition among Superconducting, Antiferromagnetic, and Charge Orders with Intervention by Phase Separation in the 2D Holstein-Hubbard Model  
Takahiro Ohgoe and Masatoshi Imada: Phys. Rev. Lett. **119** (2017) 197001.
5. Restricted Boltzmann machine learning for solving strongly correlated quantum systems  
Yusuke Nomura, Andrew S. Darmawan, Youhei Yamaji, and Masatoshi Imada: Phys. Rev. B. **96** (2017) 205152.
6. Quantum lattice model solver H Phi  
Mitsuaki Kawamura, Kazuyoshi Yoshimi, Takahiro Misawa, Youhei Yamaji, Synge Todo, and Naoki Kawashima: Compt. Phys. Commun. **217**, (2017) 180.
7. Correlation-induced superconductivity dynamically stabilized and enhanced by laser irradiation  
Kota Ido, Takahiro Ohgoe, and Masatoshi Imada: Sci. Adv. **3** (2017) e1700718 .
8. Variational Monte Carlo method for fermionic models combined with tensor networks and applications to the hole-doped two-dimensional Hubbard model  
Hui-Hai Zhao, Kota Ido, Satoshi Morita, Masatoshi Imada: Phys. Rev. B. **96** (2017) 085103.
9. Low-energy effective Hamiltonians for correlated electron systems beyond density functional theory  
Motoaki Hirayama, Takashi Miyake, Masatoshi Imada, and Silke Biermann: Phys. Rev. B. **96** (2017) 075102.
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— *Curious chemical reactions of the entangled singlet state in nanographene* VANG

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— *The radiative transport equation with FDM and FEM*

— *Transport phenomena and optical tomography*

**MAKINO, Takayuki** [ C class; 2000 (B) ] (127)

— *Study on electronic structures and density of states in perovskite-type lead-halide mixed crystals*

**MASAKI-KATO, Akiko** [ C class; 8000 (B) ] (224)

— *Excitation dynamics of two-dimensional quantum spin systems*

— *The development of the parallelizable Quantum Monte Carlo method and the application to two-dimensional quantum lattice systems*

**MATSUKAWA, Hiroshi** [ E class; 11500 (B) ] ( )

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**MATSUMOTO, Munehisa** [ C class; 5000 (B) ] (87)

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— *Study on a automatic derivation technique of first-principles effective model based on the many body electron theory*

**SASAKI, Takehiko** [ B class; 1300 (B) ] (145)

— *Dehydration process of polyalcohol in hot pressurized water studied by First Principles Calculations*

— *Materials informatics approach for catalysts' activities and properties of metal oxides obtained by First Principles Calculations*

**SATO, Tetsuya** [ C class; 3500 (B) ] (113)

— *Controlling magnetic properties of quantum-well induced ferromagnetism in Pd(100) through the lattice distortion*

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— *Generation Mechanism of Organic/Biological Molecules on Early Earth: Ab Initio Molecular Dynamics Simulation II*

**SHIMOJO, Fuyuki** [ C class; 4500 (B) ] (96,302)

— *First-Principles Molecular-Dynamics Study of Structural and Electronic Properties of Covalent Liquids and Glass under Pressure*

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— *Multiple- $Q$  states of the frustrated Heisenberg model on the honeycomb lattice*

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**SHINAOKA, Hiroshi** [ D class; 3000 (B) ] (192,346)

— *Theoretical study of strong correlations in  $Cd_2Os_2O_7$*

**SHINODA, Wataru** [ C class; 6000 (B) ] (240)

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— *Control of phonon and electron transport properties using mechanical strain*

— *Screening for Thermal Functional Materials using Materials Informatics*

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**SHIRAISHI, Kenji** [ C class; 6000 (B) ] ( )

— *Design of New Phase Change Memories Based on First Principles Calculations*

**SHUDO, Ken-Ichi** [ C class; 1000 (B) ] (147)

— *Theoretical analysis of vibronic mode and spin ordering of thin film of transition metallated porphyrin-derivative*

**SUGINO, Osamu** [ C class; 4500 (B) ] (94)

— *Functional property of solid-liquid interfaces*

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— *Ground state phase diagram of  $SU(N)$  Heisenberg model on a honeycomb lattice*

— *Ground state phase diagrams of 2D generalized Heisenberg models for  $SU(N)$  spins*

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— *Theoretical search for high-efficient monolayer water-splitting photocatalysts*

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— *Development of High-performance Perfluoropolymer Electret*

— *Study on the charge trap mechanism of electret*

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**TAKAGI, Noriaki** [ B class; 1300 (B) ] (141,143)

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— *Geometric and electronic structures of two-dimensional atomic-layered materials*

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