4 PUBLICATION LIST

Example:

LASTNAME, Firstname [project class; # points (B), # points (C)] (Page #)
Project title
1. First paper
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□ ISSP Joint Research Projects

ADACHI, Takahiro [C class; 3500 (B), 900 (C)] (250)
— *Heat Transfer Characteristics of Condensate Film Flow along Vertical Plates with Microscopic Grooves*

AKAGI, Kazuto [C class; 11000 (B), 0 (C)] (55)
— *Exploration of structure motifs characterizing the metal oxides*
1. Deep electron and hole polarons and bipolarons in amorphous oxide
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AKAI, Hisazumi [B class; 500 (B), 300 (C)] (140)
— *Electronic structure of light rare earth permanent magnets*
1. Schottky junction studied using Korringa–Kohn–Rostoker Nonequilibrium Green's function method
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2. Relevance of 4f-3d exchange to finite-temperature magnetism of rare-earth permanent magnets: an ab-initio-based spin model approach for $NdFe_{12}N$
   M. Matsumoto, H. Akai, Y. Harashima, S. Doi and T. Miyake: J. Appl. Phys. **119** (2016) 213901.
3. Electrical resistivity of substitutionally disordered hcp Fe–Si and Fe–Ni alloys: Chemically-induced resistivity saturation in the Earth's core
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   Yuta Toga, Munehisa Matsumoto, Seiji Miyashita, Hisazumi Akai, Shotaro Doi, Takashi Miyake, and Akimasa Sakuma: Phys. Rev. B **94** (2016) 174433.
5. Atomistic-model study of temperature-dependent domain walls in the neodymium permanent magnet $Nd_2Fe_{14}B$
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2. Weak Phonon-mediated pairing in BiS_2 superconductor from first principles
   C. Morice, R. Akashi, T. Koretsune, S. S. Saxena, and R. Arita: arXiv:1701.02909; submitted.

ANDO, Yasunobu [C class; 1000 (B), 0 (C)] (139)
— *First-Principles study on the electric-double layer capacitance of MXene compound Ti_2CT_x*

AOYAMA, Kazushi [B class; 1200 (B), 0 (C)] (270)
— *Effects of a magnetic field on spin-lattice-coupled orders in pyrochlore antiferromagnets*
— *Lattice distortion effects on classical Heisenberg antiferromagnets on pyrochlore lattices*

1. Spin-Lattice-Coupled Order in Heisenberg Antiferromagnets on the Pyrochlore Lattice
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ARAI, Munehito [B class; 2100 (B), 1300 (C)] (257)
— *Computational rational design of novel artificial proteins*
— *Molecular dynamics simulations of proteins*
— *Structure and dynamics of the gliding protein from Mycoplasma mobile*

ARAIDAI, Masaaki [C class; 5500 (B), 2000 (C)] (68)
— *Development and Application of Extended Ensemble Method Coupled With First-Principles Electronic Structure Calculations*

ARAKAWA, Naoya [B class; 700 (B), 0 (C)] (193)
— *Study of interaction and multiband effects in intrinsic spin-Hall effect of an interacting multiorbital metal*

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ASAI, Yoshihiro [C class; 5000 (B), 2300 (C)] (69)
— *Large scale computational simulations of non-equilibrium transport phenomena*

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DEKURA, Haruhiko [C class; 1500 (B), 0 (C)] (49)
— *First-principles calculations of iron solid solution effects on the lattice thermal conductivity of lower mantle minerals*

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— *Development and application of first-principles simulator for time-dependent electron-transport calculation*

1. First-principles study on electron transport through BN-dimer embedded zigzag carbon nanotubes
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FUCHIZAKI, Kazuhiro [C class; 6500 (B), 0 (C)] (233)
— *Melting phenomena and polyamorphism*

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— *Atomic structures and electronic properties of atomic-layered materials*

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4. Structure, Stabilities, and Electronic Properties of Smart Ceramic Composites
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— *Calculation of optical properties of ordered structures of soft materials*

FUKUI, Ken-ichi [C class; 4500 (B), 1700 (C)] (82)
— *Microscopic Structure and Dynamics of Solutions Faced to Solid Materials Using First-Principles and Classical Molecular Dynamics*
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Y. Yokota, S. Akiyama, Y. Kaneda, A. Imanishi, K. Inagaki, Y. Morikawa and K. Fukui: J. Phys. Chem. C, **120**, 8684-8692 (2016).

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— *Anomalous rheological behaviors of glassy materials and granular suspensions*
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— *Effects of heavy elements in surface nanostructures*
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— *2D Scattering Pattern Analysis on Coarse Grained MD Model of Filled Hydrogel*
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— *Development and application of the large-scale GW calculation code*

HAMAMOTO, Yuji [C class; 2000 (B), 1300 (C)] ()
— *First principles study of the influence of lattice defects on Pt cluster supported on graphene*

HARADA, Kenji [C class; 5000 (B), 0 (C)] (245)
— *Development of tensor network algorithms*

HASHIMOTO, Tamotsu [C class; 5000 (B), 0 (C)] (244)
— *Molecular dynamics simulation of ferroelectrics using a shell model II*

HATSUGAI, Yasuhiro [C class; 6000 (B), 1300 (C)] (229)
— *Numerical studies of bulk-edge correspondence*

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   Y. Takahashi, T. Kariyado, Y. Hatsugai: New J. Phys. 19, 035003 (2017).
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— *Numerical analysis on a transverse-field Ising-Kondo lattice model*

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HAYAMI, Satoru [C class; 2000 (B), 0 (C)] (189)
— *Study of skyrmion in frustrated magnets with inversion symmetry*

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

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— *Electronic State and Proximity Effects around Interface in Layered Superlattices*

HIRAYAMA, Naomi [C class; 3000 (B), 0 (C)] ()
— *Effects of Impurity Doping on Thermoelectric Transport Properties of Semiconducting Silicides*

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— *Electronic states of bioluminescence related molecules*

1. Reverse Stability of Oxyluciferin Isomers in Aqueous Solutions
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6. Critical Temperature Enhancement of Topological Superconductors: A Dynamical Mean Field Study
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— *Large-scale Monte Carlo calculation of random spin systems*

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— *Monte Carlo simulation using low-rank approximation to long range interaction matrices*
— *Parallelization and GPGPU utilization of MPS program and its application to frustrated systems*

IKUHARA, Yuichi [C class; 6500 (B), 2500 (C)] (63)
— *Study of Atomic Structures and Selective Segregation Behavior at Grain Boundaries in Functional Materials*

1. Atomic structure and electronic properties of MgO grain boundaries in tunnelling magnetoresistive devices
   J. J. Bean, M. Saito, S. Fukami, H. Sato, S. Ikeda, H. Ohno, Y. Ikuhara and K. P. McKenna: Sci. Rep. **7**, (2017) 45594.

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— *Numerical Studies on Finite-Temperature Properties of 2D Hubbard and ab initio Models for Cuprates by Finite-Temperature Variational Monte Carlo Methods*
— *Numerical Studies on Mechanisms for Critical Temperature Control at Interfaces of Superconductors*
— *Numerical study of non-equilibrium superconducting states in two-dimensional Hubbard model by the time-dependent multi-variable variational Monte Carlo method*

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   Takahiro Misawa, Yusuke Nomura, Silke Biermann, and Masatoshi Imada: Sci. Adv. **2** (2016) e1600664 .
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   Youhei Yamaji,and Masatoshi Imada: J. Phys. Soc. Jpn. **85** (2016) 094707.

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   Shiro Sakai, Marcello Civelli, and Masatoshi Imada: Phys. Rev. B.**94** (2016) 115130.
8. Stabilization of topological insulator emerging from electron correlations on honeycomb lattice and its possible relevance in twisted bilayer graphene
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INAGAKI, Kouji [C class; 5000 (B), 1800 (C)] (75)
— *First-principles meta-dynamics analysis of Catalyst Referred Etching method (dissociative adsorption reaction barrier at interface between Pt and material surface)*

INAOKA, Takeshi [C class; 2500 (B), 1100 (C)] (106)
— *Search and realization of novel electronic properties of solid surfaces and small particles*
1. STM-enhanced dynamic dipole moments coupled with adsorbate vibration at substrate or tip surfaces
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ISHII, Fumiyuki [B,C class; 8200 (B), 1300 (C)] (59, 61)
— *First-principles calculations of oxide thin-films and heterostructures*
— *First-principles study of anomalous thermoelectric effect*
— *First-principles design of thermoelectric materials based on Berry curvature landscape*
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— *Nonequilibrium phase transition in the large scale dense hard sphere molecular dynamics simulation*
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— *study on electronic structures in perovskite-type lead-halide mixed crystals*

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— *Development of Quantum Monte Carlo Methods and Application to Critical Phenomena of Dirty Bosons*
— *Development of a parallel quantum Monte Carlo Method and Study of novel quantum phenomena in quantum lattice models*

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— *Physics of Friction*

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— *First-principles analyses on crystal growth mechanism of GaN*

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