4 PUBLICATION LIST

Example:

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— *Project title*

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

ADACHI, Takahiro [C class; 8000 (A), 1000 (B), 300 (C)] (217)

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

1. Linear stability of flow in rectangular ducts in the vicinity of the critical aspect ratio
   Takahiro ADACHI: European Journal of Mechanics B/Fluids 41 (2013) 163–168
2. Velocity and temperature profiles extending over the liquid and gas phases of two-phase flow falling down vertical plates
   Takahiro ADACHI: Applied Thermal Engineering 51 (2013) 827e832
3. Heat Transfer Enhancement of the Film Flow Falling along Vertical Fluted Plates
   Shouta SATO and Takahiro ADACHI: Proceedings of 4th International Conference on Simulation and Modeling Methodologies, Technologies and Applications(Vienna, Austria,2014)

AKAI, Hisazumi [B class; 0 (A), 800 (B), 500 (C)] (135)

— *Electronic structure of rare earth magnets*

1. Role of N in a permanent magnet material $Sm_2Fe_{17}N_x$
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ANDO, Yasunobu [C class; 0 (A), 2500 (B), 1700 (C)] (104)

— *Nano-capacitance analysis based on density functional theory with applied bias*

AOKI, Hideo [C class; 0 (A), 4000 (B), 0 (C)] (163)

— *Non-equilibrium phase transitions in superconductors and electron-phonon systems*

1. Interaction quench in the Holstein model: Thermalization crossover from electron- to phonon-dominated relaxation
   Yuta Murakami, Philipp Werner, Naoto Tsuji and Hideo Aoki: Phys. Rev. B **91**, 045128 (2015).
2. Supersolid phase accompanied by a quantum critical point in the intermediate coupling regime of the Holstein model
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— *First-Principles Modeling on Emerging Memory Devices*

ARAKAWA, Naoya [B class; 0 (A), 600 (B), 0 (C)] (152)
— *Microscopic theory for transport phenomena of multi-orbital strongly correlated electron systems*

1. Orbital-cooperative spin fluctuation and orbital-dependent transport in Ru oxides
   N. Arakawa: Phys. Rev. B **90** (2014) 245103.
2. Many-body effects on the resistivity of a multiorbital system beyond Landau's Fermi-liquid theory
   N. Arakawa: arXiv:1503.06937; accepted for publication in Modern Physics Letters B as an invited brief review article.
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ARAKI, Takeaki [B class; 1800 (A), 700 (B), 0 (C)] (248)
— *Conformations of polymer chains in nematic liquid crystals II*

1. Controlled motion of a Janus particle in periodically phase-separating binary fluids
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2. Nematic caps on a colloidal particle in a nematogenic liquid under electric field
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ARITA, Ryotaro [C,D class; 0 (A), 18500 (B), 2300 (C)] (23)
— *Study of strongly-correlated multiorbital systems with continuous-time quantum Monte Carlo method*
— *Study of multi-orbital correlated electron systems by cluster dynamical mean field theory*
— *Nonempirical study of superconductivity in correlated fullerenes*

1. Effect of Hund's coupling on nonlocal correlations: a cluster DMFT study
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DEKURA, Haruhiko [C class; 0 (A), 1000 (B), 0 (C)] (140)
— *First-principles calculations of iron solid solution effects on the lattice thermal conductivity of lower mantle minerals*

EGAMI, Yoshiyuki [C class; 0 (A), 1500 (B), 3200 (C)] (97)
— *Development and application of first-principles simulator for dynamics of electron transport*

1. First-principles calculation method for electron transport based on grid Lippmann-Schwinger equation
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— *Slow Dynamical Processes in Nonequilibrium Metastable States*

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FUJIMOTO, Yoshitaka [C class; 20500 (A), 0 (B), 0 (C)] (53)
— *Atomic structures, structural stabilities, and electronic properties of impurity-doped carbon-based materials*

1. Hydrogen adsorption and anomalous electronic properties of nitrogen-doped graphene
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— *First-Principles and Classical Molecular Dynamics Investigations of Electrolyte Solution / Electrode Interfaces*

FURUKAWA, Akira [C class; 11500 (A), 6500 (B), 0 (C)] (202)
— *Hydrodynamic effects on the collective dynamics of soft matter systems*
— *Rheology of heterogeneous soft matter systems*

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— *Enhancement mechanism of dynamical spin-fluctuation in iron-based superconductors*
— *Effect of spin-orbit interactions in thermoelectric materials*

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— *First principles calculation of van der Waals interaction in Pt clusters on graphene*

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2. Disentangled Topological Numbers by a Purification of Entangled Mixed States for Non-Interacting Fermion Systems
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HIROSE, Kenji [C class; 2500 (A), 1000 (B), 700 (C)] ()
— *Multi-scale Electric and Thermal Transport Calculations*

HOSHI, Takeo [E class; 0 (A), 13500 (B), 2200 (C)] (58)
— *Parallelized ultra-large-scale electronic-structure theory based on first principle calculation and novel numerical method*

1. Novel linear algebraic theory and one-hundred-million-atom quantum material simulations on the

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IKUHARA, Yuichi [C class; 0 (A), 2500 (B), 1700 (C)] (105)
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— *First-principles meta-dynamics analysis of Catalytic Referred Etching method (Reaction barrier in etching of GaN, SiC and SiO2)*

INAOKA, Takeshi [C class; 1500 (A), 500 (B), 600 (C)] (246)

— *Physical properties of low-dimensional electron systems created at solid surfaces and their control*

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— *First-Principles Calculation of Oxide Topological Insulators*
— *First-Principles Calculation of Transition Metal Oxides Interfaces*

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— *Nonequilibirum phase transition in the large scale dense hard sphere molecular dynamics simulation*

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— *The phase transition under magnetic field of the quantum spin on the Cairo pentagon lattice*

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— *Study on physical and structural properties of defects, surfaces, and interfaces for 2D semiconductors*

KAKEHASHI, Yoshiro [C class; 0 (A), 1000 (B), 0 (C)] (261)
— *Numerical Study of Long-Range Magnetic Correlations Based on the Nonlocal Dynamical CPA*

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— *First principles calculations of ionic conductivity in solid electrolytes*

MASAKI-KATO, Akiko [C class; 2500 (A), 2000 (B), 1700 (C)] (228)

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MATSUKAWA, Hiroshi [C class; 7000 (A), 500 (B), 0 (C)] ()

— *Physics of Friction*

MATSUSHITA, Katsuyoshi [C class; 0 (A), 3000 (B), 0 (C)] (241)

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MOMIDA, Hiroyoshi [C class; 3000 (A), 2500 (B), 1400 (C)] (90)
— *First-principles study on charge-discharge reaction mechanism in cathode materials of secondary*

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MOTOYAMA, Yuichi [B class; 0 (A), 500 (B), 0 (C)] (180)

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MURASHIMA, Takahiro [E class; 0 (A), 19500 (B), 2500 (C)] (197)
— *Multiscale Simulation of Polymer Melts with Element Deformation*

NADA, Hiroki [C class; 0 (A), 3500 (B), 0 (C)] (240)
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— *Evaluation of ion conductivity at interfaces in proton conducting composite electrolyte*
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TATENO, Masaru [C class; 0 (A), 7000 (B), 0 (C)] (88)

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— *Development and Application of New Methods for First-Principles Simulation of Material Structure and Electronic Properties*

UCHIDA, Takashi [B,C class; 0 (A), 900 (B), 0 (C)] (141)
— *Temperature dependence of magnetic and electronic structure for Mn-based ordered alloys with Cu_3Au-type crystal structure*
— *Theory of magnetic and electronic structure for Mn-based ordered alloys with Cu_3Au-type crystal structure*

UDA, Yutaka [B class; 0 (A), 1000 (B), 0 (C)] (138)
— *Wear mechanism of diamond tool*

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□ CMSI Projects

DOI, Shotaro [R class; 0 (A), 0 (B), 4000 (C)] (281)
— *First-principles Electronic Structure Calculation of Permanent Magnets using the Screened KKR Green's Function Method*

IMADA, Masatoshi [R class; 0 (A), 0 (B), 10000 (C)] ()
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OGATA, Shuji [R class; 0 (A), 0 (B), 10000 (C)] (271)
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— *Ordering of topological excitations of the frustrated magnets*

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SAITO, Mineo [R class; 0 (A), 0 (B), 10000 (C)] (273)
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