

Example:

LASTNAME, Firstname [project class; # points (A), # points (B), # points (C)]
 (Page #)
 — *Project title*
 1. First paper
 Names of Authors, etc.
 2. Second paper
 ...

□ ISSP Joint Research Projects

ADACHI, Takahiro [C class; 10000 (A), 500 (B), 500 (C)] ()

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

AKAGI, Kazuto [C class; 0 (A), 6000 (B), 1500 (C)] (93)

— *Microscopic understanding of electric double layer at solid-liquid interfaces*

AMEZAWA, Koji [C class; 0 (A), 1500 (B), 0 (C)] (126)

— *First principles calculation on defect structures in mixed conducting Perovskite oxides*

ANDO, Yasunobu [E class; 0 (A), 5500 (B), 1800 (C)] (95)

— *Study on material search and electrode interfaces for next-generation secondary batteries*

AOKI, Hideo [C class; 0 (A), 5000 (B), 0 (C)] (154)

— *Numerical study of various phases and non-equilibrium phase transitions in correlated electron systems*

1. Supersolid states in a spin system — phase diagram and collective excitations
Yuta Murakami, Takashi Oka and Hideo Aoki: Phys. Rev. B **88** (2013) 224404.
2. Ordered phases in the Holstein-Hubbard model: Interplay of strong Coulomb interaction and electron-phonon coupling
Yuta Murakami, Philipp Werner, Naoto Tsuji, and Hideo Aoki: Phys. Rev. B **88** (2013) 125126.
3. Nonequilibrium dynamical mean-field theory and its applications
Hideo Aoki, Naoto Tsuji, Martin Eckstein, Marcus Kollar, Takashi Oka, and Philipp Werner: Rev. Mod. Phys. (2014), to be published (arXiv:1310.5329).

ARAKI, Takeaki [B class; 800 (A), 700 (B), 0 (C)] (236)

— *Conformations of polymer chains in nematic liquid crystals*

1. Defect science and engineering of liquid crystals under geometrical frustration
Takeaki Araki, Francesca Serrab and Hajime Tanaka: Soft Matter **9** (2013) 8107.
2. Electro-osmotic flow of semidilute polyelectrolyte solutions
Yuki Uematsu and Takeaki Araki: J. Chem. Phys. **139**, (2013) 094901.

EGAMI, Yoshiyuki [C class; 0 (A), 2000 (B), 2500 (C)] (120)

— *Development and application of first-principles electron-transport simulators for massively parallel computer*

1. First-Principles Study on Dynamic Electron-Transport Property through Low Dimensional System
Y. Egami and K. Hirose: JPS Conf. Proc. **1** (2014) 016012.
2. Ballistic electron transport through nanostructure junctions from a real-space finite-difference

approach

S. Tsukamoto, T. Ono and Y. Egami: Quantum Matter, in press.

3. First-principles calculation method for electron transport based on grid Lippmann-Schwinger equation
Y. Egami, S. Tsukamoto, T. Ono and K. Hirose: submitted to Phys. Rev. B.

FEDERICI, Filippo [C class; 0 (A), 5000 (B), 0 (C)] ()

— *Molecular Dynamics study of frictional properties of confined ionic liquids*

FUCHIZAKI, Kazuhiro [C class; 22000 (A), 5000 (B), 0 (C)] (179)

— *Slow Dynamical Processes in Nonequilibrium Metastable States*

1. Predicting the Thermodynamic Properties of the Modified Lennard-Jones Fluid from the Lennard-Jones Equation of State
K. Fuchizaki and Y. Asano: J. Phys. Soc. Jpn. **82** (2013) 124001.
2. Melting behavior of SnI₄ reexamined
K. Fuchizaki: J. Chem. Phys. **139** (2013) 244503.
3. Modified Benedict–Webb–Rubin Equation of State for the Modified Lennard-Jones Fluid
Y. Asano and K. Fuchizaki: J. Phys. Soc. Jpn. **83** (2014) 034601.

FUJII, Hitoshi [C class; 0 (A), 2000 (B), 700 (C)] ()

— *First-principles calculations of X-ray absorption spectroscopy for Transition-Metal Oxides*

FUJIMOTO, Yoshitaka [C class; 11500 (A), 0 (B), 0 (C)] (79)

— *Effects of doping on atomic structures and electronic properties of nanocarbon materials*

1. Electronic structures of carbon-doped hexagonal boron nitride sheet: A density-functional study
Y. Fujimoto, T. Koretsune and S. Saito: JPS Conference Proceedings **1**, 012066 (2014)
2. Hydrogen adsorption and anomalous electronic properties of nitrogen-doped graphene
Y. Fujimoto and S. Saito: Journal of Applied Physics, Accepted.
3. Pyridine-Type Defects in Graphene: Stability, Reactivity and Electronic Property
Y. Fujimoto: Advances in Materials Science Research (Nova Science Publishers, New York), Submitted.
4. Electronic structures of hexagonal boron-nitride monolayer: strain-induced effects
Y. Fujimoto, T. Koretsune, and S. Saito: Journal of the Ceramic Society of Japan, Accepted.

FUJIWARA, Susumu [B class; 0 (A), 600 (B), 0 (C)] (250)

— *Molecular Simulation Study of Supramolecular Structure Formation by Amphiphilic Molecules*

1. Shape transition of micelles in amphiphilic solution: A molecular dynamics study
S. Fujiwara, M. Hashimoto, T. Itoh, H. Nakamura and Y. Tamura: J. Phys.: Conf. Ser. **454** (2013) 012024.
2. Nucleation and polymorphism of trans-1,4-polyisoprene containing copper phthalocyanine
T. Tsuboi, M. Harada, K. Ishii, S. Fujiwara and T. Itoh: Polymer J. **45** (2013) 915-920.
3. One-, Two-, and Three-Dimensional Hopping Dynamics
K. M. Aoki, S. Fujiwara, K. Sogo, S. Ohnishi and T. Yamamoto: Crystals **3** (2013) 315-332.
4. Molecular Dynamics Simulations of One-, Two-, Three-dimensional Hopping Dynamics
K. M. Aoki, S. Fujiwara, K. Sogo, S. Ohnishi and T. Yamamoto: JPS Conf. Proc. **1** (2014) 012038.
5. Molecular Dynamics Simulation of Micellar Shape Transition in Amphiphilic Solution
S. Fujiwara, M. Hashimoto, Y. Tamura, H. Nakamura and R. Horiuchi: Plasma Fusion Res., in press.

FUJIWARA, Takeo [C class; 3500 (A), 3500 (B), 0 (C)] (97)

— *Expansion of the first principle electronic structure calculation with hybrid method*

1. Nanoseconds Quantum Molecular Dynamics Simulations of Lithium Superionic Conductor Li_{4-x}Ge_{1-x}P_xS₄
Shinya Nishino, Takeo Fujiwara and Hisatsugu Yamasaki, submitted to Phys. Rev. B.
2. Parametrization scheme with accuracy and transferability for tight-binding electronic structure

calculations with extended Hückel approximation and molecular dynamics simulations
S. Nishino and T. Fujiwara, *J. Molecular Modelling*. Vol.19, 2363-2373 (2013).

FUKUI, Ken-ichi [E class; 0 (A), 9500 (B), 2900 (C)] (72)

— *First-principles calculation of electrochemical properties of redox-active monolayers*

— *Counter-ion effects of First-principles calculation of electrochemical properties*

FURUKAWA, Akira [C class; 13500 (A), 5000 (B), 2000 (C)] (184)

— *Nonequilibrium dynamics of complex colloidal suspension*

1. Simple picture of the supercooled liquid dynamics: Dynamic scaling and phenomenology based on clusters

A. Furukawa: *Phys. Rev. E* **87** (2013) 062321.

2. Nonequilibrium critical Casimir interactions

A. Furukawa, A. Gambassi, S. Dietrich, and H. Tanaka: *Phys. Rev. Lett.* **111** (2013) 055701.

3. Activity-induced clustering in model dumb-bell swimmers:

The role of hydrodynamic interactions

A. Furukawa, D. Marrenduzo, and M.E. Cates: submitted to *Phys. Rev. E*

FUSEYA, Yuki [B class; 1500 (A), 0 (B), 0 (C)] (166)

— *Theory of dynamical spin fluctuation in iron-based superconductors*

GOHDA, Yoshihiro [C class; 0 (A), 5000 (B), 2200 (C)] (96)

— *Itinerant electronic states at rare-earth-magnet interfaces*

1. Strain effects on the magnetic anisotropy of $Y_2Fe_{14}B$ examined by first-principles calculations

Z. Torbatian, T. Ozaki, S. Tsuneyuki, and Y. Gohda: *Appl. Phys. Lett.*, in press.

HARADA, KENJI [C class; 2500 (A), 5500 (B), 2700 (C)] (198)

— *Numerical study of quantum liquid phase using tensor network variational method*

1. Symmetry-protected topological order and negative-sign problem for $SO(N)$ bilinear-biquadratic chains

Kouichi Okunishi and Kenji Harada, *Physical Review B* **89**, 134422 (2014).

HAMADA, Ikutaro [C class; 8000 (A), 0 (B), 0 (C)] (91)

— *Density functional theory study of stability and dynamics of metal nanoclusters on a silicon surface*

HATSUGAI, Yasuhiro [C class; 10000 (A), 3000 (B), 2000 (C)] (145)

— *Numerical study of topological order*

1. Characterization of Dimers in Graphene Flakes

D. Seki, Y. Hamamoto and Y. Hatsugai, *JPS Conf. Proc.* **1**, 012068 (2014).

2. Sharp Zero-Energy Landau Levels in Multilayer Graphene

H. Sakamoto, Y. Hatsugai, H. Aoki and T. Kawarabayashi, *JPS Conf. Proc.* **1**, 012069 (2014).

3. Emergence of Topologically Stable Dirac Dispersions in a Fermionic Shastry-Sutherland Model

T. Kariyado and Y. Hatsugai, *JPS Conf. Proc.* **1**, 012001 (2014).

4. Symmetry-protected quantization and bulk-edge correspondence of massless Dirac fermions: Application to the fermionic Shastry-Sutherland model

T. Kariyado and Y. Hatsugai, *Phys. Rev. B* **88**, 245126 (2013).

5. Chiral symmetry and fermion doubling in the zero-mode Landau levels of massless Dirac fermions with disorder

T. Kawarabayashi, T. Honda, H. Aoki and Yasuhiro Hatsugai, *AIP Conf. Proc.* **1566**, 283 (2013).

6. Spin-resolved chiral condensate as a spin-unpolarized quantum Hall state in graphene

Y. Hamamoto, T. Kawarabayashi, H. Aoki and Y. Hatsugai, *Phys. Rev. B* **88**, 195141 (2013).

7. Chiral Symmetry and Many-Body Effect in Multilayer Graphene

Y. Hatsugai; Y. Hamamoto; H. Aoki; T. Kawarabayashi, *J. Phys. Conf. Ser.* **456**, 012013 (2013).

8. Stability of zero-mode Landau levels in bilayer graphene against disorder in the presence of the trigonal warping

T. Kawarabayashi, Y. Hatsugai and H. Aoki, J. Phys. Conf. Ser. 456, 012020 (2103).

9. Symmetry Protected Weak Topological Phases in a Superlattice

T. Fukui, K.-I. Imura and Y. Hatsugai, Journal of the Physical Society of Japan 82, 073708 (2013).

HATTORI, Kazumasa [C class; 0 (A), 1500 (B), 0 (C)] (165)

— *Anomalous transport properties induced by Fermi surfaces variations*

HATTORI, Ken [B class; 1400 (A), 0 (B), 0 (C)] (127)

— *Model calculations in Si surfaces with adsorbates*

HIDA, Kazuo [B class; 800 (A), 700 (B), 0 (C)] (233)

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

1. Ground-State Phase Diagram of S=2 Heisenberg Chains with Alternating Single-Site Anisotropy

K. Hida: J. Phys. Soc. Jpn. **83** (2014) 034707.

2. Topological Phases of the Spin-1/2 Ferromagnetic-Antiferromagnetic Alternating Heisenberg Chain with Frustrated Next-Nearest-Neighbour Interaction

K. Hida, K. Takano, and H. Suzuki: J. Phys. Soc. Jpn. **82** (2013) 064703

HIRAI, Kunitomo [B class; 0 (A), 400 (B), 500 (C)] (135)

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

HIROSE, Kenji [C class; 2000 (A), 1500 (B), 800 (C)] ()

— *Multi-Scale Electric and Thermal Transport Calculations*

HOSHI, Takeo [E class; 0 (A), 16000 (B), 2300 (C)] (15)

— *Parallelized ultra-large-scale electronic-structure theory based on first principle calculation and novel numerical method*

HOSHINO, Shintaro [B class; 0 (A), 800 (B), 0 (C)] (169)

— *Quantum Monte Carlo Approach to Odd-Frequency Superconductivity*

1. Anisotropic Magnetic Response in Kondo Lattice with Antiferromagnetic Order

Taku Kikuchi, Shintaro Hoshino and Yoshio Kuramoto: arXiv:1404.5718 (2014)

2. Composite Orders and Lifshitz Transition of Heavy Electrons

Shintaro Hoshino and Yoshio Kuramoto: arXiv:1403.5634, to appear in J. Phys. Soc. Jpn. (2014)

3. Superconductivity of Composite Particles in a Two-Channel Kondo Lattice

Shintaro Hoshino and Yoshio Kuramoto: Phys. Rev. Lett. **112** (2014) 167204

4. Strong Quasi-Particle Renormalizations in Heavy-Electron Magnets

Shintaro Hoshino and Yoshio Kuramoto: to appear in JPS Conference Proceedings (2014)

5. Continuous-Time Quantum Monte Carlo Study of Strong Coupling Superconductivity in Holstein-Hubbard Model

Satoshi Yamazaki, Shintaro Hoshino and Yoshio Kuramoto: to appear in JPS Conference Proceedings (2014)

6. Itinerant Versus Localized Heavy-Electron Magnetism

Shintaro Hoshino and Yoshio Kuramoto: Phys. Rev. Lett. **111** (2013) 026401

HOTTA, Takashi [C class; 13500 (A), 0 (B), 0 (C)] (148)

— *Research for superconductivity in strongly correlated multi-orbital systems*

1. Key role of hybridization between actinide 5f and oxygen 2p orbitals for electronic structure of actinide dioxides

Yu Hasegawa, Takahiro Maehira and Takashi Hotta: J. Mod. Phys. **4** (2013)1574-1582.

2. Kondo effect emerging from a spin-vibronic state

Takahiro Fuse and Takashi Hotta: J. Phys.: Conf. Ser. **428** (2013) 012013.

3. Fermi-Surface Topology and Superconductivity Induced by Jahn-Teller Phonons

Yuji Shiba and Takashi Hotta: J. Phys.: Conf. Ser. **428** (2013) 012038.

4. Electric Dipolar Susceptibility of the Anderson-Holstein Model

Takahiro Fuse and Takashi Hotta: J. Korean Phys. Soc. **62** (2013) 1874.

HUKUSHIMA, Koji [C class; 1500 (A), 11000 (B), 2300 (C)] (190)

— *Equilibrium simulations in spin glasses*

1. Dynamics of One-Dimensional Ising Model without Detailed Balance Condition
Y. Sakai and K. Hukushima: J. Phys. Soc.Jpn **82** (2013) 064003-1-15
2. A List Referring Monte-Carlo Method for Lattice Glass Models
M.Sasaki and K. Hukushima: J. Phys. Soc.Jpn **82** (2013) 094003-1-15
3. Response to a twist in systems with Z_p symmetry: The two-dimensional p-state clock model
Y. Kumano, K.Hukushima, Y.Tomita, M.Oshikawa: Phys. Rev. B **88** (2013) 104427-1-6
4. An irreversible Markov-chain Monte Carlo method with skew detailed balance conditions
M.Sasaki and K. Hukushima: J. Phys.: Conf. Ser. **473** (2013) 12012-1-9
5. Typical Behavior of the Linear Programming Method for Combinatorial Optimization Problems: A Statistical – Mechanical Perspective
S. Takabe and K. Hukushima: J. Phys. Soc.Jpn **83** (2014) 043801-1-4

IGARASHI, Ryo [C class; 0 (A), 1000 (B), 1400 (C)] ()

— *Development of ALPS/MPS and its application to strongly correlated electron systems*

IKUHARA, Yuichi [C class; 13000 (A), 7000 (B), 3000 (C)] (53)

— *Local Quantum Design of Materials Fabricated by Bicrystal Technique* Metal-insulator Transition at Perovskite Oxide Interfaces

1. Spontaneous Structural Distortion and Quasi-One-Dimensional Quantum Confinement in a Single-Phase Compound
Z. Wang, L. Gu, M. Saito, S. Tsukimoto, M. Tsukada, F. Lichtenberg, Y. Ikuhara, and J. G. Bednorz: Adv.Mater. **25** (2013) 218.
2. Ferromagnetic Dislocations in Antiferromagnetic NiO
I. Sugiyama, N. Shibata, Z. Wang, S. Kobayashi, T. Yamamoto, and Y. Ikuhara: Nat. Nanotech. **8** (2013) 266.
titleRegulating Infrared Photoresponses in Reduced Graphene Oxide Phototransistors by Defect and Atomic Structure Control
H. X. Chang, Z. H. Sun, M. Saito, Q. H. Yuan, H. Zhang, J. H. Li, Z. C. Wang, T. Fujita, F. Ding, Z. J. Zheng, F. Yan, H. K. Wu, M. W. Chen, and Y. Ikuhara: ACS NANO **7** (2013) 6310.

IMADA, Masatoshi [C,E class; 0 (A), 22000 (B), 2200 (C)] (23)

— *Numerical studies on ab initio low-energy effective models for high-Tc cuprates*

— *Variational Monte Carlo studies of electron correlation effects on topological insulators*

1. Atomically resolved spectroscopic study of Sr₂IrO₄: Experiment and theory
Qing Li, Guixin Cao, Satoshi Okamoto, Jieyu Yi, Wenzhi Lin, Brian C. Sales, Jiaqiang Yan, Ryotaro Arita, Jan Kunes, Anton V. Kozhevnikov, Adolfo G. Eguluz, Masatoshi Imada, Zheng Gai, Minghu Pan, David G. Mandrus: Scientific Reports **3** (2013) 3073.
2. Quantum Monte Carlo Simulations for Stacked Spin-Ladder Systems Containing Low Concentrations of Nonmagnetic Impurities: Application to the Low-Temperature Broadening of NMR Spectra in SrCu₂O₃
Robert Achleitner, Hans Gerd Evertz, Masatoshi Imada, Ralf Gamillscheg, Peter Mohn: Phys. Rev. B **88** (2013) 214422.
3. Improved Multi-Variable Variational Monte Carlo Method Examined by High-Precision Calculations of One-Dimensional Hubbard Model
Ryui Kaneko, Satoshi Morita, Masatoshi Imada: J.Phys.Conf.Ser. **454** (2013) 012046.
4. Theory of Pseudogap in Underdoped Cuprates
M. Imada, S. Sakai, Y. Yamaji and Y. Motome: J. Phys. Conf. Ser. **449** (2013) 012005.
5. Derivation of Static Low-Energy Effective Models by *ab initio* Downfolding Method without Double Counting of Coulomb Correlations: Application to SrVO₃, FeSe and FeTe
M. Hirayama, T. Miyake and M. Imada: Phys. Rev. B **87** (2013) 195144.
6. Raman-scattering measurements and theory of the energy-momentum spectrum for underdoped

$\text{Bi}_2\text{Sr}_2\text{CaCuO}_8 + \delta$ superconductors: Evidence of an *s*-wave structure for the pseudogap

Shiro Sakai, Sebastien Blanc, Marcello Civelli, Yann Gallais, Maximilien Cazayous, Marie-Aude Measson, Jinsheng Wen, Zhijun Xu, Genda Gu, Giorgio Sangiovanni, Yukitoshi Motome, Karsten Held, Alain Sacuto, Antoine Georges, and Masatoshi Imada: *Phys. Rev. Lett.* **111** (2013) 107001.

7. Phase diagram structure of topological Mott transition for zero-gap semiconductors beyond conventional Landau-Ginzburg-Wilson scenario
Moyuru Kurita, Youhei Yamaji, and Masatoshi Imada: *Phys. Rev. B* **88** (2013) 115143.

INAGAKI, Kouji [C class; 19000 (A), 5500 (B), 2200 (C)] (49)

— *Clarification of reaction process in CRAE method*

— *Clarification of reaction process in CARE method for GaN, SiC and SiO₂ materials*

INAOKA, Takeshi [C class; 2000 (A), 500 (B), 400 (C)] (225)

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

1. Anisotropy of the silicon valence band induced by strain with various orientations
T. Inaoka, Y. Kinjyo, S. Yanagisawa, and K. Tomori: *J. Appl. Phys.* **113** (2013) 183718 (13 pages).
2. Exchange-correlation and temperature effects on plasmons in strongly-correlated two-dimensional electron systems: finite-temperature local-field-correction theory combined with angle-resolved Raman spectroscopy
T. Inaoka, Y. Sugiyama, and K. Sato: *Phys. Status Solidi B*, published online (2014) Doi: 10.1002/pssb.201350147 (11 pages).
3. Internal-strain effect on the valence band of strained silicon and its correlation with the bond angles
T. Inaoka, S. Yanagisawa, and Y. Kadekawa: *J. Appl. Phys.* **115** (2014) 063702 (14 pages).

ISHIHARA, Sumio [B class; 0 (A), 1500 (B), 0 (C)] (163)

— *Non-linear and non-steady dynamics in correlated electron systems*

— *Response and non-linear dynamics in correlated electron system*

1. Dynamical Jahn-Teller effect in a spin-orbital coupled system
J. Nasu and S. Ishihara: *Phys. Rev. B* **88** (2013) 094408
2. Vibronic excitation dynamics in orbitally degenerate correlated electron system
J. Nasu and S. Ishihara: *Phys. Rev. B* **88** (2013) 205110
3. Transient carrier dynamics in a Mott insulator with antiferromagnetic order
E. Iyoda and S. Ishihara: *Phys. Rev. B* **89** (2014) 125126

ISHII, Fumiyuki [B class; 0 (A), 1300 (B), 900 (C)] (121,122)

— *First-Principles Calculation of Spin Splitting at Oxide Surfaces and Interfaces*

— *First-Principles Calculation of Transition Metal Oxide Superlattices*

1. First-principles study of carrier-induced ferromagnetism in bilayer and multilayer zigzag graphene nano ribbons
K. Sawada, F. Ishii, and M. Saito: *Appl. Phys. Lett.* **104** (2014) 14311.
2. Tunable Rashba effect on strained ZnO: First-principles density-functional study
M. A. Adhib, H. Kotaka, F. Ishii, and M. Saito: *Appl. Phys. Exp.* **7** (2014) 053002.
3. Spin-Orbit Interaction Effects in the Electronic Structure of B20-type CoSi: First-Principles Density Functional Study
F. Ishii, T. Onishi, and H. Kotaka: *JPS Conf. Proc.*, in press.
4. Contribution of Berry Curvature to Thermoelectric Effects
Y.P. Mizuta and F. Ishii: *JPS Conf. Proc.*, in press.
5. First-principles study of Exchange Interaction in Ising-type Multiferroic Ca₃CoMnO₆
M. Nishida, F. Ishii, and M. Saito: *JPS Conf. Proc.*, in press.

ISOBE, Masaharu [B class; 400 (A), 300 (B), 0 (C)] (245)

— *Large scale hard sphere molecular dynamics simulation in the nonequilibrium transport phenomena*

1. Hard Disks Equation of State: First-Order Liquid-Hexatic Transition in Two Dimensions with Three Different Simulation Methods
M. Engel, J. A. Anderson, S. C. Glotzer, M. Isobe, E.P. Bernard and W. Krauth: Phys. Rev. E **87** (2013) 042134.

ISODA, Makoto [B class; 500 (A), 0 (B), 0 (C)] (252)

— *Finite temperature properties of 2-dimensional frustrated system*

1. A microscopic modeling of the instant coffee effect
M. Isoda and Y. Nishimori: J. Phys.: Conf. Ser. 490 (2014) 012030.

KAKEHASHI, Yoshiro [C class; 0 (A), 1000 (B), 0 (C)] (168)

— *Development of Nonlocal Dynamical CPA and Numerical Study of Long-Range Magnetic Correlations*

1. Nonlocal Excitations and 1/8 Singularity in Cuprates
Y. Takehashi, M.A.R. Patoary, S. Chandra: J. Korean Phys. Soc. **62** (2013) 1827-1831.
2. First-Principles Molecular Dynamics Study on the Magnetic Structure of Mn₃Pt
T. Uchida, N. Kimura, and Y. Takehashi: J. Korean Phys. Soc. **62** (2013) 1748-1752.
3. Momentum Dependent Local-Ansatz with Hybrid Wavefunction from Weak to Strong Electron Correlations
M. Atiqur R. Patoary and Y. Takehashi: J. Phys. Soc. Jpn. **82** (2013) 084710.

KAMIYA, Katsumasa [C class; 13000 (A), 3000 (B), 0 (C)] ()

— *Quantum theoretical study of the relationships among function, atomic structure, and electronic structure of bio-nano-materials*

KASAI, Hideaki [C class; 0 (A), 5500 (B), 2700 (C)] (89)

— *First principles based analysis of reactions on solid surfaces/interfaces*

1. Interplay between Plasmon Luminescence and Vibrationally Resolved Molecular Luminescence Induced by Scanning Tunneling Microscopy
Kuniyuki Miwa, Mamoru Sakaue, Hideaki Kasai: Journal of the Physical Society of Japan, **82**, 069715/1-5 (2013).
2. Vibration-assisted upconversion of molecular luminescence induced by scanning tunneling microscopy
Kuniyuki Miwa, Mamoru Sakaue, Hideaki Kasai: Nanoscale Research Letters, **8**, 204 (2013).
3. First-principles study on surface structure, thickness and composition dependence of the stability of Pt-skin/Pt₃Co oxygen-reduction reaction
Mary Clare Sison Escaño, Hideaki Kasai: Journal of Power Sources, **247**, 562-571 (2013).
4. Hydrogen absorption and hydrogen-induced reverse segregation in palladium-silver surface
Allan Abraham B. Padama. Hideaki Kasai, Yogi Wibisono Budhi: International Journal of Hydrogen Energy, **38**, 14715-14724 (2013).
5. Comparative Study on the Catalytic Activity of the TM-N₂ Active Sites (TM= Mn, Fe, Co, Ni) in the Oxygen Reduction Reaction: Density Functional Theory Study
Adhitya Gandaryus Saputro, Hideaki Kasai, Koichiro Asazawa, Hirofumi Kishi, and Hirohisa Tanaka: Journal of the Physical Society of Japan, **82**, 114704 (2013).
6. First Principles Study on the Electronic Structure and Properties of Sr- and Mg- Doped LaGaO₃
Triati Dewi Kencana Wungu, Mamoru Sakaue, Susan Meñez Aspera, Tran Linh PhanThuy, Musa Alaydrus, Hideaki Kasai, Tatsumi Ishihara: ECS Transactions, **57**(1), 2715-2722 (2013).
7. First-principles Study of the Lattice Strain Effects on the Ionic Migration Barrier of Sm-doped Ceria
Musa Alaydrus, Mamoru Sakaue, Susan Meñez Aspera, Triati Dewi Kencana Wungu, Tran Linh PhanThuy, Hideaki Kasai, Tatsumi Ishihara: ECS Transactions, **57**(1), 2733-2739 (2013).
8. Development of Novel Materials Through Computational Materials Design (CMD)
Hideaki Kasai, Susan Meñez Aspera, Adhitya Gandaryus Saputro: ECS Transactions, **53**(37), 1-6 (2013).
9. Investigations on the Structural and Electronic Properties of Pure and Doped Bulk Pr₂NiO₄ through First Principles Calculations

- Susan Meñez Aspera, Mamoru Sakaue, Musa Alaydrus, Triati Dewi Kencana Wungu, Tran Linh PhanThuy, Hideaki Kasai, Tatsumi Ishihara: ECS Transactions, **57**(1), 2753-2762 (2013).
10. Computational Studies on Ionic and Electronic Conduction of Rare-Earth-Based Oxides Based on Density Functional Theory
Mamoru Sakaue, Hideaki Kasai, Tatsumi Ishihara: ECS Transactions, **57**(1), 2411-2418 (2013).
 11. Alkaline-earth doped effect on oxygen vacancy migration in monoclinic lanthanum germanate: first-principles calculation
Tran Phan Thuy Linh, Mamoru Sakaue, Musa Alaydrus, Triati Dewi Kencana Wungu, Susan Menez Aspera, Hideaki Kasai, Tatsumi Ishihara: ECS Transactions, **57**(1), 1077-1083 (2013).
 12. Mechanistic insight into the Au-3d metal alloy-catalyzed borohydride electro-oxidation: From electronic properties to thermodynamics
Ryan Lacdao Arevalo, Mary Clare Sison Escano, Hideaki Kasai: ACS Catalysis, **3** 3031-3040 (2013).
 13. Dynamics of Mu, H, D, and T Absorption into Pd(111): Isotope Effects
Koji Shiizu, Wilson Agerico Dino, Hideaki Kasai: Journal of the Physical Society of Japan, **83**, 013601 (2014).
 14. Density functional theory study on the interaction of O₂ and H₂O₂ molecules with the active sites of cobalt-polypyrrole catalyst
Adhitya Gandaryus Saputro, Hideaki Kasai: Journal of the Physical Society of Japan, **83**, 24707-1 (2014).
 15. A density functional theory-based study on the dissociation of NO on CuO(110) surface
Joaquin Lorenzo Valmoría Moreno, Allan Abraham Bustria Padama, Hideaki Kasai: CrystEngComm, **16**, 2260-2265 (2014).
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— *Mean Field Picture of the Glass Transition*

MIYAZAKI, Kunimasa [B class; 1800 (A), 0 (B), 0 (C)] ()

— *Mean Field Picture of the Glass Transition*

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— *First-principles simulations of atomic geometries, electronic properties, and chemical reactions at interfaces*

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NOGUCHI, Hiroshi [C class; 0 (A), 5000 (B), 2300 (C)] (34,214)

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OBUSE, Hideaki [B class; 0 (A), 700 (B), 0 (C)] (248)

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ODA, Tatsuki [E class; 0 (A), 18000 (B), 1300 (C)] (59,61)

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ODAGAKI, Takashi [C class; 0 (A), 3500 (B), 1000 (C)] ()

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OGUCHI, Tamio [C class; 1500 (A), 5500 (B), 1900 (C)] (83)

— *First-Principles Calculation of Transition-Metal Compounds*

OHMURA, Satoshi [C class; 0 (A), 3500 (B), 0 (C)] (108)

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OKADA, Susumu [C class; 6000 (A), 1500 (B), 0 (C)] (94)

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— *Study on complex systems by generalized-ensemble algorithms*

OKITSU, Kouhei [C class; 10000 (A), 3000 (B), 1900 (C)] (188)

— *Study on phase determination of protein crystals based on an n -beam X-ray dynamical diffraction theory for an arbitrary number of n*

OKUBO, Tsuyoshi [C class; 3000 (A), 7000 (B), 3500 (C)] (192)

— *Ordering and dynamics of topological excitations in frustrated magnets*

— *Topological order in frustrated spin systems*

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OTANI, Minoru [E class; 0 (A), 10000 (B), 2000 (C)] (75)

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OTOMO, Junichiro [B,C class; 1300 (A), 3600 (B), 0 (C)] (100,102)

— *Synthesis of proton conducting electrolyte and evaluation of ion conductivity of interfaces*

— *Development of proton conducting solid electrolyte for intermediate temperature fuel cells*

— *Study on physicochemical properties for proton conductivity in lanthanum tungstate*

OZEKI, Yukiyasu [C class; 0 (A), 7000 (B), 1300 (C)] (201)

— *Numerical study on critical universalities for random systems including KT transition*

— *Dynamical scaling for nonequilibrium relaxation functions by the use of Bayesian inference and kernel method*

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RAEBIGER, Hannes [C class; 8500 (A), 2500 (B), 0 (C)] ()

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SAITO, Mineo [C class; 0 (A), 8500 (B), 0 (C)] (85)

— *First-Principles Calculations Concerning Spintronics*

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SAKAI, Toru [C class; 23500 (A), 8000 (B), 3800 (C)] (176,178)

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SAKURAI, Masahiro [B class; 0 (A), 1300 (B), 900 (C)] (123)

— *A study of electron self-energy using first-principles calculations*

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SATO, Toshihiro [C class; 0 (A), 5000 (B), 0 (C)] (159)

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SHIRO, Masanori [B class; 900 (A), 0 (B), 0 (C)] (241)

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— *Hybrid ab initio QM/MM calculations of biological macromolecular systems*

TATEYAMA, Yoshitaka [C,E class; 0 (A), 13500 (B), 1600 (C)] (66)

— *DFT statistical mechanics analysis of redox reaction mechanism at interfaces in catalysts and batteries*

— *DFT statistical mechanics analysis of redox reaction mechanisms at interfaces in catalysts and batteries*

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— *First-principles investigation on thermophysics of nano structures*

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— *Multipole ordering and magnetic, phononic and conduction properties of conduction systems*

WATANABE, Hiroshi [C class; 0 (A), 5000 (B), 1800 (C)] (217)

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YASUDA, Chitoshi [C class; 500 (A), 1500 (B), 400 (C)] (229)

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YOSHINO, Hajime [C,D class; 0 (A), 20500 (B), 0 (C)] (183)

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ASAI, Yoshihiro [R class; 0 (A), 0 (B), 3000 (C)] (265)— *Theory and computer simulation studies of non-equilibrium transport phenomena*

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SAITO, Mineo [R class; 0 (A), 0 (B), 5000 (C)] (262)

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YAMASHITA, Koichi [R class; 0 (A), 0 (B), 5000 (C)] (267)

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2. **THOMAS, Derek**
Theoretical study of thermoelectric properties of conical carbon nanofibers
The University of Tokyo, 2014-03-24
3. **ASANO, Yuta**
Phase diagram and equation of state of modified Lennard-Jones system
Ehime University, 2014-03-24
4. **TAE-UK, Park**
First-principles Study of Metal-atom Adsorption on Carbonic Systems
Chiba University, 2014-03-25
5. **KOBINATA, Kyouzuke**
First-principles Study of Schottky Barrier at Metal/Semiconductor Interfaces
Chiba University, 2014-03-25
6. **SAKAKIBARA, Hirofumi**
Study on the correlation between the transition temperature and the crystal structure in the cuprate superconductors
The University of Electro-Communications, 2014-03
7. **SUZUKI, Katsuhiro**
Theoretical analysis of superconductivity in multi-orbital systems
The University of Electro-Communications, 2014-03
8. **ASPERA, Susan**
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Osaka University, 2014-09-25
9. **QUANG, Nguyen**
Density Functional Theory-based Studies on Oxygen Interaction with Varied Catalytic Environments for Nano Technological Applications
Osaka University, 2014-09-25
10. **HARASHIMA, Yosuke**
Critical phenomena of the metal-insulator transition in doped semiconductors using density functional theory and local density approximation
Osaka University,
11. **KYOGOKU, Shinya**
Microscopic study on nano-scale deformation and electronic state of carbon nanotube
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12. **SHIMIZU, Ryotaro**
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13. **MOTOYAMA, Yuichi**

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□ Master Theses

1. **MIYAO, Satoaki**

Study of cuprate superconductors by element-substitution simulation
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2. **Sunnardianto Gagus Ketut**

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3. **ONISHI, Takashi**

First-principles study of spin-orbit interaction in ferroelectrics
Kawazawa University, 2014-03-22

4. **SATO, Kosuke**

Quantum dissociation processes of exciton at semiconductor hetero-interfaces
Chiba University, 2014-03-25

5. **HIRAMATSU, Tomoki**

Atom diffusion, segregation, and mixing at metal/semiconductor interfaces
Chiba University, 2014-03-25

6. **YOSHIDA, Kazuyuki**

Metal-atom diffusion in self-assembled monolayer molecules
Chiba University, 2014-03-25

7. **KIRII, Tomohiro**

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8. **KOJIMA, Yuhei**

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Tokyo Institute of Technology,

9. **MORI, Kouta**

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10. **MATSUSHIMA, Kyohei**

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11. **TAKASAKI, Eriko**

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12. **OBATA, Masao**
Development and application of electronic state calculation method based on the van der Waals density functional
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13. **SUGIHARA, Hiroki**
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14. **HAGINO, Shota**
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15. **HYUGA, Masahiko**
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16. **MOHRI, Souitirou**
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17. **HORITA, Toshiki**
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