

5 THESES

□ Doctor Theses

1. **AMAMIZU, Naoka**
Theoretical Study on Relationship between Open-Shell Electronic State and Electron Conductivity of Single Molecules and Their Aggregates toward Applications to Molecular Devices
Osaka University, 2025-03
2. **ARTUR, Akatov**
Electronic structures and their instability analysis in magnetic shape memory alloys Fe_3X ($\text{X}=\text{Pd}$, Pt) by quasiparticle self-consistent GW approach
Kanazawa University, 2025-03
3. **CHIDA, Takumi**
Green's function approach for computing physical quantities in the framework of the transcorrelated method
The University of Tokyo, 2025-03
4. **DE MELLO, Matheus**
Impact of charge distribution on the stability of ferroelectric nematic liquid crystals
Kyoto University, 2025-03
5. **DING, Mingda**
Investigation on control of graphene interlayer interaction by nanospacer insertion
Osaka University, 2025-03
6. **DOU, Ying**
Theoretical analysis of phonon behavior in group-III nitride device structures
The University of Tokyo, 2025-03
7. **ENRIQUEZ, John Isaac G.**
Quantum Engineering Design of Diamond Surfaces: Surface Facet Dependence in Oxidation and Thermal Degradation and Effectiveness of Dangling Bond Saturation on Graphitization Suppression and Control
Osaka University, 2024-07
8. **FURUTA, Tatsuhiko**
Development and application of machine learning methods for time series data in materials science: Analysis of fluorescence time series data of quantum dots and fluorescently modified DNA using hidden Markov models
Kyushu Institute of Technology, 2025-03
9. **GUO, Rulei**
Investigation of thermal conductance of complex heterogeneous interfaces using optical pump probe method
The University of Tokyo, 2025-03
10. **HARA, Keisuke**
Dynamics between transition metal oxide/dichalcogenide and adsorbed molecules
Chiba University, 2024-03
11. **HIRATA, Koichi**
Branching Structure and Mechanical Properties of Colloidal Gel Networks
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12. **IWASHITA, Wataru**
Theory of friction in macroscopic systems based on continuum analysis
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13. **KAKIZAWA, Fumiya**
Numerical approaches to many-body problems in condensed matter physics
Saitama University, 2025-03
14. **KOSHOJI, Ryotaro**
Crystal structure prediction based on space-filling principles
The University of Tokyo, 2024-03
15. **LI, Junhuan**
Fundamental study on finite-size graphene-based materials with unique electronic structures toward catalyst-assisted microfabrication of semiconductor surfaces
Osaka University, 2024-09
16. **LI, Xu**
Growth and elucidation of the structure of X-Ti-O (X = Ba, Ce, Yb) ultra-thin films on Pt(111)
Nagoya University, 2025-03
17. **LIANG, Shaoji**
Fabrication of equiaxed HCP Multi-Principal Element Alloys and elucidation of their deformation mechanisms
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18. **LUSTINEC, Jakub**
Study on first-principles electronic structures of the magnetic shape memory Heusler alloys by quasiparticle self-consistent GW method
Kanazawa University, 2024-09
19. **LYU, Xinliang**
Three-Dimensional Real Space Renormalization Group using Tensor-Network Reformulation
The University of Tokyo, 2024-09
20. **MAJUMDER, Rinku**
Study on the nanotwin boundary migration in the modulated martensite phases of magnetic shape memory alloy from first-principles
Kanazawa University, 2024-09
21. **MATSUTANI, Kenta**
Investigation of intermediate-range order in GeO₂ glass through computational simulations
Yamagata University, 2025-03
22. **MUGITA, Daigo**
Structural relaxation and development of local structure analysis methods for dense hard disk (triangle) systems using non-reversible Monte Carlo
Nagoya Institute of Technology, 2025-03
23. **NAGAHASHI, Tomoya**
Theoretical Studies on Growth Processes and Electronic Properties of SiN Used for Charge Trapping Layer of NAND Flash Memories
Nagoya University, 2025-03

24. **NEGAMI, Masahiro**
Durability improvement of thermal barrier coatings for industrial gas turbine
The University of Tokyo, 2024-09
25. **NOZAKI, Misa**
Theoretical studies on photoemission from organic materials
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26. **SEO, Insung**
Magnetic properties of rare-earth magnet compounds studied from first principles
Tokyo Institute of Technology, 2024-09
27. **YOSHIDA, Akira**
Thermodynamic characterization of small-scale mixtures and nonequilibrium phase coexistence systems
Ibaraki University, 2024-03
28. **YOSHIMURA, Masataka**
Computational analysis of protein-ligand interactions
The University of Tokyo, 2025-03

□ Master Theses

1. **ABE, Eijyu**
Magnetization process of a kagome antiferromagnet with $\{Y_3Cu_9(OH)_{19}Cl_8\}$ -type distortion
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Development of an extension program for photoelectron spectroscopy analysis to periodic materials
Chiba University, 2025-03
3. **ASHITAKA, Haruna**
Anion species dependence of liquid Madelung potentials
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4. **CHIBA, Isana**
First-principles calculation of TiO_2 surface
Iwate University, 2025-03
5. **ENDO, Ryusuke**
First-principles study on electronic structure of FePd/2D material interface
Kobe University, 2025-03
6. **FUJIMOTO, Itsuki**
First-principles magnetic anisotropy calculation in the interface PtCoO/ZnO between ferromagnetic metal and ferroelectric semiconductor
Kanazawa University, 2025-03
7. **FUNAKI, Nahoto**
First-principles analysis for effect of NO annealing on mobility of SiC MOS interface
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8. **GU, Yuhan**
Development of stretchable electret material for energy harvesting based on quantum chemistry
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9. **HASHIMOTO, Kazuki**
Magnetocrystalline anisotropy of permanent-magnet compounds
Institute of Science Tokyo, 2025-03
10. **HASHIMOTO, Kota**
A method for free-energy calculations with thermal expansion
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11. **HASHIMOTO, Masaru**
Numerical Study on the Magnetization Process of the Distorted Diamond Spin Chain
University of Hyogo, 2025-03
12. **HASHIMOTO, Taichi**
First-principles study on electron-transport properties in arsenene fluoride nanoloads
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13. **HORIGANE, Koki**
First-principles calculations of tunnel magnetoresistance effect in lattice-matched magnetic tunnel junction

Keio University, 2025-03

14. **IMAMURA, Ryo**
First-principles study of intrinsic hBN island nucleated during CVD initial growth on Cu(111)
Shimane University, 2025-03
15. **INOUE, Shinya**
Theoretical design of a fluorescence intensity-based ligand sensor protein
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16. **ITOKAZU, Shoichiro**
Microscopic theory for ferromagnetic transition in heavy fermion compound CeRh_6Ge_4
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17. **IWAKI, Kota**
First-principles study on carrier mobility in XC_6 ($\text{X}=\text{Si, Ge, Sn, Pb}$) nanoribbons
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18. **IWAMOTO, Yuya**
Theoretical design of a superlattice superconductor utilizing incipient band
Tottori University, 2025-03
19. **IWATA, Taiga**
Theoretical analysis of electrolyte decomposition process on lithium metal surface
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20. **JO, Hayate**
Free energies of β Ti-Al evaluated by first-principles cluster-expansion method
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21. **KANEMASU, Ikumi**
Ab initio Molecular Dynamics Study of the Deformation Properties and Healing Mechanisms in Calcium Silicate Hydrate
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22. **KASAI, Shoya**
Numerical Study of Superstructure Formation and Non-equilibrium Dynamics in Topological Spin Knots
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23. **KATO, Keita**
First-principles Calculations of Defect Formation Energy for $\text{Cu}_2\text{Sn}_{1-x}\text{Ge}_x\text{S}_3$
Nagaoka University of Technology, 2025-03
24. **KATO, Sae**
Theoretical design of protein folding pathways based on a statistical mechanical model
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First-principles electron-transport property simulation of C_nN_m /graphene heterostacked structures under stress
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Theoretical and Experimental Investigation of the Role of Surface Defect Sites in the Photocatal-

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Self-organized spatial inhomogeneity and final condensed states in self-propelled quasi-elastic hard disk systems
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Theoretical study on the stability of hydrogen impurity in cation-doped α -Al₂O₃
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Anharmonicity induced by thermal fluctuation and its impact on the thermal expansion of solids
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Theoretical design of nanographene realizing a 2-dimensional S=3/2 spin system derived from localized zero modes
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Development of a quantitative calculation method for electrode potential shifts
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Theoretical design of a novel bilayer nickelate superconductor
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33. **LIU, Yuxi**
High-performance Spectral Neighbor Analysis Potential for Al-Al₂O₃-H systems to investigate hydrogen embrittlement
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First-Principles study of the formation mechanism of one-dimensional silver ribbons on the Ni(110) surface using the nudged elastic band method
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35. **MATIN, Jubayer**
Study on methods to optimize the first-principles computation of phonons in materials with disordered configurations
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36. **MATSUMOTO, Ryo**
Multi-principal effect on phase transformation in TiHfNiPd shape memory alloys
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Theoretical study on electrical conduction properties of spiral graphene
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38. **MIYAKO, Yuki**
Exploration for stable surface structures and theoretical prediction of band positions for diamond and zinc-blende structures from first-principles lattice-dynamics calculations

Institute of Science Tokyo, 2025-03

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Construction of machine learning potentials toward exploration of high-entropy alloy cluster catalysts
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First-principles electronic structure calculation and carrier density analysis of manganese thin film on sapphire substrate
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41. **MURABAYASHI, Fumihito**
Microwave response of edge states in the fractional quantum Hall droplet
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Prediction of the folding and binding mechanisms of an intrinsically disordered protein using an extended statistical mechanical model
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Electronic structure calculations of novel p-type semiconductor materials with extended π -conjugated DPP derivatives
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High-throughput molecular dynamics for advanced electrolyte discovery
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Critical phenomena and network analysis in Vicsek model systems with non-reciprocal interactions
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Electronic and optical properties of non-stoichiometric lithium niobates
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48. **NODA, Hinata**
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Development and the Reaction Mechanism of CO₂ Photoreduction to Fuels/Resources Using First Row Transition Metal Nanoparticles Supported on ZrO₂
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GNN prediction of cavity-induced hopping motion in deeply supercooled binary hard disk systems
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Analyses of the aging process in scale-free networks
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Analysis of the adsorption structure and electronic state of DPh-BTBT/Ag based on multiple scattering theory
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Series expansion study of magnon spectra in triangular lattice antiferromagnets with interlayer coupling
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Phonon localization and electron transport control in two-dimensional layered materials
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Study on Enhancement of Correlation Functions due to Bond Deficit in Antiferromagnets
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Analysis of ion transport in tantalum oxide using persistent homology
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Impact of local structures of silicon grain boundaries on their interfacial thermal resistance investigated using machine learning potential
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59. **TANAKA, Junya**
Evaluation for thermal transition temperature of a quantum spin model by machine learning technique
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60. **TANG, Ruona**
Ti-Al-O ternary phase diagram constructed using machine learning
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Theoretical study of spin-fluctuation and superconductivity in incipient band systems
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64. **WADASHIMA, Shusei**
Numerical study of spin liquid and glass behavior in quantum spin models with all-to-all p -spin interactions
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65. **WATARAI, Ryota**
First-principles study on magnetocrystalline anisotropy of Co_2FeSi and Co_3Mn
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66. **YAMAI, Shin**
Crystal Structure Prediction of $\text{Li}_x\text{Ca}_{1-x}\text{Cl}_{2-x}$ Using Evolutionary Algorithm and Cluster Expansion
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67. **YAMAMOTO, Ayumu**
Rheological Analysis of Polymer Blends Using Coarse-Grained Molecular Dynamics Simulations
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Modulation in electronic states of cleaved topological insulator Bi_2Se_3 by surface reconstruction
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Multi-Objective Generative Adversarial Network for Inorganic Chemical Compositions
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70. **YAMANAKA, Masayoshi**
First-principles study of goniopolar thermoelectric material $\text{Mg}_3(\text{Sb,Bi})_2$
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71. **YONEYAMA, Haruki**
Theoretical analysis and derivation of effective model for the ladder type iron-based superconductors
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First-principles calculations for the electronic structure of Ca_2MnO_4 : Evaluation of the effect of oxygen octahedral rotation on low-energy properties
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73. **YUKI, Kanae**
First-Principles Molecular Dynamics Study of Ionic Diffusion Mechanism of RbAg_4I_5
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74. **YUSE, Ryo**
Application of machine learning to incomplete information games about Geister
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