

5 THESES

□ Doctor Theses

1. **AKAMATSU, Katsuya**
Adaptive tensor trees for generative modeling
The University of Tokyo, 2025-10
2. **BAO, Jiahui**
Theory of Nel and Hidden Orders in Perovskite Magnets
Okinawa Institute of Science and Technology, 2026-03
3. **FUJII, Akihiro**
Development of a materials design framework utilizing property-prediction models and their gradients
The University of Tokyo, 2026-03
4. **FENG, Peijie**
Nitrogen Diffusion into Iron-Based Materials under High Temperature
The University of Tokyo, 2026-01
5. **KHINEVICH, Viktor**
Developing Efficient Quantum Algorithms for State Preparation and Post-Processing in Quantum Chemistry
The University of Osaka, 2026-03
6. **LU, Shaocong**
Spin-Fluctuations in Hydride Superconductors from First Principles
The University of Tokyo, 2025-09
7. **MAHMUD Rabiatul Aliah Binti**
Theoretical and Experimental Investigations of the Enhancement of ZnO Semiconductor as a Photocatalyst: Insights into the Reduction of CO₂
The University of Osaka, 2026-04
8. **MASUDA, Shuya**
Development of metal-oxide photoelectrodes using computational materials science
Nara Institute of Science and Technology, 2026-03
9. **MATSUKIYO, Hiroki**
Numerical and theoretical study on active fluids under spatial confinements
Kyushu University, 2026-03
10. **MATSUZAKA, Mizuki**
A Study on Organic Spin Valves Using Functional Molecules
Keio University, 2026-03
11. **MIURA, Shohei**
Verification of the durability of halide perovskite materials using first-principles calculations
Kanazawa University, 2026-03
12. **MIZUHARA, Aoi**
Atomistic study of the initial stages of metal heteroepitaxial growth
Osaka Metropolitan University, 2026-03

13. **OISHI, Yasuhiro**
Computational study of conformational changes in a PASE molecule and an amyloid- β (20-34) peptide
University of Hyogo, 2026-03
14. **ONO, Mizuho**
First-Principles Study of Energy Conversion Pathway in Ultrafast Light-Matter Interaction
Tohoku University, 2026-03
15. **OSHIMA, Hisanori**
Symmetry and Topology for Measurement-Induced Phase Transitions
The University of Tokyo, 2026-03
16. **PUTRI, Salsabila Amanda**
First-Principles Study of Spin-Splitting in Janus Transition Metal Dichalcogenides
Kanazawa University, 2026-03
17. **ROJAs, Kurt Irvin Medina**
First-Principles Exploration of the Chemical and Spectral Properties of Hydrogen Boride Sheets
The University of Osaka, 2025-09
18. **SALEH, Md Abu**
Water Dynamics around Osmolytes and Polymers Using Molecular Dynamics Simulations: Insights for the Design of Effective Protein Stabilizers
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19. **SATO, Masanori**
First-principles study of Pentacene adsorption on the surfaces of the Tsai-type Ag-In-Yb quasicrystal
Kagoshima University, 2026-03
20. **SHIOTA, Tomoya**
Developing Quantum-Classical Hybrid Interfaces for Solving Realistic Atomic Scale Chemical Problems
The University of Osaka, 2025-09
21. **TAKAHARA, Wataru**
Development of a Data-Driven Approach for the Discovery of Novel Photocatalysts
Nara Institute of Science and Technology, 2026-03
22. **TEWENG, Yedija Yusua Sibuea**
First-Principles Study of the Shift Current in Perovskite CsPbI₃
Kanazawa University, 2026-03

□ Master Theses

1. **ARAI, Atsuro**
Theoretical Study on Magnetism and Superconductivity in the Kitaev-Heisenberg Ladder Model
The University of Tokyo, 2026-03
2. **ASAKURA, Yuto**
Influence of molecular torsion on the Soret effect
Kyoto University, 2026-03
3. **BANDHASO, David**
First-principles study of BaTiO₃/BaRuO₃
Kanazawa University, 2025-09
4. **CHADIZA, Nadia Maharani**
First-principles study of dielectric properties of BN multilayers
Kanazawa University, 2025-09
5. **FENG, Fan**
Electronic structures of lanthanum copper oxide using quasi-particle self-consistent GW method
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6. **FUJII, Akio**
Defect calculation of ZnM₂O₄ (M=Co,Rh,Ir) spinel by SCAN
Yokohama National University, 2025-03
7. **FUJIMORI, Shota**
Molecular Dynamics study of the electrical double layer and solvent molecules in electrolyte solutions
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8. **HAMURO, Shinasaku**
Theoretical study of p-n coexisting thermoelectric materials based on first-principles calculations
Shimane University, 2026-03
9. **HARADA, Masahiro**
Experimental and Theoretical Study of the Physical Properties of a Firefly Bioluminescence Substrate Analog: seMpai
Gunma University, 2024-03
10. **HASHIMOTO, Chika**
Fabrication of molecular nanojunctions utilizing magnetic thin-film edges and first-principles calculations
Keio University, 2026-03
11. **HATTORI, Kazuki**
Systematic First-Principles Study of Structural and Elemental Dependence of Lattice Thermal Transport in Zintl-Based Thermoelectric Materials
Keio University, 2025-03
12. **HAYASHI, Eisuke**
Diffusional characteristics and non-equilibrium phase transitions of active glass model in dense binary hard disk systems
Nagoya Institute of Technology, 2026-03

13. **HIDA, Ichika**
Research on Hydrogen Isotope Effects in Water Electrolysis/Fuel Cells Using Fe-Based Catalysts
Hokkaido University, 2026-03
14. **HIDAKA, Kotaro**
Statistical machine learning analysis of the blinking phenomenon of fluorescent molecules: Development of Poisson-emission type hidden Markov model
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15. **HIRATA, Yusaku**
Predicting the folding process of a structurally complex protein using statistical mechanical models
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16. **HOSHI, Yuto**
Theoretical analysis and material design of high- T_c superconductors by performing fluctuation exchange approximation
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17. **HOSODA, Masakage**
Molecular dynamics study of scaling law for droplet growth
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18. **HWANG, Youngseok**
Theoretical study on the stability of hydrogen impurities at the α -Al₂O₃/Fe interface
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19. **IKEGAMI, Sogen**
Quantum phenomena arising from competition between distinct topological phases in two-dimensional systems
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20. **IRIE, Yusuke**
Electrode potential in ionic liquid
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21. **ITO, Daigo**
First-principles method to calculate force constants using spherical tensors
Institute of Science Tokyo, 2026-03
22. **ITO, Sayaka**
Exploration of magnetic compounds by first-principles calculations and machine learning
Institute of Science Tokyo, 2026-03
23. **KADOWAKI, Reo**
Molecular dynamics simulations of photoresponsive membrane modulator molecules that enhance the membrane permeation of drugs with low cell-membrane permeability.
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24. **KAJIHARA, Aoi**
Theoretical study on spin current generation via topological spin textures
The University of Tokyo, 2026-03
25. **KASAI, Yuki**
Cluster-expansion method refined by Bayes compressing sensing

Institute of Science Tokyo, 2026-03

26. **KATO, Shinya**
Density Functional Theory Study of Influence of Molybdenum in Suppressing Hydrogen Embrittlement in bcc Iron
Kyoto University of Advanced Science, 2026-03
27. **KATSUTA, Takumi**
High-precision magnetic anisotropy analysis and its application to spintronics materials based on first-principles calculations
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28. **KAWATSU, Tomohide**
Magnetization Plateau of the $S=3/2$ Antiferromagnetic Chain with the Biquadratic Interaction
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29. **KIMURA, Kanta**
Verification of the accuracy of spinon variational wave-functions in the antiferromagnetic Heisenberg model -comparison with the exact diagonalization method-
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30. **KOBAYASHI, Koki**
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31. **KOBAYASHI, Mutsumi**
Analyzing the internal structure of restricted Boltzmann machines trained on classical music
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33. **KONDO, Yuki**
Flyer-Target simulation of shock waves in crystal-fluid impact in hard disk systems
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34. **KOSUGI Kaito**
Li-ion Diffusion Mechanisms in $\text{Li}_{2-2x}\text{Mg}_{1+x}\text{Cl}_4$ Studied by Molecular Dynamics Simulations
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35. **KUBO, Mahiro**
Theoretical study on work function of multilayer graphene on SiC and its origin
Shimane University, 2026-03
36. **KUMANO, Shinsuke**
Multi-orbital extended Hubbard model for $\text{GaBa}_2\text{CuO}_4\text{F}$ with stacked CuO_2 and buffer layers
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37. **KUWABARA, Shuta**
Theoretical Analysis of Electronic Properties in Transition Metal Alloys using Coherent Potential Approximation Based on Wannier Functions
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38. **MASUMI, Sao**
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39. **MASTSUDA, Kotaro**
Hydrogen Diffusion on Stepped Ru Surface
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First-principles study on stability and electronic structure of NiFe/2D material interface
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41. **MATSUMOTO, Sora**
Theoretical material design of new superconductor with malleability and ductility
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Molecular Dynamics Simulations on the Surface Segregation of CuZn Surfaces in Methanol Synthesis by using Machine-Learning Interatomic Potential
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Quantitative analysis of pedestrian counter-flow under congested conditions using a floor field model
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51. **NIWA, Haruya**
Analysis on electronic properties of spinel transition-metal oxides by first-principles GW method
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First-Principles Study of NO Detection Based on Fe-doped (6,4) Single-Walled Carbon Nanotubes
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First-principles computational study on electronic structures and optical properties in the zinc pyrovanadates
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First-principles study of tensile test for carbon nanotubes
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60. **SAKAI, Akihiro**
Mechanism of d-wave superconductivity induced by interlayer Coulomb interaction in bilayer nickelates
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61. **SAKANOE, Ryuji**
Development of a magnetic EXAFS analysis method for Co_2FeSi
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 Magnon Dispersion Analysis in Layered Nickelates Using the Frozen Magnon Method
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 Quantum Monte Carlo Study on Phase Transition Temperatures in Quasi-Two-Dimensional Ferromagnets
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68. **SHINOZAKI, Hiyori**
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69. **SHOGAN, Rikuto**
 Mechanical Property of High-Entropy MXene
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70. **SUGIYAMA, Kosei**
 First-principles study on electronic structure and conduction property of 4H-SiC/SiO₂ interface after NO annealing
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71. **SUGIYONO, Vani**
 First-principles study of ferroelectricity in BaTiO₃ thin-film
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72. **SUZUKI, Haruto**
 Theoretical Study on the Ground State of the Heisenberg Antiferromagnet on the Distorted Shastry-Sutherland Lattice
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73. **SYAWLY, Adzky Mathla**
 First-principles crystal structure prediction for SnSe
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74. **TAKAHASHI, Tomoya**
 Numerical calculations of dynamical spin structure factor using tensor networks and their application to a quasi-one-dimensional antiferromagnet YbAlO₃
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75. **TANAKA, Naotaka**
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76. **TSUGAWA, Tomoya**
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77. **USHIO, Kensei**
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78. **WATANABE, Atsuya**
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85. **YASHIMA, Givenname**
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87. **ZHANG Ziyong**
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