Terumasa Tadano

Curriculum Vitae

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Research Interests

Anharmonicity ·Thermal transport ·Thermoelectrics ·Electron–phonon interaction ·Permanent magnets ·Perovskites ·Methodology development ·Numerical algorithms

Education

- **2013** — Ph.D. in Physics, University of Tokyo (Advisor: Prof. Shinji Tsuneyuki)
- **2010** — M.Sc. in Physics, University of Tokyo (Advisor: Prof. Shinji Tsuneyuki)
- **2008** — B.Sc. in Physics, Keio University

Employment

- **Apr 2024** – Group Leader, National Institute for Materials Science (NIMS), Japan
- **Apr 2021** – **Mar 2024** — Senior Researcher, NIMS, Japan
- **Apr 2019** – **Mar 2021** — Researcher, NIMS, Japan
- **Jan 2017** – **Mar 2019** — ICYS Fellow, NIMS, Japan
- **Oct 2016** – **Dec 2016** — Postdoctoral Researcher, NIMS, Japan
- **Apr 2015** – **Sep 2016** — Postdoctoral Researcher, Dept. of Applied Physics, University of Tokyo (Advisor: Prof. Masatoshi Imada)
- **Apr 2013** – **Mar 2015** — Postdoctoral Researcher, Dept. of Physics, University of Tokyo (Advisor: Prof. Shinji Tsuneyuki)

Awards

- **Apr 2025** — The 20th NIMS President Award: Research Encouragement
- **May 2024** — HPCI Software Award for Excellence (First Prize), Development Category
- **Apr 2024** — The Young Scientists' Award, MEXT
- **Nov 2021** — Condensed-Matter Science Prize (Theory Division)
- **Mar 2019** — Young Scientist Award, Physical Society of Japan
- **Nov 2018** — Best Presentation Award, 38th Electronics Division Meeting of CerSJ
- **Sep 2017** — ECT2017 Poster Award
- **Aug 2014** — CSW2014 Young Investigator Award

Grants

- **Apr 2025 – Mar 2030** — Grant-in-Aid for Transformative Research Areas (A), "Correlation Design Science", MEXT (Co-investigator; PI: Prof. R. Arita)
- **Apr 2024 – Mar 2027** — Grant-in-Aid for Scientific Research (A), MEXT (Co-investigator; PI: Prof. R. Arita)
- **Oct 2023 – Mar 2027** — PRESTO, JST
- **Apr 2023 – Mar 2026** — Grant-in-Aid for Scientific Research (A), MEXT (Co-investigator; PI: Prof. D. Chiba)
- **Apr 2021 – Mar 2024** — Grant-in-Aid for Scientific Research (C), MEXT
- **Apr 2020 – Mar 2023** — Grant-in-Aid for Scientific Research (B), MEXT (PI: Dr. Y. Miura)
- **Oct 2019 – Mar 2022** — Elements Strategy Initiative Center for Magnetic Materials (ESICMM), MEXT
- **May 2016 – Mar 2021** — Grant-in-Aid for Scientific Research (S), MEXT (PI: Prof. M. Imada)
- **Jan 2017 – Mar 2019** — NIMS ICYS Research Grant (Internal)
- **Apr 2016 – Mar 2019** — Grant-in-Aid for Encouragement of Young Scientists (B), MEXT

Peer-reviewed Papers

1. Z. Li, H. Yuan, A. A. Belik, **T. Tadano**, Y. Tsujimoto, and K. Yamaura, "Giant lattice expansion through structural frustration release in a dense oxide", *J. Am. Chem. Soc.* **148**, 22380–22388 (2026). DOI
2. M. Ohnishi, T. Deng, P. Torres, Z. Xu, **T. Tadano**, H. Zhang, W. Nong, M. Hanai, Z. Tian, M. Hu, X. Ruan, R. Yoshida, T. Suzumura, L. Lindsay, A. J. H. McGaughey, T. Luo, K. Hippalgaonkar, and J. Shiomi, "Database and deep-learning scalability of anharmonic phonon properties by automated brute-force first-principles calculations", *npj Comput. Mater.* **12**, 150 (2026). DOI
3. K. Murayama, R. Masuki, C. Tassel, H. Sakai, T. Yanagisawa, K. Yoshida, H. Oike, S. Yoshida, X. Gu, K. Ishida, M. Namba, K. Denisova, V. Dupray, S. Clevers, O. Mentré, T. Nomoto, **T. Tadano**, C. M. Brown, P. Lemmens, R. Arita, H. Takatsu, and H. Kageyama, "Lattice softening and diffusive dynamics in the polar metal $LiReO_3$", *Sci. Adv.* **12**, eadt3886 (2026). DOI
4. R. Higuchi, X. He, T. Katase, **T. Tadano**, and T. Kamiya, "Enhanced thermoelectric performance by inverted thermal conductivity anisotropy in layered AE_2ZnN_2 (AE = Ca, Sr, Ba) with rigid interlayer bonds", *J. Phys. Chem. C* **130**, 6425–6436 (2026). DOI

5. E. Xiao and **T. Tadano**, "Accurate screening of functional materials with machine-learning potential and transfer-learned regressions: Heusler alloy benchmark", *npj Comput. Mater.* **12** (2026). DOI
6. X. Tang, Y. Miura, N. Terada, E. Xiao, S. Kobayashi, A. Döring, **T. Tadano**, A. Martin-Cid, T. Ohkochi, S. Kawaguchi, Y. Matsushita, T. Ohkubo, T. Nakamura, K. Skokov, O. Gutfleisch, K. Hono, and H. Sepehri-Amin, "Control of covalent bond enables efficient magnetic cooling", *Adv. Mater.* **38**, e14295 (2026). DOI
7. X. He, K. Ogata, **T. Tadano**, H. Hiramatsu, T. Kamiya, and T. Katase, "Simultaneous enhancement of power factor and suppression of thermal conductivity in bulk $TlFe_{1.6}Se_2$ via embedded atomically thin FeSe layers", *J. Mater. Chem. A* (2026). DOI
8. M. Morishita, **T. Tadano**, Y. Matsuoka, and T. Abe, "Mechanism of solid ammonia stabilization at ambient temperature: Insights from thermodynamics, phonon calculation, and micromechanics", *ACS Omega* **10**, 57684–57691 (2025). DOI
9. R. Asai, R. Arita, T. Chida, R. Masuki, K. Kuroki, and **T. Tadano**, "Finite-temperature ab initio structural optimization of the bilayer nickelate superconductor $La_3Ni_2O_7$", arXiv:2512.08251 (2025). arXiv
10. A. J. H. McGaughey, L. Lindsay, H. Bao, T. Hamakawa, R. Juneja, S. Li, W. Li, R. Masuki, F. Meng, H. Meng, T. Pandey, C. Shao, J. Shiomi, **T. Tadano**, A. Togo, A. Wang, and X. Zhang, "Phonon Olympics: Phonon property and lattice thermal conductivity benchmarking from open-source packages", *J. Appl. Phys.* **138** (2025). DOI
11. E. Xiao and **T. Tadano**, "High-throughput computational screening of Heusler compounds with phonon considerations for enhanced material discovery", *Acta Mater.* **297**, 121312 (2025). DOI
12. K. Oyanagi, H. Sepehri-Amin, K. Takamori, **T. Tadano**, T. Imamura, R. Nagasawa, K. Mahalingam, T. Hirai, F. Ando, Y. Sakuraba, S. Kobayashi, and K. Uchida, "Simultaneous achievement of large anomalous Nernst effect and reduced thermal conductivity in sintered polycrystalline topological Heusler ferromagnets", *Acta Mater.* **296**, 121239 (2025). DOI
13. X. He, T. Komatsu, T. Katase, **T. Tadano**, T. Honda, M. Miyazaki, M. Kitano, H. Hiramatsu, H. Hosono, and T. Kamiya, "Strong phonon scattering and enhanced thermoelectric performance in $SrTiO_3$ polycrystals by simultaneous hydrogen substitution and oxygen vacancy formation", *ACS Appl. Energy Mater.* **8**, 11447–11455 (2025). DOI
14. D. C. Sorescu, **T. Tadano**, and W. A. Saidi, "Theoretical investigations of anharmonic effects and phonon transport in the cubic phase of crystalline perovskite CsPbCl3", *J. Phys. Chem. C Nanomater. Interfaces* **129**, 13445–13456 (2025). DOI
15. R. Pohle, Y. Motome, **T. Tadano**, and S. Hoshino, "Electron-phonon coupled Langevin dynamics for Mott insulators", arXiv:2507.19764 (2025). arXiv
16. P. Wisesa, **T. Tadano**, and W. A. Saidi, "Deep-learning neural network potentials for titanate perovskites", *Comput. Mater. Sci.* **250**, 113719 (2025). DOI
17. R. Matsumoto, K. Yamane, **T. Tadano**, K. Terashima, T. Shinmei, T. Irifune, and Y. Takano, "Emergence of superconductivity at 20 K in Th_3P_4-type $In_{3-x}S_4$ synthesized by Diamond anvil cell with boron-doped Diamond electrodes", *Chem. Mater.* **37**, 1648–1656 (2025). DOI
18. M. Hiramatsu, Z. Hu, S. Yoshikawa, Z. Yang, X. He, T. Katase, J. Yamaura, H. Sagayama, **T. Tadano**, S. Ueda, H. Hiramatsu, H. Hosono, and T. Kamiya, "Nonequilibrium layered PbS stabilized by Sn doping: Bipolar semiconductors with low thermal conductivity", *ACS Appl. Electron. Mater.* **6**, 8339–8350 (2024). DOI
19. R. Masuki, T. Nomoto, R. Arita, and **T. Tadano**, "Continuous crossover between insulating ferroelectrics and polar metals: Ab initio calculation of structural phase transitions of $LiBO_3$ (B = Ta, W, Re, Os)", *Phys. Rev. B.* **110** (2024). DOI
20. G. Xing, K. Masuda, **T. Tadano**, and Y. Miura, "Chemical-substitution-driven giant anomalous Hall and Nernst effects in magnetic cubic Heusler compounds", *Acta Mater.* **270**, 119856 (2024).

DOI
21. N. Abe, Y. Hano, H. Ishizuka, Y. Kozuka, **T. Tadano**, Y. Tsujimoto, K. Yamaura, S. Ishiwata, and J. Fujioka, "Large anomalous Hall effect in spin fluctuating devil's staircase", *npj Quantum Materials* **9**, 1–8 (2024). DOI
22. M. Basini, M. Pancaldi, B. Wehinger, M. Udina, V. Unikandanunni, **T. Tadano**, M. C. Hoffmann, A. V. Balatsky, and S. Bonetti, "Terahertz electric-field-driven dynamical multiferroicity in SrTiO3", *Nature* **628**, 534–539 (2024). DOI
23. J. Yue, Y. Liu, W. Ren, S. Lin, C. Shen, H. Kumar Singh, T. Cui, **T. Tadano**, and H. Zhang, "Role of atypical temperature-responsive lattice thermal transport on the thermoelectric properties of antiperovskites Mg3XN (X = P, As, Sb, Bi)", *Materials Today Physics* **41**, 101340 (2024). DOI
24. X. He, S. Kimura, T. Katase, **T. Tadano**, S. Matsuishi, M. Minohara, H. Hiramatsu, H. Kumigashira, H. Hosono, and T. Kamiya, "Inverse-Perovskite Ba_3BO (B = Si and Ge) as a High Performance Environmentally Benign Thermoelectric Material with Low Lattice Thermal Conductivity", *Adv. Sci.*, e2307058 (2023).
25. Y. Kozuka, T. T. Sasaki, **T. Tadano**, and J. Fujioka, "Epitaxy and transport properties of alkali-earth palladate thin films", *Sci. Technol. Adv. Mater.* **24**, 2265431 (2023).
26. M. Morishita, T. Abe, T. Ohkubo, **T. Tadano**, H. Yamamoto, A. Nozaki, and H. Miyazaki, "Magnetic characterization of Sm(Fe1-x, Cox)11Ti (x = 0, 0.1) determined by heat-capacity measurement from very low to high temperatures", *Thermochim. Acta* **727**, 179573 (2023).
27. I. Kurniawan, Y. Miura, G. Xing, **T. Tadano**, and K. Hono, "Theoretical study of the effect of lattice dynamics on the damping constant of FePt at finite temperature", *Phys. Rev. B* **108**, 094426 (2023).
28. K. Kazama, M. Sakano, K. Yamagami, T. Ohkochi, K. Ishizaka, **T. Tadano**, Y. Kozuka, H. Yoshizawa, Y. Tsujimoto, K. Yamaura, and J. Fujioka, "Charge transport and thermopower in the electron-doped narrow gap semiconductor $Ca_{1-x}La_xPd_3O_4$", *Phys. Rev. Mater.* **7**, 085402 (2023).
29. G. Xing, Y. Miura, and **T. Tadano**, "First-principles prediction of phase transition of YCo_5 from self-consistent phonon calculations", *Phys. Rev. B* **108**, 014304 (2023). DOI
30. E. Fransson, P. Rosander, F. Eriksson, J. M. Rahm, **T. Tadano**, and P. Erhart, "Limits of the phonon quasi-particle picture at the cubic-to-tetragonal phase transition in halide perovskites", *Communications Physics* **6**, 1–7 (2023).
31. D. B. Khadka, Y. Shirai, M. Yanagida, **T. Tadano**, and K. Miyano, "Alleviating Defect and Oxidation in Tin Perovskite Solar Cells Using a Bidentate Ligand", *Chem. Mater.* **35**, 4250–4258 (2023).
32. A. Togo, L. Chaput, **T. Tadano**, and I. Tanaka, "Implementation strategies in phonopy and phono3py", *J. Phys. Condens. Matter* (2023).
33. C. Shen, M. Dai, X. Xiao, N. Hadaeghi, W. Xie, A. Weidenkaff, **T. Tadano**, and H. Zhang, "Impact of quartic anharmonicity on lattice thermal transport in EuTiO3: A comparative theoretical and experimental investigation", *Materials Today Physics* **34**, 101059 (2023).
34. R. Masuki, T. Nomoto, R. Arita, and **T. Tadano**, "Full optimization of quasiharmonic free energy with an anharmonic lattice model: Application to thermal expansion and pyroelectricity of wurtzite GaN and ZnO", *Phys. Rev. B Condens. Matter* **107**, 134119 (2023).
35. X. He, S. Nomoto, T. Komatsu, T. Katase, **T. Tadano**, S. Kitani, H. Yoshida, T. Yamamoto, H. Mizoguchi, K. Ide, H. Hiramatsu, H. Kawaji, H. Hosono, and T. Kamiya, "Hydride anion substitution boosts thermoelectric performance of polycrystalline $SrTiO_3$ via simultaneous realization of reduced thermal conductivity and high electronic conductivity", *Adv. Funct. Mater.* **n/a**, 2213144 (2023).
36. Z. Hu, M. Hiramatsu, X. He, T. Katase, **T. Tadano**, K. Ide, H. Hiramatsu, H. Hosono, and

T. Kamiya, "Reversible Thermal Conductivity Modulation of Non-equilibrium $(Sn_{1-x}Pb_x)S$ by 2D–3D Structural Phase Transition above Room Temperature", *ACS Appl. Energy Mater.* **6**, 3504–3513 (2023).

37. T. Amano, T. Yamazaki, R. Akashi, **T. Tadano**, and S. Tsuneyuki, "Lattice dielectric properties of rutile TiO2: First-principles anharmonic self-consistent phonon study", *Phys. Rev. B Condens. Matter* **107**, 094305 (2023).
38. R. Masuki, T. Nomoto, R. Arita, and **T. Tadano**, "Ab initio structural optimization at finite temperatures based on anharmonic phonon theory: Application to the structural phase transitions of BaTiO3", *Phys. Rev. B Condens. Matter* **106**, 224104 (2022).
39. **T. Tadano** and W. A. Saidi, "First-Principles Phonon Quasiparticle Theory Applied to a Strongly Anharmonic Halide Perovskite", *Phys. Rev. Lett.* **129**, 185901 (2022).
40. D. B. Khadka, Y. Shirai, M. Yanagida, **T. Tadano**, and K. Miyano, "Interfacial embedding for high-efficiency and stable methylammonium-free perovskite solar cells with fluoroarene hydrazine", *Adv. Energy Mater.* **12**, 2202029 (2022).
41. Y. Nishimura, X. He, T. Katase, **T. Tadano**, K. Ide, S. Kitani, K. Hanzawa, S. Ueda, H. Hiramatsu, H. Kawaji, H. Hosono, and T. Kamiya, "Electronic and lattice thermal conductivity switching by 3D–2D crystal structure transition in nonequilibrium $(Pb_{1-x}Sn_x)Se$", *Adv. Electron. Mater.* **8**, 2200024 (2022).
42. K. Cho, H. Tahara, T. Yamada, H. Suzuura, **T. Tadano**, R. Sato, M. Saruyama, H. Hirori, T. Teranishi, and Y. Kanemitsu, "Exciton-Phonon and Trion-Phonon Couplings Revealed by Photoluminescence Spectroscopy of Single CsPbBr3 Perovskite Nanocrystals", *Nano Lett.* **22**, 7674–7681 (2022).
43. A. Togo, H. Hayashi, **T. Tadano**, S. Tsutsui, and I. Tanaka, "LO-mode phonon of KCl and NaCl at 300 K by inelastic x-ray scattering measurements and first principles calculations", *J. Phys. Condens. Matter* **34**, 365401 (2022).
44. M. Ohnishi, **T. Tadano**, S. Tsuneyuki, and J. Shiomi, "Anharmonic phonon renormalization and thermal transport in the type-I Ba8Ga16Sn30 clathrate from first principles", *Phys. Rev. B Condens. Matter* **106**, 024303 (2022).
45. M. Hirayama, M. T. Schmid, **T. Tadano**, T. Misawa, and M. Imada, "*Ab initio* material design of Ag-based oxides for high-T_c superconductor", arXiv:2207.12595 (2022). arXiv
46. X. He, H. Zhang, T. Nose, T. Katase, **T. Tadano**, K. Ide, S. Ueda, H. Hiramatsu, H. Hosono, and T. Kamiya, "Degenerated Hole Doping and Ultra-Low Lattice Thermal Conductivity in Polycrystalline SnSe by Nonequilibrium Isovalent Te Substitution", *Adv. Sci.* **9**, e2105958 (2022).
47. G. Xing, Y. Miura, and **T. Tadano**, "Lattice dynamics and its effects on magnetocrystalline anisotropy energy of pristine and hole-doped YCo5 from first principles", *Phys. Rev. B Condens. Matter* **105**, 104427 (2022).
48. R. Masuki, T. Nomoto, R. Arita, and **T. Tadano**, "Anharmonic Grüneisen theory based on self-consistent phonon theory: Impact of phonon-phonon interactions neglected in the quasiharmonic theory", *Phys. Rev. B Condens. Matter* **105**, 064112 (2022).
49. P. Torres, S. Wu, S. Ju, C. Liu, **T. Tadano**, R. Yoshida, and J. Shiomi, "Descriptors of intrinsic hydrodynamic thermal transport: screening a phonon database in a machine learning approach", *J. Phys. Condens. Matter* **34**, 135702 (2022).
50. T. Katase, X. He, **T. Tadano**, J. M. Tomczak, T. Onozato, K. Ide, B. Feng, T. Tohei, H. Hiramatsu, H. Ohta, Y. Ikuhara, H. Hosono, and T. Kamiya, "Breaking of Thermopower-Conductivity Trade-Off in LaTiO3 Film around Mott Insulator to Metal Transition", *Adv. Sci.* **8**, e2102097 (2021).
51. K. Masuda, **T. Tadano**, and Y. Miura, "Crucial role of interfacial s−d exchange interaction in the temperature dependence of tunnel magnetoresistance", *Phys. Rev. B Condens. Matter* **104**,

L180403 (2021).
52. M. Kimura, X. He, T. Katase, **T. Tadano**, J. M. Tomczak, M. Minohara, R. Aso, H. Yoshida, K. Ide, S. Ueda, H. Hiramatsu, H. Kumigashira, H. Hosono, and T. Kamiya, "Large phonon drag thermopower boosted by massive electrons and phonon leaking in LaAlO3/LaNiO3/LaAlO3 heterostructure", *Nano Lett.* **21**, 9240–9246 (2021).
53. K. Ishioka, **T. Tadano**, M. Yanagida, Y. Shirai, and K. Miyano, "Anharmonic organic cation vibrations in the hybrid lead halide perovskite CH3NH3PbI3", *Phys. Rev. Mater.* **5**, 105402 (2021).
54. G. Xing, T. Ishikawa, Y. Miura, T. Miyake, and **T. Tadano**, "Lattice dynamics effects on finite-temperature stability of R1−Fe (R = Y, Ce, Nd, Sm, and Dy) alloys from first principles", *J. Alloys Compd.* **874**, 159754 (2021).
55. K. Cho, T. Yamada, H. Tahara, **T. Tadano**, H. Suzuura, M. Saruyama, R. Sato, T. Teranishi, and Y. Kanemitsu, "Luminescence fine structures in single lead Halide perovskite nanocrystals: Size dependence of the exciton–phonon coupling", *Nano Lett.* **21**, 7206–7212 (2021).
56. M. Charlebois, J. Morée, K. Nakamura, Y. Nomura, **T. Tadano**, Y. Yoshimoto, Y. Yamaji, T. Hasegawa, K. Matsuhira, and M. Imada, "Ab initio derivation of low-energy Hamiltonians for systems with strong spin-orbit interaction: Application to Ca5Ir3O12", *Phys. Rev. B Condens. Matter* **104**, 075153 (2021).
57. S. Ju, R. Yoshida, C. Liu, S. Wu, K. Hongo, **T. Tadano**, and J. Shiomi, "Exploring diamondlike lattice thermal conductivity crystals via feature-based transfer learning", *Phys. Rev. Mater.* **5**, 053801 (2021).
58. T. Ishikawa, T. Fukazawa, G. Xing, **T. Tadano**, and T. Miyake, "Evolutionary search for cobalt-rich compounds in the yttrium-cobalt-boron system", *Phys. Rev. Mater.* **5**, 054408 (2021).
59. K. Nakamura, Y. Yoshimoto, Y. Nomura, **T. Tadano**, M. Kawamura, T. Kosugi, K. Yoshimi, T. Misawa, and Y. Motoyama, "RESPACK: An ab initio tool for derivation of effective low-energy model of material", *Comput. Phys. Commun.* **261**, 107781 (2021).
60. T. Katase, Y. Takahashi, X. He, **T. Tadano**, K. Ide, H. Yoshida, S. Kawachi, J. Yamaura, M. Sasase, H. Hiramatsu, H. Hosono, and T. Kamiya, "Reversible 3D-2D structural phase transition and giant electronic modulation in nonequilibrium alloy semiconductor, lead-tin-selenide", *Sci Adv* **7**, eabf2725 (2021).
61. S. Kawano, **T. Tadano**, and S. Iikubo, "Effect of Halogen Ions on the Low Thermal Conductivity of Cesium Halide Perovskite", *J. Phys. Chem. C* **125**, 91–97 (2021).
62. Z. Zeng, S. Li, **T. Tadano**, and Y. Chen, "Anharmonic lattice dynamics and thermal transport of monolayer InSe under equibiaxial tensile strains", *J. Phys. Condens. Matter* **32**, 475702 (2020).
63. T. Tanimoto, K. Suekuni, T. Tanishita, H. Usui, **T. Tadano**, T. Kamei, H. Saito, H. Nishiate, C. H. Lee, K. Kuroki, and M. Ohtaki, "Enargite Cu_3PS_4: A Cu–S-based thermoelectric material with a wurtzite-derivative structure", *Adv. Funct. Mater.* **30**, 2000973 (2020).
64. Y. Wu, W. A. Saidi, J. K. Wuenschell, **T. Tadano**, P. Ohodnicki, B. Chorpening, and Y. Duan, "Anharmonicity Explains Temperature Renormalization Effects of the Band Gap in SrTiO3", *J. Phys. Chem. Lett.* **11**, 2518–2523 (2020).
65. M. Hirayama, **T. Tadano**, Y. Nomura, and R. Arita, "Materials design of dynamically stable d9 layered nickelates", *Phys. Rev. B Condens. Matter* **101**, 075107 (2020).
66. I. Errea, F. Belli, L. Monacelli, A. Sanna, T. Koretsune, **T. Tadano**, R. Bianco, M. Calandra, R. Arita, F. Mauri, and J. A. Flores-Livas, "Quantum crystal structure in the 250-kelvin superconducting lanthanum hydride", *Nature* **578**, 66–69 (2020).
67. Y. Nomura, M. Hirayama, **T. Tadano**, Y. Yoshimoto, K. Nakamura, and R. Arita, "Formation of a two-dimensional single-component correlated electron system and band engineering in the nickelate superconductor NdNiO2", *Phys. Rev. B Condens. Matter* **100**, 205138 (2019).

68. Y. Oba, **T. Tadano**, R. Akashi, and S. Tsuneyuki, "First-principles study of phonon anharmonicity and negative thermal expansion in ScF3", *Phys. Rev. Mater.* **3**, 033601 (2019).
69. **T. Tadano**, Y. Nomura, and M. Imada, "Ab initio derivation of effective Hamiltonian for $La_2CuO_4/La_{1.55}Sr_{0.45}CuO_4$ heterostructure", *Phys. Rev. B* **99**, 155148 (2019). DOI
70. **T. Tadano** and S. Tsuneyuki, "Ab initio prediction of structural phase-transition temperature of SrTiO3 from finite-temperature phonon calculation", *J. Ceram. Soc. Jpn.* **127**, 404–408 (2019).
71. **T. Tadano** and S. Tsuneyuki, "First-Principles Lattice Dynamics Method for Strongly Anharmonic Crystals", *J. Phys. Soc. Jpn.* **87**, 041015 (2018).
72. **T. Tadano** and S. Tsuneyuki, "Quartic Anharmonicity of Rattlers and Its Effect on Lattice Thermal Conductivity of Clathrates from First Principles", *Phys. Rev. Lett.* **120**, 105901 (2018).
73. P. Norouzzadeh, J. S. Krasinski, and **T. Tadano**, "Thermal conductivity of type-I, type-II, and type-VIII pristine silicon clathrates: A first-principles study", *Phys. Rev. B Condens. Matter* **96**, 245201 (2017).
74. A. Rohskopf, H. R. Seyf, K. Gordiz, **T. Tadano**, and A. Henry, "Empirical interatomic potentials optimized for phonon properties", *npj Computational Materials* **3**, 1–7 (2017).
75. W. Sano, T. Koretsune, **T. Tadano**, R. Akashi, and R. Arita, "Effect of Van Hove singularities on high-Tc superconductivity in H3S", *Phys. Rev. B Condens. Matter* **93**, 094525 (2016).
76. **T. Tadano** and S. Tsuneyuki, "Self-consistent phonon calculations of lattice dynamical properties in cubic SrTiO3 with first-principles anharmonic force constants", *Phys. Rev. B Condens. Matter* **92**, 054301 (2015).
77. **T. Tadano**, Y. Gohda, and S. Tsuneyuki, "Impact of rattlers on thermal conductivity of a thermoelectric clathrate: a first-principles study", *Phys. Rev. Lett.* **114**, 095501 (2015).
78. **T. Tadano** and S. Tsuneyuki, "First-principles analysis of anharmonic nuclear motion and thermal transport in thermoelectric materials", AIP Publishing LLC (2015).
79. **T. Tadano**, Y. Gohda, and S. Tsuneyuki, "Anharmonic force constants extracted from first-principles molecular dynamics: applications to heat transfer simulations", *J. Phys. Condens. Matter* **26**, 225402 (2014).

Reviews & Book Chapters

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2. **T. Tadano**, "第一原理計算を用いた熱伝導・電気伝導予測の前線", セラミックス **59**, 779–783 (2024).
3. R. Masuki, T. Nomoto, R. Arita, and **T. Tadano**, "非調和フォノン理論に基づいた有限温度における結晶構造の第一原理計算", *Kotai Butsuri* **58**, 419–432 (2023).
4. **T. Tadano**, "非調和フォノン理論が拓く有限温度物性の第一原理計算", 日本物理学会誌 **78**, 542–547 (2023).
5. **T. Tadano**, "熱電材料研究に資する第一原理格子動力学", 計算科学を活用した熱電変換材料の研究開発動向, シーエムシー・リサーチ (2022).
6. **T. Tadano**, "格子熱伝導の基礎理論と第一原理シミュレーション", マイクロ・ナノ熱工学の進展, エヌ・ティー・エス (2021).
7. Y. Nomura, M. Hirayama, M. Kitatani, **T. Tadano**, and R. Arita, "ニッケル酸化物新超伝導体の発見：現状と展望", *Kotai Butsuri* **55**, 491 (2020).
8. **T. Tadano**, T. Koretsune, and R. Arita, "原子核の量子ゆらぎが支える高圧下 LaH10 の高温超伝導", *Kotai Butsuri* **55**, 425 (2020).
9. **T. Tadano**, "非調和効果を取り込める新しいフォノン計算ツールの開発", シミュレーション **39** (2020).
10. **只野央将**, "非調和フォノン物性の第一原理計算", 応用物理 **89**, 35–39 (2020).

11. **T. Tadano** and S. Tsuneyuki, “第一原理からの非調和フォノンと格子熱伝導”, 固体物理 **52**, 637–646 (2017).
12. **T. Tadano**, “第一原理フォノン伝導計算”, マイクロ・ナノスケールの次世代熱制御技術フォノンエンジニアリング, エヌ・ティー・エス (2017).

Invited Talks & Seminars

1. **T. Tadano**, “First-Principles and Machine-Learning Exploration of Energy Harvesting Heusler Alloys”, TYC 8th Energy Materials workshop: From Electron and Phonon Interactions to Net Zero, London, UK, Jun 1, 2026.
2. **只野央将**, “有限温度における構造最適化法の開発とニッケル酸化物超伝導体への応用”, 新規超伝導体を舞台とする超伝導科学のフロンティア, 京都大学基礎物理学研究所, Dec 22, 2025.
3. **T. Tadano**, “Anharmonic lattice dynamics and thermal transport in type-I clathrates studied by first-principles calculation”, 2025 MRS Fall Meeting, Boston, MA, USA, Dec 1, 2025.
4. **T. Tadano**, “First-Principles and Data-Driven Approaches for the Computational Design of Functional Heusler Alloys”, Materials Science from First Principles: Materials Scientist Toolbox, Sorbonne University, Paris, France, Nov 7, 2025.
5. **只野央将**, “非調和フォノン計算を活用した相転移温度の非経験予測”, 日本物理学会第 80 回年次大会, 広島大学, Sep 17, 2025.
6. **只野央将**, “第一原理計算とデータ駆動手法による機能性ホイスラー合金の探索”, スーパーコンピュータワークショップ 2024 − AI/ML に基づく材料設計と開発：理論と実験の接点−, 岡崎コンファレンスセンター・ハイブリッド開催, Jan 15, 2025.
7. **T. Tadano**, “Simulating structural change and phase transitions at finite temperatures: A phonon-based approach”, The 25th Asian Workshop on First-Principles Electronic Structure Calculations (ASIAN-25), University of Ulsan, Haesong Hall, Oct 28, 2024.
8. **T. Tadano**, “Computational Exploration of Functional Materials at Finite Temperatures”, LANL-NIMS Quantum and Functional Materials 2024, WPI-MANA Bldg. , Namiki-site, National Institute for Materials Science (NIMS), Oct 15, 2024.
9. **只野央将**, “計算科学とデータ駆動による磁性材料開発”, DDCoMS-PCoMS-RISME 計算物質科学セミナーシリーズ 2024, オンライン, Jul 29, 2024.
10. **T. Tadano**, “Anharmonic phonon theory in condensed matter physics”, RIKEN Symposium Second Workshop on Fundamentals in Density Functional Theory (DFT2024), Auditorium, Integrated Innovation Building (IIB), RIKEN Kobe Campus, Feb 20, 2024.
11. **只野央将**, “第一原理フォノン計算を用いた有限温度における構造最適化”, 第 36 期 CAMM フォーラム本例会, Jun 9, 2023.
12. **T. Tadano**, “Ab initio calculation of phonons and crystal structures at finite temperatures: A self-consistent phonon approach”, ISSP Theory Seminar, ISSP, University of Tokyo, Aug 19, 2022.
13. **T. Tadano**, “First-principles calculations of phonons and crystal structures at finite temperatures”, Recent Progress in Thermal Transport Theory and Experiments, Online, May 30, 2022.
14. **只野央将**, “自己無撞着フォノン理論による構造相転移温度の第一原理計算”, 物性研究所スパコン共同利用・CCMS 合同研究会「計算物質科学の新展開, ISSP, University of Tokyo, May 13, 2022.
15. **只野央将**, “フォノン計算を活用した熱伝導の非経験予測”, 透明酸化物光･電子材料第 166 委員会第 92 回研究会, Online, Mar 11, 2022.
16. **T. Tadano**, “Extending first-principles structural optimization method to finite temperatures”, APW-RIKEN-Tsinghua-Kavli workshop ‘’Highlights on condensed matter physics’, Online, Oct 23, 2021.

17. **T. Tadano**, “Ab initio phonon calculation at finite temperature toward computational exploration of metastable phases”, The Twelfth International Conference on the Science and Technology for Advanced Ceramics (STAC12), Online, Jul 8, 2021.
18. **只野央将**, “高圧下ランタン水素化物 LaH_x における原子核の量子ゆらぎと超伝導”, 京大基研研究会「高温超伝導・非従来型超伝導研究の最前線: 多様性と普遍性」, Online, Oct 26, 2020.
19. **只野央将**, “第一原理フォノン計算の前線：非調和効果と電子格子相互作用”, 第 121 回フロンティア材料研究所講演会, 東京工業大学, Feb 5, 2020.
20. **T. Tadano**, “Phonon lifetime and thermal transport in complex thermoelectric clathrates and tetrahedrites from first principles”, Phonon lifetime from disordered and complex systems—Measurement and Interpretation, 4 rue A. Einstein Villeurbanne, Dec 20, 2019.
21. **T. Tadano**, “Phonon anharmonicity and thermal transport in complex thermoelectric materials from first principles”, Colloquium at TU-Darmstadt, TU Darmstadt, Dec 9, 2019.
22. **T. Tadano**, “Development and application of ALAMODE software”, The 5th Workshop on ab initio phonon calculations, Institute of Nuclear Physics PAN, Dec 3, 2019.
23. **T. Tadano**, “Phonon anharmonicity from first principles”, 第 35 回コンピュテーショナル・マテリアルズ・デザインワークショップ, 大阪大学, Sep 6, 2019.
24. **T. Tadano**, “Ab initio phonon calculations of strongly anharmonic solids”, Seminar at Samsung Advanced Institute of Technology (SAIT), SAIT, May 23, 2019.
25. **只野央将**, “クラスレートのフォノンと熱伝導の第一原理解析”, 第三回大型実験施設とスーパーコンピュータとの連携利用勉強会, SPring-8, Feb 25, 2019.
26. **T. Tadano**, “Efficient ab initio prediction of thermal properties of solids assisted by machine learning”, JST International Symposium on Materials Informatics, University of Tokyo, Feb 11, 2019.
27. **只野央将**, “第一原理からの有限温度フォノン計算：手法開発とエネルギー材料への応用”, 第 83 回フロンティア材料研究所講演会, 東京工業大学, Nov 26, 2018.
28. **只野央将**, “第一原理からの熱伝導・相安定性予測：フォノンの精密な取り扱い”, 日本金属学会 2018 秋期大会, 東北大学川内北キャンパス・仙台国際センター, Sep 20, 2018.
29. **T. Tadano**, “Ab initio lattice dynamics methods for modeling strong phonon anharmonicity in solids”, The International Summer workShop 2018 on First-Principles Electronic Structure Calculations (ISS2018), ISSP, University of Tokyo, Jul 12, 2018.
30. **只野央将**, “フォノンの非調和効果の高精度・高効率計算”, 第 31 期 CAMM フォーラム本例会, 東京・表参道「アイビーホール」, May 11, 2018.
31. **只野央将**, “フォノンと格子熱伝導率の第一原理計算”, 第 38 回 Kyutech 物性セミナー・応用物理学会特別講演会「超伝導と熱伝導」, 九州工業大学戸畑キャンパス, Mar 30, 2018.
32. **T. Tadano**, “Microscopic origin of anomalous thermal transport in intermetallic clathrates: A first-principles study”, Seminar at Institut Lumière matière, Institut Lumière matière, Jan 16, 2018.
33. **T. Tadano**, “Understanding the role of quartic anharmonicity in solids using first-principles lattice dynamics”, CECAM workshop on ‘’Anharmonicity and thermal properties of solids’, Institut Henri Poincaré, Jan 10, 2018.
34. **只野央将**, “第一原理計算によるフォノンの非調和効果の予測と解析”, 大阪大学黒木研究室セミナー, 大阪大学, Dec 8, 2017.
35. **只野央将**, “第一原理計算でのフォノンの非調和性の取り扱い”, 電子格子相互作用：基礎物理からデバイス応用まで, 奈良先端科学技術大学院大学, Jul 31, 2017.
36. **T. Tadano**, “Thermal conductivity and lattice anharmonicity from first principles: Theoretical developments and applications”, International Workshop of Materials Informatics and Materials Data (MIMD), NIMS, Apr 6, 2017.
37. **只野央将**, “非調和フォノン物性の第一原理計算：プログラム開発とマテリアルズインフォマティクスへ向けた取り組み”, 第 3 回材料系ワークショップ, 秋葉原 UDX, Feb 23, 2017.

38. **T. Tadano**, “First-principles modeling of phonon transport and lattice anharmonicity in energy harvesting materials”, The 4th Workshop for Extreme Materials Science “Thermal Conductivity of Earth”, RIKEN, Dec 13, 2016.
39. **T. Tadano**, “Thermal conductivity and lattice anharmonicity of materials from first-principles calculations”, 19th ASIAN workshop, National Chiao Tung University, Oct 31, 2016.
40. **只野央将**, “第一原理フォノン伝導計算：その最前線とポスト「京」/マテリアルズインフォマティクス時代への展望”, 第 63 回応用物理学会春期学術講演会特別シンポジウム, 東京工業大学, Mar 22, 2016.
41. **T. Tadano**, “Non-equilibrium heat transfer simulation with first-principles anharmonic lattice model”, 22th GREEN Open Seminar, NIMS, Sep 20, 2012.