

# Terumasa TADANO (只野央将)

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## PERSONAL DATA

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## RESEARCH INTERESTS

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

## EDUCATION

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MARCH 2013    Ph.D., Department of Physics, University of Tokyo, Japan  
Advisor: Prof. Shinji TSUNEYUKI

MARCH 2010    M.Sc., Department of Physics, University of Tokyo, Japan  
Advisor: Prof. Shinji TSUNEYUKI

MARCH 2008    B.Sc., Department of Physics, Keio University, Japan

## EMPLOYMENT

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APR 2024–    | Group Leader, 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–    | Postdoctoral researcher,  
DEC 2016    | National Institute for Materials Science (NIMS), Japan

APR 2015–    | Postdoctoral researcher, Department of Applied Physics,  
SEP 2016    | University of Tokyo, Japan (Advisor: Prof. Masatoshi IMADA)

APR 2013–    | Postdoctoral researcher, Department of Physics,  
MAR 2015    | University of Tokyo, Japan (Advisor: Prof. Shinji TSUNEYUKI)

## AWARDS

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APR 2025	The 20th NIMS President Awards : Research Encouragement
MAY 2024	HPCI Software Award for Excellence (First Prize) in the Development Category
APR 2024	The Young Scientists' Award by MEXT
NOV 2021	Condensed-Matter Science Prize (Theory division)
MAR 2019	Young Scientist Award of the Physical Society of Japan
NOV 2018	Best Presentation Award at the 38th Electronics division meeting of CerSJ
SEP 2017	ECT2017 Poster Award
AUG 2014	CSW2014 Young Investigator Award

## GRANTS

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APR 2025–MAR 2030	Grant-in-Aid for Transformative Research Areas (A) “Correlation Design Science”, MEXT, Japan (Co-investigator, PI : Prof. Arita)
APR 2024–MAR 2027	Grant-in-Aid for Scientific Research (A), MEXT, Japan (Co-investigator, PI : Prof. Arita)
OCT 2023–MAR 2027	PRESTO, JST, MEXT, Japan
APR 2023–MAR 2026	Grant-in-Aid for Scientific Research (A), MEXT, Japan (Co-investigator, PI : Prof. Chiba)
APR 2021–MAR 2024	Grant-in-Aid for Scientific Research (C), MEXT, Japan
APR 2020–MAR 2023	Grant-in-Aid for Scientific Research (B), MEXT, Japan (PI: Dr. Miura)
OCT 2019–MAR 2022	Elements Strategy Initiative Center for Magnetic Materials (ESICMM), MEXT, Japan
MAY 2016–MAR 2021	Grant-in-Aid for Scientific Research (S), MEXT, Japan (PI: Prof. Imada)
JAN 2017–MAR 2019	NIMS ICYS Research Grant (Internal grant)
APR 2016–MAR 2019	Grant-in-Aid for Encouragement of Young Scientists (B), MEXT, Japan

## PAPERS

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1. R. Asai, R. Arita, T. Chida, R. Masuki, K. Kuroki, and **T. Tadano**, “*Finite-Temperature ab initio Structural Optimization of the Bilayer Nickelate Superconductor  $\text{La}_3\text{Ni}_2\text{O}_7$* ”, arXiv:2512.08251 (2025).
  2. E. Xiao and **T. Tadano**, “*Accurate Screening of Functional Materials with Machine-Learning Potential and Transfer-Learned Regressions: Heusler Alloy Benchmark*”, arXiv:2508.20556 (2025).
  3. R. Pohle, Y. Motome, **T. Tadano**, and S. Hoshino, “*Electron-phonon coupled Langevin dynamics for Mott insulators*”, arXiv:2507.19764 (2025).
  4. M. Ohnishi, T. Deng, P. Torres, Z. Xu, **T. Tadano**, H. Zhang, W. Nong, M. Hanai, Z. Wang, 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*”, arXiv:2504.21245 (2025).
  5. 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.
  6. 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).
  7. 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, H. Sepehri-Amin, “*Control of covalent bond enables efficient magnetic cooling*”, Adv. Mater. **e14295** (2025).

8. 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, X. Zhang, “Phonon Olympics: Phonon property and lattice thermal conductivity benchmarking from open-source packages”, *J. Appl. Phys.* **138**, 135108 (2025).
9. E. Xiao and **T. Tadano**, “High-throughput computational screening of Heusler compounds with phonon considerations for enhanced material discovery”, *Acta Mater.* **297**, 121312 (2025).
10. K. Oyanagi, H. Sepehri-Amin, K. Takamori, **T. Tadano**, T. Imamura, R. Nagasawa, K. Mahalingam, T. Hirai, F. Ando, Y. Sakuraba, S. Kobayashi, K.-I. Uchida, “Simultaneous achievement of large anomalous Nernst effect and reduced thermal conductivity in sintered polycrystalline topological Heusler ferromagnets”, *Acta Mater.* **296**, 121239 (2025).
11. 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  $\text{SrTiO}_3$  polycrystals by simultaneous hydrogen substitution and oxygen vacancy formation”, *ACS Appl. Energy Mater.* **8**, 11447–11455 (2025).
12. D. Sorescu, **T. Tadano**, and W. A. Saidi, “Theoretical investigations of anharmonic effects and phonon transport in the cubic phase of crystalline perovskite  $\text{CsPbCl}_3$ ”, *J. Phys. Chem. C* **129**, 13445–13456 (2025).
13. R. Matsumoto, K. Yamane, **T. Tadano**, K. Terashima, T. Shinmei, T. Irifune, and Y. Takano, “Emergence of superconductivity at 20 K in  $\text{Th}_3\text{P}_4$ -type  $\text{In}_{3-x}\text{S}_4$  synthesized by Diamond anvil cell with boron-doped Diamond electrodes”, *Chem. Mater.* **37**, 1648–1656 (2025).
14. P. Wisesa, **T. Tadano**, and W. A. Saidi, “Deep-learning neural network potentials for titanate perovskites”, *Comput. Mater. Sci.* **250**, 113719 (2025).
15. M. Hiramatsu, Z. Hu, S. Yoshikawa, Z. Yang, X. He, T. Katase, J. Yamaura, H. Sagayama, **T. Tadano**, S. Ueda, H. Hiramatsu, H. Hosono, T. Kamiya, “Nonequilibrium Layered  $\text{PbS}$  Stabilized by Sn Doping: Bipolar Semiconductors with Low Thermal Conductivity”, *ACS Appl. Electron. Mater.* **6**, 8339 (2024).
16. R. Masuki, T. Nomoto, R. Arita, and **T. Tadano**, “Continuous crossover between insulating ferroelectrics and the polar metals: Ab initio calculation of structural phase transitions of  $\text{LiBO}_3$  ( $B = \text{Ta}, \text{W}, \text{Re}, \text{Os}$ )”, *Phys. Rev. B* **110**, 094102 (2024).
17. 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 Mater.* **9**, 41 (2024).
18. 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).
19. M. Basini, M. Pancaldi, B. Wehinger, M. Udina, **T. Tadano**, M. C. Hoffmann, A. V. Balatsky, and S. Bonetti, “Terahertz electric-field driven dynamical multiferroicity in  $\text{SrTiO}_3$ ”, *Nature* **628**, pages 534–539 (2024).
20. J. Yue, Y. Liu, W. Ren, S. Lin, C. Shen, H. K. Singh, T. Cui, **T. Tadano**, H. Zhang, “Role of atypical temperature-responsive lattice thermal transport on the thermoelectric properties of antiperovskites  $\text{Mg}_3\text{XN}$  ( $X = \text{P}, \text{As}, \text{Sb}, \text{Bi}$ )”, *Mater. Today Phys.* **41**, 101340 (2024).
21. Y. Kozuka, T. T. Sasaki, **T. Tadano**, J. Fujioka, “Epitaxy and transport properties of alkali-earth palladate thin films”, *Sci. Tech. Adv. Mater.* **24**, 2265431 (2023).
22. X. He, S. Kimura, T. Katase, **T. Tadano**, S. Matsuishi, M. Minohara, H. Hiramatsu, H. Kumigashira, H. Hosono, T. Kamiya, “Inverse-Perovskite  $\text{Ba}_3\text{BO}$  ( $B = \text{Si}$  and  $\text{Ge}$ ) as a

High Performance Environmentally Benign Thermoelectric Material with Low Lattice Thermal Conductivity”, *Adv. Sci.* **2307058** (2023).

23. M. Morishita, T. Abe, T. Ohkubo, **T. Tadano**, H. Yamamoto, A. Nozaki, H. Miyazaki, “Magnetic characterization of  $\text{Sm}(\text{Fe}_{1-x}\text{Co}_x)_{11}\text{Ti}$  ( $x = 0, 0.1$ ) determined by heat-capacity measurement from very low to high temperatures”, *Thermochimica Acta.* **727**, 179573 (2023).
24. I. Kurniawan, Y. Miura, G. Xing, **T. Tadano**, 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).
25. K. Kazama, M. Sakano, K. Yamagami, T. Ohkuchi, K. Ishizaka, **T. Tadano**, Y. Kozuka, H. Yoshizawa, Y. Tsujimoto, K. Yamaura, J. Fujioka, “Charge transport and thermopower in the electron-doped narrow gap semiconductor  $\text{Ca}_{1-x}\text{La}_x\text{Pd}_3\text{O}_4$ ”, *Phys. Rev. Mater.* **7**, 085402 (2023).
26. G. Xing, Y. Miura, and **T. Tadano**, “First-principles prediction of phase transition of  $\text{YCo}_5$  from self-consistent phonon calculations”, *Phys. Rev. B* **108**, 014304 (2023).
27. E. Frasson, P. Rosander, F. Eriksson, M. Rahm, **T. Tadano**, P. Erhart, “Limits of the phonon quasi-particle picture at the cubic-to-tetragonal phase transition in halide perovskites”, *Commun. Phys.* **6**, 173 (2023).
28. 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 (2023).
29. A. Togo, L. Chaput, **T. Tadano**, I. Tanaka, “Implementation strategies in phonopy and phono3py”, *J. Phys.: Condens. Matter* **35**, 353001 (2023).
30. C. Shen, M. Dai, X. Xiao, N. Hadaeghi, W. Xie, A. Weidenkaff, **T. Tadano**, H. Zhang, “Impact of Quartic Anharmonicity on Lattice Thermal Transport in  $\text{EuTiO}_3$ : A Comparative Theoretical and Experimental Investigation”, *Mater. Today Phys.* **34**, 101059 (2023).
31. 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  $\text{GaN}$  and  $\text{ZnO}$ ”, *Phys. Rev. B* **107**, 134119 (2023).
32. 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, T. Kamiya, “Hydride Anion Substitution Boosts Thermoelectric Performance of Polycrystalline  $\text{SrTiO}_3$  via Simultaneous Realization of Reduced Thermal Conductivity and High Electronic Conductivity”, *Adv. Func. Mater.* **2213144** (2023).
33. T. Amano, T. Yamazaki, R. Akashi, **T. Tadano**, S. Tsuneyuki, “Lattice dielectric properties of rutile  $\text{TiO}_2$ : First-principles anharmonic self-consistent phonon study”, *Phys. Rev. B* **107**, 094305 (2023).
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35. 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  $\text{BaTiO}_3$ ”, *Phys. Rev. B* **106**, 224104 (2022).
36. **T. Tadano** and W. A. Saidi, “First-Principles Phonon Quasiparticle Theory Applied to a Strongly Anharmonic Halide Perovskite”, *Phys. Rev. Lett.* **129**, 185901 (2022).

37. 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 CsPbBr<sub>3</sub> Perovskite Nanocrystals”, *Nano Lett.* **22**, 7674 (2022).
38. 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.* **2202029** (2022).
39. M. Ohnishi, **T. Tadano**, S. Tsuneyuki, and J. Shiomi, “Anharmonic phonon renormalization and thermal transport in the type-I Ba<sub>8</sub>Ga<sub>16</sub>Sn<sub>30</sub> clathrate from first principles”, *Phys. Rev. B* **106**, 024303 (2022).
40. 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).
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<sub>1–x</sub>Sn<sub>x</sub>)Se”, *Adv. Electron. Mater.* **2200024** (2022).
42. G. Xing, Y. Miura, and **T. Tadano**, “Lattice dynamics and its effects on magnetocrystalline anisotropy energy of pristine and hole-doped YCo<sub>5</sub> from first principles”, *Phys. Rev. B* **105**, 104427 (2022).
43. X. He, H. Zhang, T. Nose, T. Katase, **T. Tadano**, K. Ide, S. Ueda, H. Hiramatsu, H. Hosono, T. Kamiya, “Degenerated Hole Doping and Ultra-Low Lattice Thermal Conductivity in Polycrystalline SnSe by Nonequilibrium Isovalent Te Substitution”, *Adv. Sci.* **2105958** (2022).
44. R. Masuki, T. Nomoto, R. Arita, and **T. Tadano**, “Anharmonic Grüneisen theory based on self-consistent phonon theory: Impact of phonon-phonon interaction neglected in the quasi-harmonic theory”, *Phys. Rev. B* **105**, 064112 (2022).
45. 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. Mater* **34**, 135702 (2022).
46. 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* **104**, L180403 (2021).
47. K. Ishioka, **T. Tadano**, M. Yanagida, Y. Shirai, K. Miyano, “Anharmonic Organic Cation Vibrations in Hybrid Lead Halide Perovskite CH<sub>3</sub>NH<sub>3</sub>PbI<sub>3</sub>”, *Phys. Rev. Materials* **5**, 105402 (2021).
48. 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 LaAlO<sub>3</sub>/LaNiO<sub>3</sub>/LaAlO<sub>3</sub> heterostructure”, *Nano Lett.* **21**, 9240–9246 (2021).
49. 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 LaTiO<sub>3</sub> film around Mott insulator to metal transition”, *Adv. Sci.* **2102097** (2021).
50. M. Charlebois, J. Morée, K. Nakamura, Y. Nomura, **T. Tadano**, Y. Yoshimoto, Y. Yamaji, T. Hasegawa, K. Matsuhira, M. Imada, “Ab initio Derivation of Low-Energy Hamiltonians for Systems with Strong Spin-Orbit Interaction and Its Application to Ca<sub>5</sub>Ir<sub>3</sub>O<sub>12</sub>”, *Phys. Rev. B* **104**, 075153 (2021).

51. 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).
52. T. Ishikawa, T. Fukazawa, G. Xing, **T. Tadano**, and Takashi Miyake, “*Evolutionary search for cobalt-rich compounds in the yttrium-cobalt-boron system*”, *Phys. Rev. Materials* **5**, 054408 (2021).
53. G. Xing, T. Ishikawa, Y. Miura, T. Miyake, and **T. Tadano**, “*Lattice dynamics effects on finite-temperature stability of  $R_{1-x}Fe_x$  ( $R = Y, Ce, Nd, Sm, \text{ and } Dy$ ) alloys from first principles*”, *J. Alloys Compd.* **874**, 159754 (2021).
54. S. Ju, R. Yoshida, C. Liu, K. Hongo, **T. Tadano**, J. Shiomi, “*Exploring diamond-like lattice thermal conductivity crystals via feature-based transfer learning*”, *Phys. Rev. Materials* **5**, 053801 (2021).
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56. 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).
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58. 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. Mater* **32**, 475702 (2020).
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60. 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).
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62. 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 K Superconducting Lanthanum Hydride*”, *Nature* **578**, 66–69 (2020).
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64. **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).
65. **T. Tadano** and S. Tsuneyuki, “*Ab initio prediction of structural phase-transition temperature of  $SrTiO_3$  from finite-temperature phonon calculation*”, *J. Ceram. Soc. Jpn.* **127**, 404 (2019).
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## BOOK CHAPTERS & INVITED REVIEW

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2. 只野央将：「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』 Vol. 59, 779-783, 2024 年.
3. 増木亮太, 野本拓也, 有田亮太郎, 只野央将：「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」, 『固体物理』 Vol. 58, 419-432, 2023 年.
4. 只野央将：「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』 Vol. 78, 542-547, 2023 年.
5. 只野央将：「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 (株式会社 シーエムシー・リサーチ), 2022 年.
6. 只野央将：「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 (株式会社 エヌ・ティー・エス), 2021 年.
7. 野村悠祐, 平山元昭, 北谷基治, 只野央将, 有田亮太郎：「ニッケル酸化物新超伝導体の発見：現状と展望」, 『固体物理』 Vol. 55, 491-503, 2020 年.
8. 只野央将, 是常隆, 有田亮太郎：「原子核の量子ゆらぎが支える高圧下  $LaH_{10}$  の高温超伝導」, 『固体物理』 Vol. 55, 425-434, 2020 年.
9. 只野央将：「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』 Vol. 39, No. 1, 2020 年.
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』 Vol. 89, No. 1, 2019 年.
11. 只野央将：「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 (株式会社エヌ・ティー・エス), 2017 年.
12. 只野央将, 常行真司：「第一原理からの非調和フォノンと格子熱伝導」, 『固体物理』 (アグネ技術センター) Vol. 52, No. 11, 637, 2017 年.

## INVITED TALKS & SEMINARS

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1. 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, 2025 年 12 月 22 日.
2. T. Tadano, “Anharmonic lattice dynamics and thermal transport in type-I clathrates studied by first-principles calculation”, 2025 MRS Fall Meeting, Boston, USA, Dec. 1, 2025.
3. T. Tadano, “First-Principles and Data-Driven Approaches for the Computational Design of Functional Heusler Alloys”, Materials Science from First Principles: Materials Scientist Toolbox, Paris, France, Nov. 3-7, 2025.
4. 只野央将:「第一原理計算とデータ駆動による磁性材料設計」, 第 3 回ナノエラストロニクスワークショップ, 2025 年 10 月 20 日.
5. 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」, 計算科学研究センター・計算物質科学スーパーコンピュータ共用事業合同ワークショップ「AI/ML に基づく材料設計と開発: 理論と実験の接点」, 2025 年 01 月 16 日.
6. 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), Ulsan, South Korea, Oct 28, 2024.
7. T. Tadano, “Computational Exploration of Functional Materials at Finite Temperatures”, LANL-NIMS Quantum and Functional Materials 2024, Tsukuba, Japan, Oct 15, 2024.
8. 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, Jul 29, 2024.
9. T. Tadano, “Anharmonic Phonon Theory in Condensed Matter Physics with Applications based on DFT”, DFT2024 (RIKEN Symposium), Kobe, Japan, Feb. 22, 2024.
10. 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, 2023 年 6 月 9 日.
11. 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) and online (hybrid), Aug. 19, 2022.
12. 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.
13. 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」, 東京大学物性研究所, 2022 年 5 月 13 日.
14. 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, オンライン, 2022 年 3 月 11 日.
15. T. Tadano, “Extending first-principles structural optimization method to finite temperatures”, APW-RIKEN-Tsinghua-Kavli workshop “Highlights on condensed matter physics”, Online, Oct. 21-23, 2021.
16. 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. 6-8, 2021.
17. 只野央将:「高圧下ランタン水素化物  $\text{LaH}_x$  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」, 湯川記念館パナソニック国際交流ホール + オンライン, 2020 年 10 月 26 日



18. 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，2020 年 2 月 5 日。
19. 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”, Lyon, France, Dec. 19–20, 2019.
20. T. Tadano, “Phonon anharmonicity and thermal transport in complex thermoelectric materials from first principles”, Colloquium at TU-Darmstadt, Dec. 9, 2019.
21. T. Tadano, “Development and application of ALAMODE software”, The 5th Workshop on ab initio phonon calculations, Krakow, Poland, Dec. 3–6, 2019.
22. 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，2019 年 9 月 6 日。
23. T. Tadano, “Ab initio phonon calculations of strongly anharmonic solids”, Seminar at Samsung Advanced Institute of Technology (SAIT), Suwon-si, Korea, May 23, 2019.
24. 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-8，2019 年 2 月 25 日。
25. T. Tadano, “Efficient ab initio prediction of thermal properties of solids assisted by machine learning”, JST International Symposium on Materials Informatics, Tokyo, Japan, Feb. 9–11, 2019.
26. 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，2018 年 11 月 26 日。
27. 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，2018 年 9 月。
28. 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), Kashiwanoha, Japan, Jul. 12, 2018.
29. 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，2018 年 5 月 11 日。
30. 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，九州工業大学戸畑キャンパス，2018 年 3 月 30 日。
31. T. Tadano, “Microscopic origin of anomalous thermal transport in intermetallic clathrates: A first-principles study”, Seminar at Institut Lumière matière, Lyon, France, Jan. 16, 2018.
32. T. Tadano, “Understanding the role of quartic anharmonicity in solids using first-principles lattice dynamics”, CECAM workshop on “Anharmonicity and thermal properties of solids”, Paris, France, Jan. 10–12, 2018.
33. 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，2017 年 12 月 8 日。
34. 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（奈良市），2017 年 7 月 31—8 月 1 日。
35. T. Tadano, “Thermal conductivity and lattice anharmonicity from first principles: Theoretical developments and applications”, International Workshop of Materials Informatics and Materials Data (MIMD), Tsukuba, Japan, Apr. 6–7, 2017.
36. 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（千代田区），2017 年 2 月。

37. 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 (Wakou), Japan, Dec. 13, 2016.
38. T. Tadano, "Thermal conductivity and lattice anharmonicity of materials from first-principles calculations", ASIAN-19, Hsinchu, Taiwan, Oct. 31-Nov. 2 2016.
39. 只野央将, 常行真司:「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 (目黒区), 2016 年 3 月
40. T. Tadano and S. Tsuneyuki, "Non-equilibrium heat transfer simulation with first-principles anharmonic lattice model", 22th GREEN Open Seminar, Tsukuba, Japan, Sep. 2012.