

Terumasa TADANO (只野央将)

Updated: January 18, 2023

PERSONAL DATA

PLACE AND DATE OF BIRTH: Japan | 18 December 1984
ADDRESS: 1-2-1 Sengen, Tsukuba, Ibaraki 305-0047, Japan
PHONE: +81 29 859 2332 (ext. 2332)
EMAIL: terumasa.tadano@gmail.com

RESEARCH INTERESTS

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

EDUCATION

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

APR 2021– | 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,
National Institute for Materials Science (NIMS), Japan

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

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

AWARDS

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

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

COMPUTER SKILLS

Basic Knowledge:	HTML, LINUX, \LaTeX
Intermediate Knowledge:	C++, Fortran, Python, MPI, OpenMP

PAPERS

-
1. E. Frasson, P. Rosander, F. Eriksson, M. Rahm, **T. Tadano**, P. Erhart, “Probing the limits of the phonon quasi-particle picture: The transition from underdamped to overdamped dynamics in CsPbBr_3 ”, (submitted).
 2. 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 EuTiO_3 : A Comparative Theoretical and Experimental Investigation”, (submitted).
 3. 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 SrTiO_3* ”, (submitted).
 4. 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*”, (submitted).
 5. 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 BaTiO_3* ”, Phys. Rev. B **106**, 224104 (2022).
 6. **T. Tadano** and W. A. Saidi, “*First-Principles Phonon Quasiparticle Theory Applied to a Strongly Anharmonic Halide Perovskite*”, Phys. Rev. Lett. **129**, 185901 (2022).
 7. 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_3 Perovskite Nanocrystals*”, Nano Lett. **22**, 7674 (2022).
 8. 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 Matter. **2202029** (2022).
 9. M. Ohnishi, **T. Tadano**, S. Tsuneyuki, and J. Shiomi, “*Anharmonic phonon renormalization and thermal transport in the type-I $\text{Ba}_8\text{Ga}_{16}\text{Sn}_{30}$ clathrate from first principles*”, Phys. Rev. B **106**, 024303 (2022).
 10. 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).

11. 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. **2200024** (2022).
12. 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 **105**, 104427 (2022).
13. 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).
14. 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).
15. 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).
16. 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).
17. K. Ishioka, **T. Tadano**, M. Yanagida, Y. Shirai, K. Miyano, “*Anharmonic Organic Cation Vibrations in Hybrid Lead Halide Perovskite CH₃NH₃PbI₃*”, Phys. Rev. Materials **5**, 105402 (2021).
18. 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).
19. 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. **2102097** (2021).
20. 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 Ca₅Ir₃O₁₂*”, Phys. Rev. B **104**, 075153 (2021).
21. 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).
22. 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).
23. 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, and Dy) alloys from first principles*”, J. Alloys Compd. **874**, 159754 (2021).
24. 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).

25. 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).
26. 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).
27. 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).
28. 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).
29. Y. Wu, W. Saidi, J. 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).
30. 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 Cu₃PS₄: A Cu–S-Based Thermoelectric Material with a Wurtzite-Derivative Structure”, *Adv. Funct. Mater.* **30**, 2000973 (2020).
31. M. Hirayama, **T. Tadano**, Y. Nomura, and R. Arita, “Materials design of dynamically stable *d*⁹ layered nickelates”, *Phys. Rev. B* **101**, 075107 (2020).
32. 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).
33. Y. Nomura, M. Hirayama, **T. Tadano**, Y. Yoshimoto, K. Nakamura, and R. Arita, “Formation of 2D single-component correlated electron system and band engineering in the nickelate superconductor NdNiO₂”, *Phys. Rev. B* **100**, 205138 (2019).
34. **T. Tadano**, Y. Nomura, and M. Imada, “*Ab initio* derivation of effective Hamiltonian for La₂CuO₄/La_{1.55}Sr_{0.45}CuO₄ heterostructure”, *Phys. Rev. B* **99**, 155148 (2019).
35. **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 (2019).
36. Y. Oba, **T. Tadano**, R. Akashi, and S. Tsuneyuki, “First-principles study of phonon anharmonicity and negative thermal expansion in ScF₃”, *Phys. Rev. Materials* **3**, 033601 (2019).
37. **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).
38. **T. Tadano** and S. Tsuneyuki, “First-principles lattice dynamics method for strongly anharmonic crystals”, *J. Phys. Soc. Jpn.* **87**, 041015 (2018).
39. 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* **96**, 245201 (2017).
40. A. Rohskopf, H. R. Seyf, K. Gordiz, **T. Tadano**, and A. Henry, “Empirical Interatomic Potentials Optimized for Phonon Properties”, *npj Computational Materials* **3**, 27 (2017).
41. W. Sano, T. Koretsune, **T. Tadano**, R. Akashi, and R. Arita, “Effect of van Hove singularities on high-T_c superconductivity in H₃S”, *Phys. Rev. B* **93**, 094525 (2016).

42. T. Tadano and S. Tsuneyuki, “Self-consistent phonon calculations of lattice dynamical properties in cubic SrTiO_3 with first-principles anharmonic force constants”, *Phys. Rev. B* **92**, 054301 (2015).
43. 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).
44. 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).

BOOK CHAPTERS & INVITED REVIEW

1. 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.
2. 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.
3. 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.
4. 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.
5. 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.
6. 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.
7. 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.
8. 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

1. 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.
2. 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.
3. 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.
4. 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.
5. 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.
6. 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.
7. 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」，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

8. 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。
9. 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.
10. T. Tadano, “Phonon anharmonicity and thermal transport in complex thermoelectric materials from first principles”, Colloquium at TU-Darmstadt, Dec. 9, 2019.
11. T. Tadano, “Development and application of ALAMODE software”, The 5th Workshop on ab initio phonon calculations, Krakow, Poland, Dec. 3–6, 2019.
12. 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。
13. T. Tadano, “Ab initio phonon calculations of strongly anharmonic solids”, Seminar at Samsung Advanced Institute of Technology (SAIT), Suwon-si, Korea, May 23, 2019.
14. 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。
15. 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.
16. 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。
17. 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。
18. 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.
19. 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。
20. 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。
21. 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.
22. 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.
23. 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。
24. 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。
25. 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.
26. 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。

27. 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.
28. T. Tadano, "Thermal conductivity and lattice anharmonicity of materials from first-principles calculations", ASIAN-19, Hsinchu, Taiwan, Oct. 31-Nov. 2 2016.
29. 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
30. T. Tadano and S. Tsuneyuki, "Non-equilibrium heat transfer simulation with first-principles anharmonic lattice model", 22th GREEN Open Seminar, Tsukuba, Japan, Sep. 2012.