

Zherui Han

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Email: zrhan@stanford.edu • <https://zrhan.notion.site> • Phone (US): 765-714-5832

Postdoctoral Scholar, Department of Electrical Engineering, Stanford University

Current office: 420 Via Palou, [Allen Center for Integrated Systems](#), Room 303X, Stanford, CA 94305

Education

Purdue University

2019 – 2024

Ph.D. in Mechanical Engineering

Thesis: First-principles predictions of high-order and nonequilibrium phonon thermal transport

Advisor: Professor Xiulin Ruan, *GPA: 4.00/4.00*.

Huazhong University of Science and Technology

2015 – 2019

B.Eng. in Energy and Power Engineering

Mentor: Professor Kun Wang, *GPA: 3.96/4.00*.

Appointment

Stanford University

June 2024 – Present

Postdoctoral Scholar, Department of Electrical Engineering

Advisor: Professor Eric Pop

Publications

[Google Scholar Profile](#)

(* Equal contributions; under review in grey)

- [22] Victoria M. Ravel, Robert K. A. Bennett, Sarah R. Evans, [Zherui Han](#), Samantha K. Holmes, Tara Peña, Eric Pop, Aaron D. Franklin, "Geometric Effects of Contacts to Two-Dimensional Semiconductors", *under review*, (2026).
- [21] [Zherui Han](#), Robert K. A. Bennett, Davide Donadio, Maritha A. Wang, Tara Peña, Mikaël Cassé, Martin Vanbrabant, Valeriya Kilchytska, Jean-Pierre Raskin, Eric Pop, "Band Tail States: Speed Bump or End of the Road for Two-Dimensional Semiconductors?", *under review*, (2026).
- [20] Jianfeng Jiang, Peng Wu, Hao-Yu Lan, [Zherui Han](#), Eric Pop, Lian-Mao Peng, "Rethinking Schottky-barrier height extraction at two-dimensional semiconductor contacts", *under review*, (2026).
- [19] Theresia Knobloch, Quentin Smets, Anton E. O. Persson, Pedram Khakbaz, Christoph Wilhelmer, Dennis Lin, [Zherui Han](#), Yunyan Chung, Kevin P. O'Brien, Chelsey Dorow, Cormac OCoileain, Mario Lanza, Dominic Waldhoer, Alexander Karl, Kailang Liu, Tianyou Zhai, Hailin Peng, Congwei Tan, Xiao Renshaw Wang, Georg S. Duesberg, John Robertson, Uygur Avci, Iuliana Radu, Eric Pop, Cesar J. Lockhart de la Rosa, Tibor Grasser, "Industrial Requirements for Gate Dielectrics in Two-Dimensional Semiconductor Devices," *Nat. Nanotechnol.*, in press (2026).
- [18] Xun Li, [Zherui Han](#), Xiulin Ruan, Li Shi, "Effects of four-phonon scattering on phonon hydrodynamics in monolayer graphene", *Phys. Rev. B* 112 (10), L100302 (2025).
- [17] Jordi Tur-Prats, [Zherui Han](#), Albert Beardo, Xiulin Ruan, F. Xavier Alvarez, "High-Order Anharmonicities Shape Phonon Hydrodynamic Effects in Graphene", *Nano Lett.* 25, 11203 (2025).

- [16] Krutarth Khot, Boyuan Xiao, **Zherui Han**, Ziqi Guo, Zixin Xiong, Xiulin Ruan, “Phonon local non-equilibrium at Al/Si interface from machine learning molecular dynamics”, *J. Appl. Phys.* 137, 115301 (2025).
- [15] Abdulaziz Alkandari, **Zherui Han**, Ziqi Guo, Thomas E Beechem, Xiulin Ruan, “Anisotropic anharmonicity dictates the thermal conductivity of $\beta - \text{Ga}_2\text{O}_3$ ”, *Phys. Rev. B* 111, 094308 (2025).
- [14] Daniel Carne, Joseph Peoples, Ziqi Guo, Dudong Feng, **Zherui Han**, Xiaojie Liu, Xiulin Ruan, “FOS: A fully integrated open-source program for Fast Optical Spectrum calculations of nanoparticle media”, *Com. Phys. Commun.* 307 (2025) 109393.
- [13] Ziqi Guo, Peter Sokalski, **Zherui Han**, Yanhua Cheng, Li Shi, Takashi Taniguchi, Kenji Watanabe, Xiulin Ruan, “First-principles prediction of zone-center optical phonon linewidths and IR spectra of hexagonal boron nitride”, *Appl. Phys. Lett.* 125, 231106 (2024).
- [12] Ziqi Guo, **Zherui Han**, Abdulaziz Alkandari, Krutarth Khot, Xiulin Ruan, “First-principles prediction of thermal conductivity of bulk hexagonal boron nitride”, *Appl. Phys. Lett.* 124, 163906 (2024).
- [11] Dudong Feng, Xiaolong Yang, **Zherui Han** and Xiulin Ruan, “Near-field radiation in BAs and BSb dominated by four-phonon scattering”, *Phys. Rev. B* 109, L081409 (2024).
- [10] Ziqi Guo, **Zherui Han**, Dudong Feng, Guang Lin, Xiulin Ruan, “Sampling-accelerated prediction of phonon scattering rates for converged thermal conductivity and radiative properties”, *npj Comput. Mater.* 10, 31 (2024).
- [9] **Zherui Han**^{*}, Zixin Xiong^{*}, William T. Riffe, Hunter B. Schonfeld, Mauricio Segovia, Jiawei Song, Haiyan Wang, Xianfan Xu, Patrick E. Hopkins, Amy Marconnet, and Xiulin Ruan, “Predictions and measurements of thermal conductivity of ceramic materials at high temperature”, *Phys. Rev. B* 108, 184306 (2023).
- [8] **Zherui Han**, Xiulin Ruan, “Thermal conductivity of monolayer graphene: Convergent and lower than diamond”, *Phys. Rev. B* 108, L121412 (2023).
- [7] **Zherui Han**, Changkyun Lee, Jiawei Song, Haiyan Wang, Peter Bermel, and Xiulin Ruan, “Temperature-Dependent Full Spectrum Dielectric Function of Semiconductors from First Principles”, *Phys. Rev. B* 107, L201202 (2023).
- [6] **Zherui Han**, Peter Sokalski, Li Shi and Xiulin Ruan, “Prediction of Hot Zone-center Optical Phonons in Laser Irradiated Molybdenum Disulfide with a Semiconductor Multitemperature Model”, *Phys. Rev. B* 107, L041407 (2023).
- [5] Peter Sokalski, **Zherui Han**, Gabriella Coloyan Fleming, Brandon Smith, Sean E. Sullivan, Rui Huang, Xiulin Ruan and Li Shi, “Effects of hot phonons and thermal stress in micro-Raman spectra of molybdenum disulphide”, *Appl. Phys. Lett.* 121, 182202 (2022)
- [4] **Zherui Han**^{*}, Xiaolong Yang^{*}, Sean E. Sullivan, Tianli Feng, Li Shi, Wu Li, and Xiulin Ruan, “Raman Linewidth Contributions from Four-Phonon and Electron-Phonon Interactions in Graphene”, *Phys. Rev. Lett.* 128, 045901 (2022).
- [3] **Zherui Han**, Xiaolong Yang, Tianli Feng, Wu Li, and Xiulin Ruan, “FourPhonon: An extension module to ShengBTE for computing four-phonon scattering rates and thermal conductivity”, *Com. Phys. Commun.* 270, 108179 (2022).

- [2] Yanhua Cheng, Xiaolong Yang, **Zherui Han**, Wenzhuo Wu, Xiaobing Luo and Xiulin Ruan, "Abnormal in-plane thermal conductivity anisotropy in bilayer α -phase tellurene", *Int. J. Heat Mass Transf.* 192, 122908 (2022).
- [1] **Zherui Han**, Kun Wang, Luyi Lu, Yunsheng Wu, and Chao Wang, "Fatigue damage assessment method of turbine shafts' torsional vibrations under SSO incidents", *Eng. Fail. Anal.* 105, 627 (2019).

Honors and Awards

Outstanding Graduate Student Research Award (Purdue College of Engineering), 2024
 Bilsland Dissertation Fellowship (Purdue University), 2023
 Best Poster at the Hawkins Student Poster Session (Purdue Mechanical Engineering), 2022
 Best student poster award (Symposium EN03, Materials Research Society), 2021
 Ross Fellowship (Purdue University), 2019
 iSURE scholarship (University of Notre Dame), 2017
 National scholarship (Ministry of Education, PRC), 2016 & 2017

Conference Proceedings and Abstracts (refereed)

(First-author is the presenter)

- [18] **Z. Han**, R.K.A. Bennett, D. Donadio, M.A. Wang, T. Peña, M. Cassé, M. Vanbrabant, V. Kilchytska, J.-P. Raskin, E. Pop, "Band Tail States as Energy-Efficient Limits for Two-Dimensional Electronics", ASME International Mechanical Engineering Congress & Exposition (IMECE), Nov 2026, Vancouver, Canada
- [17] **Z. Han**, T. Peña, C. Nattoo, W. Zhou, A. T. Hoang, A. J. Mannix, E. Pop, "Defects and Inhomogeneities of Two-dimensional Materials Probed by Raman Spectroscopy", MRS Spring Meeting, April 2026, Honolulu, HI
- [16] **Z. Han**, Y.-M. Lee, R.K.A. Bennett, E. Pop, "Band Tail States in Two-Dimensional Transistors", MRS Spring Meeting, April 2026, Honolulu, HI
- [15] H. Su, S. Alaei, Á. Friðriksdóttir, S. Fultz-Waters, X. Wu, D. Zhong, T. Peña, **Z. Han**, G. Pitner, P.C. McIntyre, Y. Suzuki, S.X. Wang, E. Pop, "Width-Scaling of Topological Semimetal NbP Nanoribbons from Room Temperature to Superconducting Behavior", MRS Spring Meeting, Apr 2026, Honolulu HI
- [14] K. Khot, P. Sokalski, **Z. Han**, X. Li, L. Shi, X. Ruan, "Mode-Resolved Electron-Phonon Dynamics in MoS₂ Field-Effect Transistors—Bridging First Principles to Device Simulations", MRS Spring Meeting, Apr 2026, Honolulu HI
- [13] H. Su, S. Gowda, X. Wu, S. Fultz-Waters, Y.S. Song, **Z. Han**, S.X. Wang, P.E. Hopkins, E. Pop, "Thermal Properties of Topological Semimetal NbP Thin Films and Nanoribbons", APS Global Physics Summit, Mar 2026, Denver CO
- [12] **Z. Han**, R.K.A. Bennett, E. Pop, "Band Tail States in Two-Dimensional Transistors", IEEE Semicon. Interface Specialists Conf. (SISC), December 2025, San Diego, CA

- [11] Y.S. Song, H. Su, T. Peña, A.E.O. Persson, K. Yang, E. Yalon, R.K.A. Bennett, **Z. Han**, K. Neilson, J. Kang, J.A. Yang, H.-S.P. Wong, S.X. Wang, E. Pop, "First Comparative Thermal Evaluation of 2D Semiconductor vs. Silicon Nanosheet Transistors", IEEE Intl. Electron Devices Meeting (IEDM), Dec 2025, San Francisco CA
- [10] Y.S. Song, H. Su, Y.-M. Lee, **Z. Han**, R.K.A. Bennett, M.A. Wang, L.G. Min, M. Asheghi, K.E. Goodson, S.X. Wang, E. Pop, "Investigation and Reduction of Thermal Resistance in Gate-All-Around Indium Tin Oxide Nanosheet Field-Effect Transistors", IEEE Device Research Conference (DRC), Jun 2025, Durham NC
- [9] **Z. Han**, E. Pop, "Thermal Transport in Layered Materials, Devices and Systems", MRS Spring Meeting, April 2025, Seattle, WA
- [8] T. Peña, A.T. Hoang, A. Fridriksdottir, **Z. Han**, K. Neilson, S. Lai, J. Wang, C.A. Nattoo, T.F. Heinz, P.C. McIntyre, A.J. Mannix, E. Pop, "Opto-Electronic Properties of Isotopically Purified Monolayer MoS₂", MRS Spring Meeting, Apr 2025, Seattle WA
- [7] Z. Guo, **Z. Han**, D. Feng, A. Alkandari, K. Khot, G. Lin and X. Ruan, "ML-assisted acceleration of Phonon Scattering Simulation: Methods and Applications", MRS Spring Meeting, Apr 2025, Seattle WA
- [6] **Z. Han**, X. Ruan, "Is Thermal Conductivity of Graphene Divergent and Higher Than Diamond?", ASME Summer Heat Transfer Conference, July 2023, Washington, D.C.
- [5] **Z. Han**, P. Sokalski, L. Shi, X. Ruan, "Hot Zone-center Optical Phonons in Laser Irradiated Molybdenum Disulfide Predicted by a Semiconductor Multitemperature Model", ASME Summer Heat Transfer Conference, July 2023, Washington, D.C.
- [4] **Z. Han**, X. Yang, S.E. Sullivan, T. Feng, L. Shi, W. Li, C. Lee, J. Song, H. Wang, P. Bermel, X. Ruan, "First-principles Predictions of Temperature-dependent Raman and Optical Responses", MRS Spring Meeting, May 2022, Honolulu, HI
- [3] **Z. Han**, Z. Xiong, J. Song, H. Wang, A. Marconnet, X. Ruan, "Thermal Conductivity Prediction of Ceramic Materials at High Temperature", MRS Spring Meeting, May 2022, Honolulu, HI
- [2] **Z. Han**, X. Ruan, "Thermal Conductivity Prediction of Ceramic Materials at High Temperature", MRS Fall Meeting, December 2021, Boston, MA
- [1] **Z. Han**, X. Yang, S.E. Sullivan, T. Feng, L. Shi, W. Li, X. Ruan, "Raman Linewidth Contributions from Four-Phonon and Electron-Phonon Interactions in Graphene" (poster), MRS Fall Meeting, December 2021, Boston, MA

Teaching Experience

Hands-on sessions lecturer, ME 697R: Computational Methods for Nanoscale Energy Transport, Spring 2022 and Spring 2024

Several hands-on sessions on computational methods and how to perform basic first-principles calculations using GULP and ABINIT. *Videos recorded.*

Instructor: Prof. Xiulin Ruan

Teaching assistant (lecture), ME 315: Heat and Mass Transfer, Spring 2023

Instructor: Prof. Thomas Beechem

Mentoring, Outreach and Service

Lead developer of FourPhonon, a phonon transport solver [\[link\]](#)

GitHub repository, online forum and tutorials

Conference session co-chair

Symposium EN03: “*Thermal Materials, Modeling and Technoeconomic Impacts for Thermal Management and Energy Application*”, MRS Fall meeting 2021, Boston, Massachusetts

Mentor

Purdue Summer Undergraduate Research Fellowship (SURF): Alison Brown

Stanford Undergraduate Research Experience (REU): Brian Chen

Graduate students in research groups: Krutarth Khot, Ziqi Guo, Abdulaziz Alkandari, Sreerag Sundaram; Maritha Wang, Young Suh Song, Haotian Su

Reviewer

APS Physical Review series; APL; JAP; Science Adv; Nat. Comm.; npj series; Nat. Rev. EE

References

Eric Pop

Pease-Ye Professor of Electrical Engineering and (by courtesy) of Applied Physics and Materials Science & Engineering, Stanford University

Email: epop@stanford.edu

Postdoc advisor

Xiulin Ruan

Professor of Mechanical Engineering, University Faculty Scholar, Purdue University

Email: ruan@purdue.edu

PhD advisor

Li Shi

Professor of Walker Department of Mechanical Engineering and Texas Materials Institute

Ernest Cockrell Sr. Chair in Engineering, The University of Texas at Austin

Email: lishi@mail.utexas.edu

Project: High-Order Phonon Scattering and Highly Nonequilibrium Carrier Transport in Two-dimensional Electronic and Optoelectronic Materials, NSF

Amy Marconnet

Professor of Mechanical Engineering and (by courtesy) of Materials Engineering, Perry Academic Excellence Scholar, Purdue University

Email: amarconn@purdue.edu

Project: Prediction-guided Hierarchically Structured Coatings for High Temperature Thermal Radiation Control, DARPA

Guang Lin

Full Professor, Department of Mathematics, School of Mechanical Engineering, Purdue University

Email: guanglin@purdue.edu

Project: FourPhonon: A Computational Tool for Higher-Order Phonon Anharmonicity and Thermal Properties, NSF