# Tianli Feng

(as of Jan 2024)

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### **Professional Appointments**

08/2021 - Present	Assistant Professor, Mechanical Engineering, University of Utah, USA
11/2020 - 07/2021	R&D Associate Staff Scientist, Oak Ridge National Laboratory, USA
08/2017 - 10/2020	Postdoc, Oak Ridge National Laboratory, USA

### **Education**

08/2017 Ph.D. in Mechanical Engineering, Purdue University, West Lafayette, IN, USA

- Thesis: Theoretical phonon spectroscopy using predictive atomistic simulations

12/2013 M.S. in Mechanical Engineering, Purdue University, West Lafayette, IN, USA

- Thesis: Accurate prediction of spectral phonon relaxation time and thermal conductivity of intrinsic and perturbed materials

07/2011 B.S. in Physics, University of Science and Technology of China (USTC), Hefei, China

### **Selected Honors/Awards**

- 2024 NSF CAREER Award
- 2023 Brillouin Medal
  - The Brillouin Medal is awarded every two years to 1-3 researchers who make significant contributions to the research of phonons.
- 2023 ORAU Ralph E. Powe Junior Faculty Enhancement Award
  - This award annually honors the 35 most promising junior faculty members, selected from a pool of over 150 universities.
- 2021 ES Energy & Environment Best Paper Award
- 2016-2017 Bilsland Dissertation Fellowship, Purdue University

### **Research Interests**

- Ultra-high or low thermal conductivity materials, semiconductors, interfacial thermal transport across solid heterostructures, thermal management of electronics, thermal interface materials
- Ultra-high-temperature thermal transport, hypersonic materials, thermal barrier coatings, high temperature energy harvesting, thermal transport in Earth mantle materials
- Building energy efficiency, thermal insulation materials, building envelope air leakage detection, thermal energy storage, passive cooling, thermoelectrics.
- Quantum materials, lithium-ion materials, heat in quantum computing, 2D materials

### **Research Projects**

### Current @ University of Utah (as a tenure-track assistant professor)

- NSF CAREER, "Prediction and understanding of thermal transport across successive interfaces". 2/2024 -1/2029. (Role: Principal Investigator)
- **DOE**, ORNL, "Building envelope air leakage detection and quantification by a novel transient IR imaging method". 1/2024 9/2024. (Role: Co-Principal Investigator)

- **DOE**, INL-LDRD, "Phonon transport in superior heat conductors under irradiation". 10/2022 9/2025. (Role: Co-Principal Investigator)
- NSF, "Prediction of thermal transport in nonmetallic materials at ultra-high temperatures". 6/2022 -5/2025. (Role: Principal Investigator)
- **DOE**, ORNL, "Develop multiscale simulation and machine learning models to predict the thermal conductivity of porous insulation materials". 5/2022 9/2025. (Role: Co-Principal Investigator)

### Past @ University of Utah (as a tenure-track assistant professor)

• **Qorvo**, industry, "Demonstrate high thermal conductivity (15-16 W/mK) of the AlN-filled epoxy materials with appropriate moldability on Si wafer", 4/2023-6/2023. (Role: Principal Investigator)

### Past @ Oak Ridge National Laboratory (as a postdoc/ staff scientist)

- **DOE**, BTO, "A New Approach to Encapsulate Salt Hydrate PCM", 2021. (Role: Researcher)
- **DOE**, BTO, "Models to Evaluate and Guide the Development of Low Thermal Conductivity Materials for Building Envelopes", 2018-2021. (Role: Researcher)
- **DOE**, BTO, "Facer barriers for aged foam boards with > R8/in", 2021. (Role: Researcher)
- **DOE**, BTO, "Active insulation systems, simulations, and prototype development", 2021. (Role: Researcher)
- **DOE**, BTO, "Developing the Metrology for Accurately Assessing the R-value of Super Insulation", 2018-2021. (Role: Researcher)
- **DOE**, BES, "Physics of Complex Materials Systems Through Theory and Microscopy/EELS", 2017-2019. (Role: Researcher)

# Past @ Purdue University (as a graduate student)

- **DARPA**, "First Principles-Based Prediction and Design of Thermoelectric Materials and Interfaces under Large Temperature Gradients", 2015-2017. (Role: Researcher)
- NSF, "First Principles-Enabled Prediction of Thermal Conductivity and Radiative Properties of Solids", 2012-2017. (Role: Researcher)

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# **PUBLICATIONS**

	All	Since 2018
Citations	4184	3826
h-index	35	34
i10-index	58	58
		980
		735
		490
_		245
2016 2017 2018	3 2019 2020 2021	2022 2023 0

Google Scholar Profile: https://shorturl.at/jozJ0 as of 2023

### Patents / Invention disclosure

- [2]. Tianli Feng, Zhenglai Shen, Som S Shrestha, Provisional patent application "Building Air Leakage Detection and Quantification Using Transient Infrared Imaging" 63 542 999 (2023).
- [1]. Som S. Shrestha, Mikael Salonvaara, Emishaw D. Iffa, Niraj Kunwar, Diana Hun, Philip R. Boudreaux, and Tianli Feng, Non-Provisional Utility Patent Application UTB Ref. No. ID202004771.US.01, Fox Ref. No. 157379.11801 (6321-547), "Solid-State Thermal Switch Panel For Thermal Storage". (2023)

# **Developed Simulation Tools**

- [5]. **Tianli Feng**, Som Shrestha, Diana Hun, Daniel Howard, Amit Rai, <u>ThermoPI</u> is a Windows APP and Online tool that can calculate the thermal conductivity of porous thermal insulation materials given the structural information. This tool is to help researchers develop the next-generation thermal insulation materials used in building envelopes, pipeline thermal protection, food, drug, and vaccine transportation and storage, etc. (2022) <a href="https://thermopi.ornl.gov/about">https://thermopi.ornl.gov/about</a>
- [4]. Zherui Han, Xiaolong Yang, Wu Li, **Tianli Feng**, Xiulin Ruan, "FourPhonon: An extension module to ShengBTE for computing four-phonon scattering rates and thermal conductivity", <a href="Comp. Phys. Comm.">Comp. Phys. Comm.</a> 270, 108179 (2022). <a href="https://github.com/FourPhonon/FourPhonon">https://github.com/FourPhonon/FourPhonon</a>
- [3]. **Tianli Feng**, Divya Chalise, Xiulin Ruan (2015), Nanohub tool: Spectral phonon relaxation time calculation tool by using normal mode analysis based on molecular dynamics, <a href="https://nanohub.org/resources/phononlifetime/usage">https://nanohub.org/resources/phononlifetime/usage</a>
- [2]. **Tianli Feng**, Xiulin Ruan (2015), Nanohub tool: Lorentzian fitting tool for phonon spectral energy density, <a href="https://nanohub.org/resources/lorentzfit/usage">https://nanohub.org/resources/lorentzfit/usage</a>
- [1]. **Tianli Feng**, Yang Zhong, Divya Chalise, Xiulin Ruan, Nanohub tool: Spectral analysis of nonequilibrium molecular dynamics, <a href="https://nanohub.org/resources/spectralnemd">https://nanohub.org/resources/spectralnemd</a>

# **Book Chapters / Review Articles**

- [4]. T. Feng\*, H. Zhou, Z. Cheng, L. Larkin, M. Neupane, "A Critical Review of Thermal Boundary Conductance across Wide and Ultrawide Bandgap Semiconductor Interfaces", <u>ACS Applied Materials & Interfaces</u>, 15, 25, 29655 (2023).
- [3]. T. Feng, X. Ruan\*, "Higher-order phonon scattering: advancing the quantum theory of phonon linewidth, thermal conductivity and thermal radiative properties" in Nanoscale Energy Transport 2-1-2-44 (IOP Publishing, 2020). https://doi.org/10.1088/978-0-7503-1738-2ch2.
- [2]. B. Xu, T. Feng, Z. Li, W. Zheng, Y. Wu\*, "Large-Scale, Solution-Synthesized Nanostructured Composites for Thermoelectric Applications", <u>Advanced Materials.</u>, 30, 1801904 (2018).
- [1]. T. Feng, X. Ruan\*, "Prediction of spectral phonon mean free path and thermal conductivity with applications to thermoelectrics and thermal management: a review", <u>Journal of Nanomaterials</u> 2014, 206370 (2014).

# Peer-Reviewed Journal Articles (underline: Feng group members. \*corr. authors)

- [79] <u>H. Zhou, J. Tiwari,</u> T. Feng\*, "On the flattening trend of thermal conductivity of La<sub>2</sub>Zr<sub>2</sub>O<sub>7</sub> at ultrahigh temperatures", under review.
- [78]. T. Feng\*, Z. Shen, S. Shrestha, D. Hun, "A novel transient infrared imaging method for non-intrusive, low-cost, fast, and accurate air leakage detection in building envelopes", under review.
- [77] <u>J. Tiwari</u>, T. Feng\*, "Accurate prediction of thermal conductivity of Al<sub>2</sub>O<sub>3</sub> at ultrahigh temperatures", arXiv preprint, arXiv:2312.11755
- [76]. <u>J. Tiwari</u>, S. Shrestha, T. Feng\*, "Computational design of isotropic and anisotropic ultralow thermal conductivity foams", under review.

[75]. M. Hoque, E. Hoglund, B. Zhao, D. Bao, H. Zhou, S. Thakur, E. Osei-Agyemang, K. Hattar, E. Scott, M. Surendran, J. Tomko, J. Gaskins, K. Aryana, S. Makarem, G. Balasubramanian, A. Giri, T. Feng, J. Hachtel, J. Ravichandran, S. Pantelides, P. Hopkins, "Ruddlesden-Popper chalcogenides push the limit of mechanical stiffness and glass-like thermal conductivity in crystals", arXiv preprint, arXiv:2312.02534

#### 2023:

- [74]. <u>H. Zhou</u>, S. Zhou, Z. Hua, K. Bawane, **T. Feng\***, "Extreme sensitivity of higher-order interatomic force constants and thermal conductivity to the energy surface roughness of exchange-correlation functionals", <u>Appl. Phys. Lett.</u> 123, 192201 (2023).
  - This work is selected as a Featured Article by Applied Physics Letters!
- [73]. T. Feng\*, H. Zhou, Z. Cheng, L. Larkin, M. Neupane, "A Critical Review of Thermal Boundary Conductance across Wide and Ultrawide Bandgap Semiconductor Interfaces", <u>ACS Applied Materials & Interfaces</u>, 15, 25, 29655 (2023).
- [72]. Y. Lou, X. Li, Z. Shi, <u>H. Zhou</u>, **T. Feng**, B. Xu, "General Syntheses of High-Performance Thermoelectric Nanostructured Solids without Post-Synthetic Ligand Stripping", <u>Nano Lett.</u> 23, 11, 5317 (2023).
- [71]. <u>J. Tiwari</u>, **T. Feng\***, "Intrinsic thermal conductivity of ZrC from low to ultra-high temperatures: A critical revisit", <u>Phys. Rev. Materials</u> 7, 065001 (2023).
- [70]. <u>H. Zhou</u>, **T. Feng\***, "Theoretical upper limits of the thermal conductivity of Si<sub>3</sub>N<sub>4</sub>", <u>Appl. Phys.</u> <u>Lett.</u>, 122, 182203 (2023).
- [69]. Y. Zhang, W. M. Postiglione, R. Xie, C. Zhang, H. Zhou, V. Chaturvedi, K. Heltemes, H. Zhou, T. Feng, C. Leighton, X. Wang, Large tunability in thermal conductivity of La0.5Sr0.5CoO3-films through electrolyte gating, Nat. Comm. 14, 2626 (2023).
- [68]. Z. Shen, S Shrestha, D. Howard, **T. Feng**, D. Hun, B. She, Machine learning–assisted prediction of heat fluxes through thermally anisotropic building envelopes, <u>Building and Environment</u>, 234, 110157 (2023).
- [67]. S. Shrestha, <u>J. Tiwari</u>, A. Rai, D. E Hun, D. Howard, A. O Desjarlais, M. Francoeur, **T. Feng\***, Solid and Gas Thermal Conductivity Models Improvement and Validation in Various Porous Insulation Materials, <u>Int. J. Therm. Sci.</u>, 187, 108164 (2023).

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- [65]. X. Li, Y. Lou, K. Jin, L. Fu, P. Xu, Z. Shi, **T. Feng**, B. Xu\*, Realizing zT > 2 in environment-friendly monoclinic Cu2S tetragonal Cu<sub>1.96</sub>S nano phase junctions for Thermoelectrics, <u>Angew. Chem. Int. Ed.</u>, 2022, e202212885.
- [64]. R. Xie, J. Tiwari, T. Feng\*, Impacts of various interfacial nanostructures on spectral phonon thermal boundary conductance, J. Appl. Phys. 132, 115108 (2022).
- [63]. W. Zhang, Y. Lou, H. Dong, F. Wu, <u>J. Tiwari</u>, Z. Shi, **T. Feng**, S. T. Pantelides, B. Xu, Phase-engineered high-entropy metastable FCC Cu<sub>2-y</sub>Ag<sub>y</sub>(In<sub>x</sub>Sn<sub>1-x</sub>)Se<sub>2</sub>S nanomaterials with high thermoelectric performance, <u>Chem. Sci.</u>, 13, 10461 (2022).
- [62]. K. Jin, <u>J. Tiwari</u>, **T. Feng\***, Y. Lou\*, B. Xu\*, Realizing high thermoelectric performance in ecofriendly Bi<sub>2</sub>S<sub>3</sub> with nanopores and Cl-doping through shape-controlled nano precursors, <u>Nano Energy</u> 100, 107478, (2022).
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- [60]. X. Yang, **T. Feng**, J. Li, X. Ruan, Evidence of five-order and higher-order phonon scattering entropy of zone-center optical phonons, <u>Phys. Rev. B</u> 105, 115205 (2022).
- [59]. Z. Zhu, <u>J. Tiwari</u>, T. Feng, Z. Shi, Y. Lou\*, B. Xu\*, "High thermoelectric properties with low thermal conductivity due to the porous structure induced by the dendritic branching in n-type PbS", <u>Nano Research</u> 15, 4739 (2022).

- [58]. 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", <u>Physical Review Letters</u> 128, 045901 (2022).
- [57]. Q. Guo, **T. Feng**, M.J. Lance, K.A. Unocic, S.T. Pantelides, E. Lara-Curzio\*, "Evolution of the structure and chemical composition of the interface between multi-component silicate glasses and yttriastabilized zirconia after 40,000-hour exposure in air at 800°C", <u>J. Eur. Ceram. Soc.</u> 42, 1576 (2022).
- [56]. Y. Zhang, M. Eslamisaray, T. Feng, U. Kortshagen, X. Wang\*, "Observation of Suppressed Diffuson and Propagon Thermal Conductivity of Hydrogenated Amorphous Silicon Films', Nanoscale Advances 4, 87 (2022).
- [55]. Z. Han, X. Yang, W. Li, **T. Feng**, X. Ruan\*, "FourPhonon: An extension module to ShengBTE for computing four-phonon scattering rates and thermal conductivity", <u>Computer Physics Communications</u> 270, 108179 (2022).

#### 2021:

- [54]. J. Xu, Y. Hu, X. Ruan, X. Wang, **T. Feng\***, H. Bao\*, "Nonequilibrium phonon transport induced by finite sizes: the effect of phonon-phonon coupling", <a href="Physical Review B">Physical Review B</a>, 104, 104310 (2021).
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  This paper is covered by News Media: Heat conduction record with tantalum nitride
- [52]. A. Rai, T. Feng, D. Howard, D. Hun, M. Zhang, H. Zhou, S. S. Shrestha, "Conduction Heat Transfer through Solid in Porous Materials: A Comparative Study by Finite-Element Simulations and Effective Medium Approximations", Comp. Therm. Sci., 13, 19, 2021.
- [51]. Q. Zheng#, T. Feng#, J. A. Hachtel#, R. Ishikawa, J. C. Idrobo, J. Yan, N. Shibata, Y. Ikuhara, B. C. Sales, S. T. Pantelides, M. Chi, "Direct Visualization of Anionic Electrons in an Electride Reveals Inhomogeneities", Science Advances 7, eabe6819 (2021). (#contributed equally)
- [50]. P. R. Chowdhury, J. Shi, T. Feng, X. Ruan, "Prediction of Bi2Te3/Sb2Te3 interfacial conductance and superlattice thermal conductivity using molecular dynamics simulations", <u>ACS Appl. Mater. & Interfaces</u>, 10.1021/acsami.0c17851 (2021).
- [49]. T. Feng, A. Rai, D. Hun, S. S Shrestha, "Molecular dynamics simulations of energy accommodation between gases and polymers for ultra-low thermal conductivity insulation", <u>International Journal of Heat and Mass Transfer</u>, 164, 120459 (2021).
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- [47]. T. Feng, J. He, A. Rai, D. Hun, J. Liu, S. S Shrestha, "Size Effects in the Thermal Conductivity of Amorphous Polymers", <a href="Physical Review Applied">Physical Review Applied</a> 14, 044023 (2020).
- [46]. S. Neumayer, L. Tao, A. O'Hara, J. Brehm, M. Si, P.-Y. Liao, T. Feng, S. V Kalinin, D Y. Peide, S. T Pantelides, P. Maksymovych, N. Balke, "Alignment of Polarization against an Electric Field in van der Waals Ferroelectrics", <u>Physical Review Applied</u> 13, 064063 (2020).
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- [44]. T. Feng\*, A. O'Hara, S. T. Pantelides\*, "Quantum prediction of the Ultra-Low Thermal Conductivity of Lithium Intercalation Materials", Nano Energy 75, 104916 (2020).
- [43]. Y. Luo, X. Yang, T. Feng, J. Wang, X. Ruan, "Vibrational hierarchy leads to dual-phonon transport in low thermal conductivity crystals", <u>Nature Communications</u> 11, 2554 (2020).

- [42]. Y. Hu#, T. Feng#, X. Gu, Z. Fan, X. Wang, M. Lundstrom, S. S. Shrestha, H. Bao, "Unification of nonequilibrium molecular dynamics and the mode-resolved phonon Boltzmann equation for thermal transport simulations", <a href="Phys. Rev. B">Phys. Rev. B</a> 101, 155308 (2020). (#contributed equally)
- [41]. X. Yang#, T. Feng#, J. S. Kang, Y. Hu, J. Li, X. Ruan\*, "Observation of strong higher-order lattice anharmonicity in Raman and infrared response", <a href="Phys. Rev. B">Phys. Rev. B</a> 101, 161202(R) (2020). (#contributed equally)
  - This work is selected as Editors' Suggestions (top 5%) in Physical Review B.
- [40]. Z. Tong, X. Yang, T. Feng, H. Bao, X. Ruan, "First-principles predictions of temperature-dependent infrared dielectric function of polar materials by including four-phonon scattering and phonon frequency shift", Phys. Rev. B 101, 125416 (2020).
- [39]. P. R. Chowdhury, C. Reynolds, A. Garrett, T. Feng, S. P. Adiga,\* X. Ruan,\* "Machine learning maximized Anderson localization of phonons in aperiodic superlattices", <u>Nano Energy</u> 69, 104428 (2020).
- [38]. T. Feng#, X. Wu#, X. Yang, P. Wang, L. Zhang, X. Du, X. Wang\*, S. T. Pantelides\*, "Thermal conductivity of HfTe5: a critical revisit", <u>Advanced Functional Materials</u>, 30, 1907286 (2020). (Image is selected as the inside back cover of the issue.) (#contributed equally)
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- [32]. A. Oyedele#, S. Yang#, T. Feng#, A. V. Haglund, Y. Gu, A. A. Puretzky, D. Briggs, C. M. Rouleau, M. F. Chisholm, R. R. Unocic, D. Mandrus, H. M. Meyer, S. T. Pantelides, D. B. Geohegan, K. Xiao\*, "Defect-mediated phase transformation in anisotropic 2D PdSe<sub>2</sub> crystals for seamless electrical contact devices", <u>Journal of the American Chemical Society</u>, 141, 22, 8928-8936 (2019).
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  - This work is honored as a "Highly Cited" paper by Web of Science (top 1%).
- [29]. M. Hong, Y. Wang, T. Feng, Q. Sun, S. Xu, S. Matsumura, S. T. Pantelides, J. Zou\*, Z. Chen\*, and ZhiGang Chen, Strong Phonon-Phonon Interactions Securing Extraordinary Thermoelectric Ge<sub>1-x</sub>Sb<sub>x</sub>Te with Zn-Doping Induced Band Alignment, <u>Journal of the American Chemical Society</u>, 141 (4), 1742 (2019).
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#### 2018:

- [25]. B. Xu#, T. Feng#, Z. Li, L. Zhou, S. T. Pantelides, Y. Wu\*, "Creating Zipper-like van der Waals Gap Discontinuity in Low-Temperature-Processed Nanostructured PbBi<sub>2n</sub>Te<sub>1+3n</sub> for Enhanced Phonon Scattering and Improved Thermoelectric Performance", <u>Angewandte Chemie International Edition</u> 57, 10938 (2018). (#contributed equally)
- [24]. J. Zhu#, T. Feng#, S. Mills, P. Wang, X. Wu, L. Zhang, S. T. Pantelides, X. Du, and X. Wang\*, "Record-Low and Anisotropic Thermal Conductivity of Quasi-1D Bulk ZrTe<sub>5</sub> Single Crystal", ACS Applied Materials and Interfaces 10, 47, 40740 (2018). (#contributed equally)
- [23]. B. Xu, T. Feng, Z. Li, W. Zheng, Y. Wu\*, "Large-Scale, Solution-Synthesized Nanostructured Composites for Thermoelectric Applications", <u>Advanced Materials</u> 30, 1801904 (2018).
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  - This paper won the Best Paper Award from Engineered Science Publisher.
- [21]. B. Xu, T. Feng, Z. Li, S. Pantelides, Y.Wu\*, "Constructing Highly Porous Thermoelectric Monoliths with High-Performance and Improved Portability from Solution-Synthesized Shape-Controlled Nanocrystals", Nano Letters 18, 4034-4039 (2018).
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  - Our prediction was directly verified by experiment in three Science papers: Kang et al. Science 2018; Tian et al. Science 2018; Li et al. Science 2018;

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- [13]. J. Kaiser\*, T. Feng, J. Maassen, X.Wang, X. Ruan, M. Lundstrom, "Thermal transport at the nanoscale: A Fourier's law vs. phonon Boltzmann equation study", <u>Journal of Applied Physics</u>, 121, 044302 (2017).
- [12]. B. Xu, T. Feng, M. T Agne, L. Zhou, X. Ruan, G J. Snyder, Y. Wu\*, "Highly Porous Thermoelectric Nanocomposite with Low Thermal Conductivity and High Figure of Merit from Large-Scale Solution-Synthesized Bi<sub>2</sub>Te<sub>2.5</sub>Se<sub>0.5</sub> Hollow Nanostructures", <u>Angewandte Chemie International Edition</u> 129, 3600-3605 (2017).
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- [11]. B. Xu, M. Agne, T. Feng, T. C. Chasapis, X. Ruan, Y. Zhou, H. Zheng, J. Bahk\*, M. G. Kanatzidis, J. G. Snyder\*, Y. Wu\*, "Nanocomposites from solution-synthesized PbTe-BiSbTe nano-heterostructure with unity figure of merit at low-medium temperatures (500-600 K)", <u>Advanced Materials</u> 29, 1605140 (2017).
  - <u>Selected as the inside front cover of Advanced Materials, Vol 29, Iss 10, 2017</u> **Before 2016:**
- [10]. T. Feng and X. Ruan\*, "Ultra-low thermal conductivity in graphene nanomesh", <u>Carbon</u> 101, 107-113 (2016).
- [9]. T. Feng and X. Ruan\*, "Quantum mechanical prediction of four-phonon scattering rates and reduced thermal conductivity of solids", <a href="Physical Review B">Physical Review B</a> 93, 045202 (2016).
  - This work is honored as a "Highly Cited" paper by Web of Science (top 1%).
- [8]. H. Fang, J. Bahk, T. Feng, Z. Cheng, A. Mohammed, X. Wang, X. Ruan, A. Shakouri, Y. Wu\*, "Thermoelectric properties of solution synthesized n-type Bi<sub>2</sub>Te<sub>3</sub> nanocomposites modulated by Se: An experimental and theoretical study", Nano Research 9, 117-127 (2016).
- [7]. T. Feng, B. Qiu, X. Ruan\*, "Coupling between phonon-phonon and phonon-impurity scattering: A critical revisit of the spectral Matthiessen's rule", <a href="Physical Review B">Physical Review B</a> 92, 235206 (2015).
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- [5]. T. Feng, B. Qiu, X. Ruan\*, "Anharmonicity and necessity of phonon eigenvectors in the phonon normal mode analysis", Journal of Applied Physics 117, 195102 (2015).
- [4]. Z. Wang, T. Feng, X. Ruan\*, "Thermal conductivity and spectral phonon properties of freestanding and supported silicene", <u>Journal of Applied Physics</u> 117, 084317 (2015).
- [3]. Z. Ye, B. Cao\*, W. Yao, T. Feng, X. Ruan\*, "Spectral phonon thermal properties in graphene nanoribbons", <u>Carbon</u> 93, 915-923 (2015).
- [2]. T. Feng, X. Ruan\*, "Prediction of spectral phonon mean free path and thermal conductivity with applications to thermoelectrics and thermal management: a review", <u>Journal of Nanomaterials</u> 2014, 206370 (2014).
- [1]. H. Fang, T. Feng, H. Yang, X. Ruan, Y. Wu\*, "Synthesis and Thermoelectric Properties of Compositional Modulated Lead Telluride-Bismuth Telluride Nanowire Heterostructures", Nano Letters 13, 2058 (2013).

# **Peer-Reviewed Conference Papers**

- [2]. Z. Shen, S. Shrestha, D. Howard, T. Feng, B. She, D. Hun, "A Machine Learning Assisted Framework to Control Thermally Anisotropic Building Envelopes in Residential Buildings", 2022 Buildings XV Conference, 2022.
- [1]. S. Shrestha, A. Rai, T. Feng, M. Zhang, D. Hun, K. Biswas, A. Desjarlais, "Review of Models to Evaluate and Guide the Development of Low-Thermal-Conductivity Materials." ASHRAE Topical Conference Proceedings. American Society of Heating, Refrigeration and Air Conditioning Engineers, Inc., 2019.

# **Major Media Exposure**

- 06/2023 Brillouin Medal! Prof. Feng, together with Prof. Xiulin Ruan, received the 2023 Brillouin Medal, which is awarded every 2 years to 1-3 people who make significant contributions to phonon research. Prof. Ruan will deliver a Brillouin talk at Phononics 2023 in Manchester, UK (June 12-16, 2023). More news will come out soon. <a href="https://www.mech.utah.edu/tianlifeng-receives-2023-brillouin-medal/">https://www.mech.utah.edu/tianlifeng-receives-2023-brillouin-medal/</a> https://phononics2023.org/conf/index.php/phononics/2023/pages/view/Medals
- Our research work on Thermal Conductivity at Ultra-High Temperatures is reported by <a href="https://www.mech.utah.edu/thermal-conductivity-at-ultra-high-temperatures">https://www.mech.utah.edu/thermal-conductivity-at-ultra-high-temperatures</a>
- 03/2021 Our paper about finding new ultra-high thermal conductivity material tantalum nitride, published in Physical Review Letters, was reported by many new media: https://aps.altmetric.com/details/102012911/news
- 11/2020 Our paper that finds the heat transport ability of lithium-ion battery cathodes is much lower than previously determined, published in Nano Energy, was reported by news media: <a href="https://www.ornl.gov/news/batteries-catching-heat">https://www.ornl.gov/news/batteries-catching-heat</a>
- 04/2020 Our paper that demonstrated four-phonon scattering in infrared and Raman for the first time, published in Physical Review B, was reported by news media: <a href="https://engineering.purdue.edu/ME/News/2020/fourphonon-scattering-affects-materials-infrared-and-raman-spectra">https://engineering.purdue.edu/ME/News/2020/fourphonon-scattering-affects-materials-infrared-and-raman-spectra</a>
- 03/2018 Our work that realized nanoscale temperature measurement using an electron probe for the first time, published in Physical Review Letters, was reported by many News Media: https://aps.altmetric.com/details/34290601/news
- 12/2017 Our breakthrough of four-phonon scattering thermal conductivity prediction, published in Physical Review B: rapid communications, was reported by many news media: https://aps.altmetric.com/details/28312669/news

# **TEACHING**

### **Mentored Students**

- Mentored Ph.D. Students
  - 2023-now, Tanvirul Abedien, University of Utah
  - 2023-now, Jacob Crossley, University of Utah
  - 2023-now, Khalid Adnan, University of Utah
  - 2022-now, Hao Zhou, University of Utah
  - 2021-now, Janak Tiwari, University of Utah
  - 2017-2018, Xiaolong Yang. Visiting scholar at Purdue University
  - 2015-2016, Wenjun Yao. Visiting scholar at Purdue University
- Mentored M.S. Students

- 2021-2023, Rui Xie, University of Utah, Thesis: "Interfacial Phonon Transport by Molecular Dynamics Simulations Based on Classical and Machine Learning Potentials"
- 2013-2015, Vignesh Gouthaman, Purdue University. Now in Trelleborg Vibracoustic, MI.
- 2013-2015, Eshaan Mathew, Purdue University. Now in Digital Energy, CA.
- Mentored Undergraduate Students
  - 2023-now, Wyatt Jones, University of Utah
  - 2023-now, Bryce Rundell, University of Utah
  - 2023-now, Yara Ahmed, University of Utah
  - 2017, Yang Zhong, Purdue University. Position after graduation: Ph.D. student at MIT.
  - 2017, Divya Chalise, Purdue University. Position after graduation: UC Berkeley.
- Mentored High-school Internship Students
  - 2023, Audrey Bradley, "First principles-based machine learning molecular dynamics simulations", University of Utah
  - 2023, Adam Clark, "First principles-based machine learning molecular dynamics simulations", University of Utah

# **Courses Taught**

- Advanced Conduction, ME EN 7650 (Fall 23)
- Thermodynamics, ME EN 2300 (Spring 23, Spring 24)
- Intermediate Heat Transfer, ME EN 5560/6560 (Fall 22, Fall 21)

# **Short Courses and Workshops Taught**

- Two lectures (each 60 mins), September 2023, to high school students on the topic of "Control The Heat" to the high school students in Farmington Bay Youth Center, Farmington, Utah.
- Three lectures (each 80 mins), February 2023, to high school students on the topic of "Control The Heat" to the high school students in the Decker Lake Youth Center, West Valley City, Utah.
- Half-day tutorial at Materials Research Society (MRS) conference, Boston, MA, November 2021. "Four-Phonon Scattering - A Critical Process Determining Thermal and Radiative Properties". The audience was expected to (1) be familiar with the background of three- and four-phonon scattering and their roles in thermal and radiative properties of materials, (2) understand the various characteristics of four-phonon scattering mechanism in different systems and scenarios, (3) understand the broad impact of four-phonon scattering on thermal transport and radiative properties in various materials, (4) be able to tell in which types of materials and scenarios will four-phonon scattering be critical, (5) be able to use the open-source code FourPhonon together with ShengBTE to calculate four-phonon scattering rates (linewidth) and thermal conductivities for materials. The outline of this tutorial is as follows.
  - 1:30-2:05 Overview, background, and formalism
  - 2:05-2:20 Characteristics of four phonon scattering
  - 2:20-2:30 First principles predictions
  - 2:45-3:10 Materials with large acoustic optical phonon band gaps
  - 3:10-3:30 Optical phonons and radiative properties
  - 4:00-4:15 Two dimensional materials with reflection symmetry
  - 4:15-4:30 Impact of phonon renormalization
  - 4:30-4:50 Usage of FourPhonon with ShengBTE
  - 4:50-5:00 Q&A
- One lecture (50 mins), October 2021, to high school students on the topic of "Control The Heat" to the high school students in the Millcreek Youth Center, Ogden, Utah.

# **Mentored Capstone Projects**

• The senior students mentored by Dr. Rao, Dr. Shiri, and Dr. Feng won the 2023 IEEE/EPS ASME K16 Student Heat Sink Design Challenge! Congratulations, Xander Lehnardt, Chandler Elliott, Preston Bodily, Taylor Cox, and Zachary Julien! This is a part of the capstone course.

#### **Outreach Activities**

- 11/2023 Gave three talks (each 30 mins) on Engineering Day to the high school students in Utah to help them understand the significance of heat transfer in cutting-edge applications.
- 09/2023 Gave two lectures (each 60 mins) to high school students on the topic of "Control The Heat" in Farmington Bay Youth Center, Farmington, Utah.
- 06/2023 Mentored two high school students for 8-week Summer Research Internship (SRI) in my lab.
- 06/2023 Showed high school students our lab and our research in the Hi-GEAR (Girls Engineering Abilities Realized) summer camp.
- 02/2023 Gave three lectures (each 80 mins) to high school students on the topic of "Control The Heat" in the Decker Lake Youth Center, West Valley City, Utah.
- 11/2022 Gave three talks (each 50 mins) on Engineering Day to the high school students in Utah to help them understand what research in engineering looks like. The students were well engaged.
- Gave two talks (each 50 mins) on Engineering Day to the high school students in Utah to help them understand what research in engineering looks like. The students were well engaged.
- 10/2021 Gave a lecture (50 mins) about my research to the high school students at Mill Creek Youth Center in Ogden. The activity was organized by STEM Community Alliance Program (STEMCAP), which forges novel connections through inquiry-based and interactive STEM programming to put scientists, artists and community educators inside Youth-In-Custody (YIC) facilities. https://stemcap.org/archive/past-presentations
- 10/2021 Gave a talk to undergraduate students at Brigham Young University (BYU), Provo, Utah, for the graduate recruitment of our ME department.

# PROFESSIONAL ACTIVITIES

# **Editorial Activities**

- Advisor of Materials Research Letters (Impact Factor of 8.5), Article Collection: Micro and Nanoscale Thermal Transport in Materials, 2023.
- **Associate Editor**, Frontiers in Thermal Engineering, Micro- and Nano-Scale Heat Transfer section, 2022 present
- Editorial board member, Energy and Environment Focus, American Scientific Publisher, 2021 Present
- Early-Career Editorial board member, ES Energy & Environment, a journal of Engineered Science, 2021 present

# **Conference Organizational Activities**

- **Organizer and Session Chair** of the ASME International Mechanical Engineering Congress and Exposition (IMECE) conference, New Orleans, LA, Nov. 2023.
- Session Chair of the Materials Research Society (MRS) Spring Conference, San Francisco, CA, Apr. 2023.
- Session Chair of The 47th International Conference and expo on Advanced Ceramics and Composites (ICACC2023), Daytona Beach, Florida, Jan, 2023.
- **Organizer and Session Chair** of the ASME International Mechanical Engineering Congress and Exposition (IMECE) conference, Columbus, Ohio, Nov. 2022.

- Organizer of the ASME Summer Heat Transfer Conference (SHTC) 2022.
- Committee member of the ASME HTD K-9 Nanoscale Thermal Transport since November 2021.
- **Topic Organizer** of the ASME International Mechanical Engineering Congress and Exposition (IMECE), November 2019.
- **Session Chair** of the ASME International Mechanical Engineering Congress and Exposition (IMECE), Pittsburgh, PA, November 2018.

# Reviewer and Judge Services:

- Reviewer for journal papers: ACS Applied Materials and Interfaces; Acta Materialia; Advanced Functional Materials; AIP Advances; Applied Physics Letters; Case Studies in Construction Materials; Ceramics International; Chemical Physics Letters; Computer Physics Communications; Crystals; Diamond and Related Materials; Energies; ES Energy & Environment; International Journal of Heat and Mass Transfer; International Journal of Thermophysics; International Heat Transfer Conferences; Journal of Applied Physics; Journal of Heat Transfer; Journal of Materials Chemistry A; Journal of Molecular Liquids; Materials; Materials Horizons; Materials Today Physics; Nano Energy; Nano Letters; Nanomaterials; Nanoscale; Nanoscale and Microscale; Thermophysical Engineering; Nature Communications; npj Computational Materials; Philosophical Magazine; Physica B; Physical Chemistry Chemical Physics; Physical Review Applied; Physical Review B; Physical Review Letters; Physical Review Materials; Proceedings of National Academic Science; Results in Physics; Scientific Reports; Science China; The Journal of Physical Chemistry C; The Journal of Physical Chemistry Letters.
- Reviewer for 2024 NSF Graduate Research Fellowship Program (GRFP)
- **Reviewer** for proposals of DOE and DOD.
- **Judge** for the student poster competition at the ASME InterPACK (International Technical Conference and Exhibition on Packaging and Integration of Electronic and Photonic Microsystems), San Diego, CA, Oct. 2023.
- **Judge** for the NSF student poster competition at the ASME International Mechanical Engineering Congress and Exposition (IMECE), Columbus, Ohio, Nov. 2022.
- **Judge** for the NSF student poster competition at the ASME International Mechanical Engineering Congress and Exposition (IMECE), Pittsburgh, PA, November 2018.

# INVITED TALKS & CONFERENCE PRESENTATIONS

### **Invited Talks**

- 9. Tianli Feng, "Accurate first-principles prediction of thermal and mechanical properties of ultrahigh temperature ceramics", **47th International Conference and Exposition on Advanced Ceramics and Composites** in Daytona Beach, Florida, USA, Jan. 2023.
- 8. Tianli Feng, "Pushing the Frontiers of Thermal Transport Predictions", **University of California**, **Riverside**, ECE Colloquium, Oct. 2022.
- 7. Tianli Feng, "Four-Phonon Scattering A Critical Process Ignored for Half Century", **University of Utah**, MSE seminar series, Mar. 2022.
- 6. Tianli Feng, "Progress in Four-Phonon Scattering Calculations", **Materials Quantum Characteristics and Computational Condensed Matter Physics Conference**, Chongqing, (Online) December 2021.
- 5. Tianli Feng, "Four-Phonon Scattering A Critical Process Determining Thermal and Radiative Properties", **Materials Research Society** (MRS) Fall Meeting, Boston, MA, November 2021.
- 4. Tianli Feng (together with Prof. Xiulin Ruan) "Four-phonon scattering: an ignored phonon scattering mechanism for decades", **IMECE**, Pittsburgh, November 2018.

- 3. Tianli Feng, "Theoretical phonon spectroscopy using predictive atomistic simulations", Condensed Matter & Optics Seminars, Vanderbilt University, February 2018.
- 2. Tianli Feng, "Theoretical Phonon Spectroscopy Using Predictive Atomistic Simulations", University of Minnesota Twin Cities, August 2017.
- 1. Tianli Feng, "Theoretical Phonon Spectroscopy Using Predictive Atomistic Simulations", Computational Material Online Seminar, July 2017.

### **Conference Presentations**

### Feng group members' presentations:

- Hao Zhou, Tianli Feng, "Thermal conductivity of BAs under irradiation", IMECE, New Orleans, LA, Nov. 2023
- Janak Tiwari, Tianli Feng, "First-principles prediction of thermal conductivity of Al2O3 at ultrahigh temperatures", IMECE, New Orleans, LA, Nov. 2023
- Hao Zhou, Tianli Feng, "On the flattening trend of thermal conductivity of La2Zr2O7 at ultra-high temperatures", IMECE, New Orleans, LA, Nov. 2023

### **Tianli Feng's Presentations**

- Tianli Feng, "High thermal conductivity of cubic SiC", ASME InterPACK International Technical Conference and Exhibition on Packaging and Integration of Electronic and Photonic Microsystems, San Diego, CA, Oct. 2023.
- Janak Tiwari, Xiaolong Yang, Tianli Feng, "First principles prediction of thermal conductivity at ultrahigh temperatures", Materials Research Society (MRS) Spring Meeting, San Francisco, CA, April 2023.
- Rui Xie, Janak Tiwari, Tianli Feng, "Spectral Phonon Transport Across Interfaces: The Effects of Interfacial Engineering", Materials Research Society (MRS) Spring Meeting, San Francisco, CA, April 2023.
- Rui Xie, Janak Tiwari, Tianli Feng, "Spectral Phonon Transport Across Interfaces: The Effects of Interfacial Engineering", IMECE, Columbus, Ohio, Nov. 2022
- Janak Tiwari, Tianli Feng, "First Principles Prediction of Thermal Conductivity at Ultra-High Temperatures", IMECE, Columbus, Ohio, Nov. 2022
- Janak Tiwari, Tianli Feng, "First principles prediction of thermal conductivity of ZrC and HfC at ultrahigh temperatures", Ultra-High Temperature Ceramics (UHTC): Materials for Extreme Environment Applications V, An ECI Conference Series, Snowbird, Utah, June 2022.
- Xiaolong Yang, Janak Tiwari, Tianli Feng, "First principles prediction of thermal conductivity of UO2 over a wide temperature range", Materials Research Society (MRS) Spring Meeting, Honolulu, Hawaii, May 2022.
- Tianli Feng, A. O'Hara, S. T. Pantelides, "Quantum prediction of ultra-low thermal conductivity in lithium intercalation materials", Materials Research Society (MRS) Fall Meeting, Boston, MA, November 2021.
- Tianli Feng, A. Rai, D. Hun, S. S Shrestha, "Revealing Energy Accommodation Between Gases and Polymers for High-Efficiency Thermal Insulation", ASME 2020 International Mechanical Engineering Congress & Exposition (IMECE), Virtual Conference.
- T. Feng, J. He, A. Rai, D. Hun, J. Liu, S. S Shrestha, "Discovering Size Effect of Thermal Conductivity of Amorphous Polymers", ASME 2020 International Mechanical Engineering Congress & Exposition (IMECE), Virtual Conference.
- Tianli Feng, Y. Zhong, J. Shi, X. Ruan, "Unexpected high inelastic phonon transport across solid-solid interface: Modal nonequilibrium molecular dynamics simulations and Landauer analysis", Materials Research Society (MRS) Spring Meeting, Phoenix, AZ, April 2019.

- Tianli Feng, X. Wu, X. Yang, P. Wang, L. Zhang, X. Du, X. Wang, S. T. Pantelides, "Ultra-Low and Anisotropic Thermal Conductivities of Quasi-1D ZrTe5 and HfTe5 Single Crystals", Materials Research Society (MRS) Spring Meeting, Phoenix, AZ, April 2019.
- Tianli Feng and Sokrates Pantelides, "Ultra-low and anisotropic thermal conductivity of quasi-1D single-crystalline ZrTe5", Materials Research Society (MRS) Fall Meeting, Boston, MA, November 2018.
- Tianli Feng, Xiaolong Yang, Xiulin Ruan and Sokrates Pantelides, "First-Principles Prediction of Temperature Dependent Phonon Energy Shifts of Boron Nitride", ASME 2018 International Mechanical Engineering Congress & Exposition (IMECE), Pittsburgh, PA, November 2018.
- Tianli Feng and Sokrates Pantelides, "Accurate First-Principles Prediction of Temperature-Dependent Phonon Energy Shifts", American Physical Society (APS) March Meeting, Los Angeles, CA, March 2018.
- Tianli Feng and Xiulin Ruan, "Phonon transport in defected graphene and graphene nanomesh", ASME 2016 International Mechanical Engineering Congress & Exposition (IMECE), Phoenix, AZ, November 2016.
- Tianli Feng and Xiulin Ruan, "First principles prediction of importance of four-phonon scattering in Si and BAs", ASME 2016 International Mechanical Engineering Congress & Exposition (IMECE), Phoenix, AZ, November 2016.
- Tianli Feng, Wenjun Yao, Zuyuan Wang, Jingjing Shi, Chuang Li, Bingyang Cao, and Xiulin Ruan, "Spectral phonon temperature as an effective tool to predict the ballistic and diffusive transport in nanomaterials and across interfaces", ASME 2016 International Mechanical Engineering Congress & Exposition (IMECE), Phoenix, AZ, November 2016.
- Tianli Feng, Bo Qiu, and Xiulin Ruan, "Coupling between Phonon-Phonon and Phonon-Impurity Scattering: A Critical Revisit of the Spectral Matthiessen's Rule", ASME 2015 International Mechanical Engineering Congress & Exposition (IMECE), Houston, TX, November 2015.
- Tianli Feng and Xiulin Ruan, "Quantum mechanical prediction of four-phonon scattering rates and reduced thermal conductivity of solids", ASME 2015 International Mechanical Engineering Congress & Exposition (IMECE), Houston, TX, November 2015.
- Tianli Feng, Bo Qiu, and Xiulin Ruan, "Coupling between Phonon-Phonon and Phonon-Impurity Scattering: A Critical Revisit of the Matthiessen Rule", 32nd International Thermal Conductivity Conference (ITCC) & 20th International Expansion Symposium (IES), West Lafayette, IN, April 2014.