Nanoscale Energy Transport

Emerging phenomena, methods and applications

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Preface

Nanoscale energy transport is a fast-developing research field that studies the transport processes of fundamental energy carriers, including electrons, phonons, photons, magnons, etc, in devices and material structures with characteristic sizes in the nanometer range. Fundamentally, new physical phenomena emerge at the nanoscale due to the classical and quantum confinement effects of the energy carriers, leading to the breakdown of macroscopic constitutive laws, such as Fourier's law of heat conduction and Planck's law of blackbody radiation. Practically, as the advancement of nanotechnology has enabled routine fabrication of devices and materials at the nanoscale, a fundamental understanding of energy transport in these systems is crucial for achieving better efficiency and performance. Indeed, the improved understanding of nanoscale energy transport in the past two decades has led to better thermal management for microelectronic devices, more efficient thermoelectric modules and new strategies to efficiently harvest the full spectrum of solar power, to name a few examples. Therefore, nanoscale energy transport is a field of both fundamental interest and practical relevance. In this light, this multi-contributor volume aims to cover new developments in both the scientific basis and the practical relevance of nanoscale energy transport, with a particular emphasis on the emerging effects at the nanoscale that qualitatively differ from those at the macroscopic scale.

Excellent texts and monographs on nanoscale energy transport are available, for example by Chen [1], Zhang [2], Fisher [3], Volz [4] and others, where the fundamentals and the research developments at the time of publication are clearly elaborated. However, as this is an active field of research, new effects, experimental and computational methods, and applications are emerging at a fast pace. Complementary to these existing books, the goal of this volume is to cover recent developments in the theory, methods and applications of nanoscale energy transport from the past few years, and help researchers in this field obtain an overview of the current frontiers. To this end, I have invited active researchers in nanoscale energy transport to contribute chapters on their specialty topics and offer their expert perspectives on the important advancements in the past decade as well as future directions. In the end, 17 chapters were selected for this multi-contributor volume that cover a broad range of topics. In terms of microscopic energy carriers, the transport of phonons, electrons, photons and magnons in the nanoscale are discussed in various chapters. In terms of methods, state-of-the-art computational and experimental approaches are reviewed, including a chapter on the emerging material informatics method (chapter 5). In terms of material systems, a broad range from interfaces and molecular junctions to nanostructured bulk materials is included. While I believe this volume is a comprehensive survey of the state of the art of nanoscale energy transport, by no means does this book cover all significant new developments in the field. Notable omissions include spin caloritronics, where the coupling effects of phonons and magnons are investigated, and the energy

transport in two-dimensional materials. For these topics, the interested reader is referred to excellent recent review articles such as [5] and [6].

The chapters are organized into two parts. Part I focuses on emerging theory and computational methods. Chapter 1 by Sangyeop Lee's group at the University of Pittsburgh discusses hydrodynamic phonon transport, particularly in two-dimensional materials, where normal phonon–phonon scatterings dominate Umklapp scatterings and the phonon thermal transport mimics fluid flow. Chapter 2, by Tianli Feng from Oak Ridge National Laboratory and Xiulin Ruan from Purdue University, reviews the recent development of calculating higher order phonon scattering rates, e.g. four-phonon processes, and its relevance to thermal transport in technologically important materials. Chapter 3, by Tengfei Luo's group at the University of Notre Dame, provides a detailed account of how bulk phonon scattering events affect interfacial thermal transport from first-principles and molecular dynamics simulations. Chapter 4, by Zhiting Tian's group at Cornell University, gives an introduction to the state-of-the-art atomistic Green's function (AGF) method for calculating interfacial phonon transport properties and interfacial thermal resistance. Chapter 5, by Junichiro Shiomi's group at the University of Tokyo, elaborates on using material informatics methods, in particular Bayesian optimization, for nanoscale thermal transport problems. This is an emerging front in computational materials science that has attracted intense interest recently due to the fast advancement of data science and machine learning methods. Chapter 6, by Chengyun Hua at Oak Ridge National Laboratory, reviews the current status of resolving the phonon mean free path distribution in real materials from both the computational and experimental perspectives, which is essential for engineering materials at the nanoscale to achieve desirable thermal transport properties. Chapter 7, by Keivan Esfarjani's group at the University of Virginia, provides a historic view of incorporating the lattice anharmonicity into first-principles phonon calculations at finite temperature, which is necessary to correctly describe phonon softening and phase transitions.

Part II focuses on the developments of experimental techniques and practical applications enabled by fundamental advancements. Chapter 8, by Professors Edgar Meyhofer and Pramod Reddy's group at the University of Michigan, details state-of-the-art measurement techniques to resolve thermal and thermoelectric transport across atomic and molecular junctions with extreme sensitivity. Chapter 9, by Xiaojia Wang's group at the University of Minnesota, reviews the recent applications of emerging time-resolved magneto-optical Kerr effect (TR-MOKE) spectroscopy to characterize both phonon and magnetization dynamics. Chapter 10, by Keshav Dani's group at Okinawa Institute of Science and Technology in Japan, introduces a class of powerful tools—ultrafast electron microscopy, in particular time-resolved photoemission electron microscopy (TR-PEEM)—and their applications in nanoscale energy transport. Chapter 11, by Chen Li's group at the University of California, Riverside summarizes recent results utilizing the inelastic neutron scattering (INS) technique to understand phonons and magnons in energy materials. Chapter 12, by Renkun Chen's group at the University of California, San Diego, reviews the historic development and recent applications of suspended

micro-devices to characterize the thermal transport properties of nanomaterials. Chapters 13 and 15, by Nenad Miljkovic's group at the University of Illinois, Urbana–Champaign, discuss how micro- and nanostructured surfaces can significantly enhance condensation heat transfer and help combat frosting and icing in practical energy systems. Chapter 14, by Mona Zebarjadi's group at the University of Virginia, introduces the mechanisms and current frontiers of using thermionic emission to convert thermal energy into electricity as an alternative to thermoelectric conversion. Chapter 16, by Zhifeng Ren's group at the University of Houston, addresses a critical problem at the current development stage of thermoelectric materials—how to reliably measure the thermoelectric transport properties and energy conversion efficiency of thermoelectric materials. Chapter 17, by Andrej Lenert's group at the University of Michigan, reviews the recent development of thermophotovoltaic energy conversion, including both the material and the device aspects, and particularly the opportunities offered by the recent advancement of nanophotonics.

I wish to acknowledge all the authors for their valuable input and hard work, which have made this volume possible. I also want to thank the Institute of Physics Publishing for providing me the opportunity to work on this project, in particular Michael Slaughter and John Navas who initiated this project, and Caroline Mitchell, Daniel Heatley and Robert Trevelyan for their generous help (and patience) during the editing and production process. Last, but not least, I want to thank the support for research provided by the US Department of Energy, National Science Foundation and US Army Research Office.

Bolin Liao
University of California, Santa Barbara
November 2019

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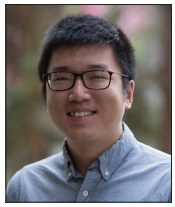
Editor biography

Bolin Liao



Bolin Liao is currently an assistant professor in the Department of Mechanical Engineering at the University of California, Santa Barbara. His main research interest is in nanoscale energy transport and its application to sustainable energy technologies. Specifically, his research aims to understand the transport and interaction processes of fundamental energy carriers, such as electrons, phonons, photons and magnons, at the smallest length and time scales, and then use this knowledge to develop more efficient clean energy devices, e.g. thermoelectric modules and photovoltaic cells. Current projects include first-principles and multiscale simulation of energy carrier transport, visualization of photophysics in space and time with scanning ultrafast electron microscopy, ultrafast optical techniques for thermal and thermoelectric characterization, and applied clean energy devices and systems.

Bolin obtained his PhD in mechanical engineering from MIT in March 2016, advised by Gang Chen. He was a Kavli Postdoctoral Fellow at the California Institute of Technology from May 2016 to June 2017, hosted by the late Ahmed Zewail, where he worked on scanning ultrafast electron microscopy.

Contributors

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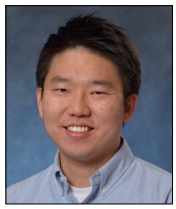
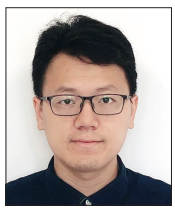
Xun Li received his BS degree in energy engineering from Zhejiang University, the People's Republic of China, in 2015. He is currently a PhD candidate in the Department of Mechanical Engineering and Materials Science at the University of Pittsburgh, PA. His research focuses on the computational study of first-principles based phonon transport in graphitic materials and interfacial phonon transport in semiconductors.

Sangyeop Lee



Sangyeop Lee is an Assistant Professor in the Department of Mechanical Engineering and Materials Science at the University of Pittsburgh, PA. He received his PhD from the Department of Mechanical Engineering at Massachusetts Institute of Technology in 2015. His current research interests are first-principles based simulation of hydrodynamic phonon transport and thermal transport in partially/fully disordered phases.

Tianli Feng



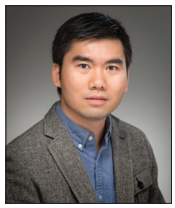
Tianli Feng is a postdoctoral fellow at Oak Ridge National Laboratory, TN. He received his BS in physics from the University of Science and Technology of China in 2011. He received his MS and PhD in mechanical engineering from Purdue University, IN in 2013 and 2017, respectively. His research interests include developing new atomistic-scale predictive simulation methods for thermal energy transport, and using these methods to guide the development of high-performance materials.

Xiulin Ruan

Xiulin Ruan is a Professor in the School of Mechanical Engineering and the Birck Nanotechnology Center at Purdue University, IN. He received his BS and MS in engineering thermophysics from Tsinghua University in 2000 and 2002, respectively. He received an MS in electrical engineering and a PhD in mechanical engineering from the University of Michigan at Ann Arbor in 2006 and 2007, respectively. His research interests include multiscale multiphysics simulations and experiments of phonon, electron, and photon transport and interactions, for various emerging applications. Ruan has been recognized with

many awards, including the NSF CAREER Award (2012), the ASME Heat Transfer Division Best Paper Award (2015) and the Air Force Summer Faculty Fellowship (2010, 2011 and 2013). He currently serves as an associate editor for the ASME *Journal of Heat Transfer*.

Tengfei Luo



Tengfei Luo is the Dorini Family Collegiate Chair and Associate Professor in the Department of Aerospace and Mechanical Engineering (AME) at the University of Notre Dame (UND), IN. Before joining UND, he was a postdoctoral associate at Massachusetts Institute of Technology from 2009 to 2011, after obtaining his PhD from Michigan State University in 2009. At UND, Luo leads an interdisciplinary group focusing on nanoscale thermal transport, electronics thermal management, novel material design and manufacturing, and water treatment.

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Eungkyu Lee is the Research Assistant Professor in the Department of Aerospace and Mechanical Engineering (AME) at the University of Notre Dame (UND), IN. He was a postdoctoral associate at the Department of AME at UND. He obtained his PhD from Seoul National University in 2015. At UND, Lee studies light–matter interaction involving nanophotonics and multiphase thermofluids and interfacial thermal transport.

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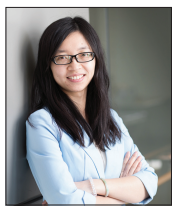
Ruiyang Li is currently pursuing a PhD degree at the University of Notre Dame, IN under the supervision of Tengfei Luo. He received his BS degree in energy and power engineering from Huazhong University of Science and Technology in 2018. His research interests include nanoscale thermal transport at semiconductor material interfaces, and the prediction of thermal properties using machine learning based techniques.

Zhiting Tian



Zhiting Tian is an Assistant Professor and a Eugene A Leinroth Sesquicentennial Faculty Fellow in the Sibley School of Mechanical and Aerospace Engineering at Cornell University, NY. Between 2014 and 2018 she was an Assistant Professor of Mechanical Engineering at Virginia Tech. Zhiting obtained her PhD in mechanical engineering from MIT in 2014. Zhiting's research focuses on the fundamental understanding of nanoscale thermal

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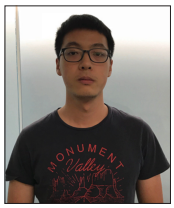
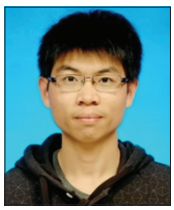
Renjiu Hu



Renjiu Hu is a PhD student in the Sibley School of Mechanical and Aerospace Engineering at Cornell University, NY. His research focuses on interfacial thermal transport and Anderson localization.

Jiang Guo



Jiang Guo is currently a PhD student in the Department of Mechanical Engineering at the University of Tokyo, working on tailoring thermal radiative properties for energy applications via optimizing metamaterials using machine learning methods.

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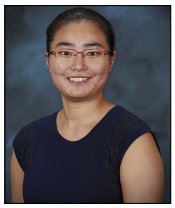
Chengyun Hua



Chengyun Hua received her BS in engineering physics from the University of Michigan in 2011, and her PhD in mechanical engineering from the California Institute of Technology in 2016. She joined the Oak Ridge National Laboratory, TN, in 2016 as a Liane B Russell Fellow and is currently working as an R&D associate. Her research focuses on gaining a comprehensive picture of how heat is transported in a solid at the scales of heat carriers, i.e. electrons and phonons (quantized vibrations in the lattice). Using both computation and experiments, she is currently working on using structures at the nanoscale as a tunable physical parameter to control and manipulate heat.

Keivan Esfarjani

Keivan Esfarjani obtained his general-engineering degree at the Ecole Centrale de Paris in France. He then pursued his studies in theoretical solid-state physics with a Master's (DEA) from the University of Paris followed by a PhD at the University of Delaware and a postdoc at Washington University in Saint Louis, MO. During his career, Esfarjani has held various positions at the Institute for Materials Research of Tohoku University, Sharif University of Technology, University of California Santa Cruz, MIT and Rutgers University. Currently he is an Associate Professor at the Departments of Mechanical Engineering, Materials Science and Physics at the University of Virginia. His research interests include the electronic structure calculation of materials from first-principles, lattice dynamics and phase change, electrical and thermal transport, and finally the storage and conversion of energy and information.

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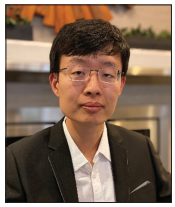

Yuan Liang received his BSc in applied physics from the University of Science and Technology of China, in Hefei, Anhui, in 2015. He was a member of the YAN Ji-Ci Elite Program in Physics, School of Gifted Young, working on the super-hydrophobicity of nano-membranes. He is currently working on his PhD in physics at the University of Virginia, Charlottesville. His current research interests include free energy computation and phase transition studies based on self-consistent phonon theory, computational schemes to extract anharmonic force constants in finite temperature—specifically stochastically designing a sampling method of lattice snapshots— and material properties analysis by applications of deep learning neural network packages.

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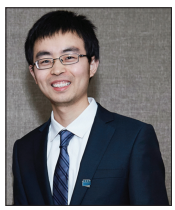


Longji Cui joined the faculty of the Mechanical Engineering and Materials Science and Engineering program of CU Boulder, CO, as an Assistant Professor in January 2020. Cui received his PhD in mechanical engineering in 2018 from the University of Michigan, Ann Arbor, under the supervision of Pramod Reddy and Edgar Meyhofer. From August 2018, he served as a Visiting Assistant Professor in the Mechanical Engineering department of CU and has been the J Evans Attwell-Welch Fellow of Rice University, and performed postdoctoral research in the Smalley-Curl Institute and Department of Physics and Astronomy (Natelson Research Group) at Rice University. Cui is a recipient of the

Robert M Caddell Memorial Award, the Richard and Eleanor Towner Prize for Outstanding PhD Research at U-M, the Chinese Government Award for Outstanding Student Abroad and the Material Research Society (MRS) Graduate Student Gold Medal.

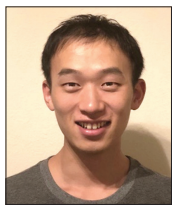
Dustin Lattery

Dustin Lattery is currently a PhD student in mechanical engineering at the University of Minnesota, Twin Cities. He received his Bachelor's and Master's degrees in mechanical engineering from the University of Minnesota, Twin Cities in 2014 and 2017, respectively. His research focuses on magnetization dynamics in thin films. During his research, Lattery has optimized the signal from time-resolved magneto-optical Kerr effect measurements of perpendicular magnetic thin films, successfully combining both experimental and numerical methods. He has applied this method to a range of technologically important magnetic materials, for extracting information about their magnetic anisotropy and Gilbert damping.

Jie Zhu

Jie Zhu is currently an Associate Professor in the School of Energy and Power Engineering at Dalian University of Technology in China. He was previously a research associate in the Department of Mechanical Engineering at the University of Minnesota, Twin Cities. He received his BS in thermal science and energy engineering in 2004 from the University of Science and Technology of China, and a PhD from the Institute of Engineering Thermophysics, Chinese Academy of Sciences in 2011. Zhu's research interests include ultrafast non-equilibrium heat transfer, thermal transport across interfaces, the thermophysical properties of novel materials and the development of related experimental methods.

Dingbin Huang



Dingbin Huang is currently a PhD student in mechanical engineering at the University of Minnesota, Twin Cities. Mr Huang received his Master's degree in mechanical engineering from Shanghai Jiao Tong University in 2018, and a Bachelor's degree from Xi'an Jiaotong University in 2015. Mr Huang's research interests are the time-resolved study of magnetization dynamics and spin-heat coupling of novel materials for spintronic and data storage applications.

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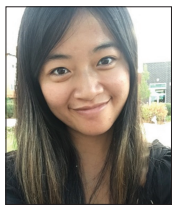
Professor Xiaojia Wang is an assistant professor in the Department of Mechanical Engineering at the University of Minnesota, Twin Cities. Prior to this, she was a postdoctoral research associate in the Department of Materials Science and Engineering at the University of Illinois at Urbana–Champaign. She received her PhD in mechanical engineering from the Georgia Institute of Technology in 2011. She received her MS in 2007 and BS in 2004 from Xi'an Jiaotong University, China, studying mechanical engineering. Her current research explores thermal and magnetic transport in functional materials and across material interfaces, using ultrafast optical techniques. These investigative efforts have a wide range of applications, including solid-state energy conversion and harvesting, data storage and spintronic devices.

Rebecca Wong

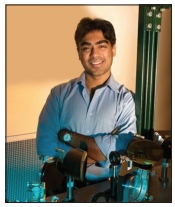


Rebecca Wong obtained her Bachelor's degree in physics and environmental science from Grinnell College. She has worked on various energy-related research projects at universities and national laboratories in the United States and abroad, and has experience in optics research at Osaka University and more recently the Okinawa Institute of Science and Technology Graduate University. Her research interests include novel semiconductor materials and devices, in particular for solar and renewable energy.

Michael Man

Michael Man received his Masters and PhD from Hong Kong University of Science and Technology. He moved to Okinawa and joined the Okinawa Institute of Science and Technology (OIST) as a postdoctoral researcher in 2012. Currently, he is a staff scientist in the Femtosecond Spectroscopy Unit at OIST. His research focuses on the development of ultrafast techniques in photoemission electron microscopy and in the study of electron dynamics and ultrafast phenomena in two-dimensional materials. He also has expertise in the field of surface science, covering phase transition, growth and magnetism in ultrathin films and two-dimensional materials.

Keshav Dani



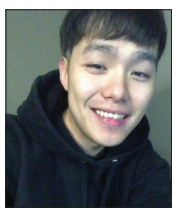
Keshav Dani is currently an Associate Professor at the Okinawa Institute of Science and Technology (OIST), Graduate University in Okinawa, Japan. He joined OIST in November 2011 as a tenure-track Assistant Professor after completing a Director's Postdoctoral Fellowship at the Center for Integrated Nanotechnologies at Los Alamos National Laboratory, NM. Keshav graduated from UC Berkeley in 2006 with a PhD in physics, where he explored the nonlinear optical response of the quantum Hall system under the supervision of Daniel Chemla at LBNL. Prior to his PhD, he obtained a BS from Caltech in mathematics with a senior thesis in quantum information theory under John Preskill and Hideo Mabuchi. His current research interests lie in the use of ultrafast techniques to study the electron dynamics of two-dimensional materials and energy materials, develop optoelectronic applications in the terahertz regimes, and pursue interdisciplinary projects with OIST colleagues in neuroscience and art conservation.

Chen Li

Chen Li joined the Department of Mechanical Engineering and Materials Science and Engineering Program at the University of California, Riverside as an assistant professor in July 2016. Prior to joining UCR, Li worked as a research scientist for EFree (Energy Frontier Research in Extreme Environment Center), a DOE Energy Frontier Research Center (EFRC) centered at the Geophysical Laboratory of the Carnegie Institute of Washington and a joint faculty at Spallation Neutron Source (SNS) at Oak Ridge National Laboratory, TN.

Li obtained a BSc in physics from the Department of Physics, Peking University, and a PhD in materials science from the Department of Applied Physics and Materials Science, California Institute of Technology. After graduation, he worked as a postdoc for the Scattering and Thermophysics Group, Materials Science and Technology Division, at Oak Ridge National Laboratory.

Qiyang Sun



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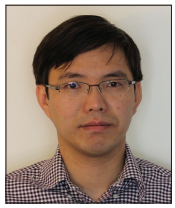
Renkun Chen



Renkun Chen is an Associate Professor in the Department of Mechanical and Aerospace Engineering at the University of California, San Diego (UCSD). He received his BS in thermophysics from Tsinghua University, Beijing in 2004, and his PhD in mechanical engineering from the University of California, Berkeley in 2008. He was a postdoctoral researcher at Berkeley prior to joining UCSD in 2009. His research group at UCSD is interested in the fundamentals and applications of thermal energy transport and conversion, including nanoscale energy transport phenomena, thermoelectric and solar–thermal energy conversion, phase-change heat transfer and thermal insulation technologies.

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Hyeongyun Cha received BS and MS degrees in mechanical engineering from the University of Illinois at Urbana–Champaign in 2014 and 2016, respectively, where he is currently pursuing a PhD degree in mechanical engineering. His current research focuses on the study of functional coating degradation using scanning probe microscopy techniques.

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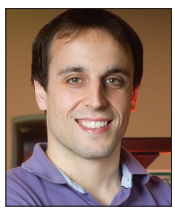
Nenad Miljkovic



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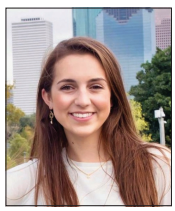
Tobias Burger is a PhD candidate in chemical engineering at the University of Michigan. He received his MSE in chemical engineering from the University of Michigan and his BS in chemical engineering from the New Mexico Institute of Mining and Technology. He is working to develop thin-film PV devices for more affordable, high-performance thermophotovoltaic generators.

Caroline Sempere



Caroline Sempere is pursuing a BSE in chemical engineering at the University of Michigan. Her research experience includes the modeling of novel self-doped semiconductors and spectral control methods for thermophotovoltaic systems.

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Andrej Lenert is an Assistant Professor in the Department of Chemical Engineering at the University of Michigan. He completed his PhD at MIT in 2014, under the supervision of Evelyn Wang. He was a postdoctoral fellow at the University of Michigan, working with the Nanoscale Transport Laboratory and the Center for Photonic and Multiscale Nanomaterials. In 2016, he was named on the Forbes 30 under 30 list in Science for his contributions to the field of thermophotovoltaic energy conversion.