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Webinar #3

Prof. Keivan Esfarjani

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University of Virginia, USA

Title: High-temperature heat transport in anharmonic systems at the Nanoscale

26th October 2021, 8.30 am – 10.00 am IST

About speaker

Prof. Keivan Esfarjani has completed General Engineering in Ecole Centrale de Paris in 1986, M.S. in University of Paris VII, 1987, and Ph.D. in University of Delaware in 1991. He has done his Post-doc in Washington University in 1992. He has worked as assistant and associate professor at Institute for Materials Research. Tohoku University in Japan, where his research focused on understanding and modeling properties of carbon-based materials and clusters, using first-principles methods. Thereafter, he has worked in Sharif University, UC Santa Cruz, MIT, and Rutgers University. Currently, he is working as associate professor in Dept. of mechanical and aerospace Engg., University of Virginia. His research has covered non-linear lattice dynamics, density functional theory methods, and modeling of electronic properties and transport of charge and heat in nanoscale systems. He has pioneered a method to compute phonon lifetimes and thermal conductivity of solids from density functional calculation of force constants. His recent work has been to include anharmonicity via the self-consistent phonon theory in the thermodynamic and transport formalism at high temperatures. His work on electron cloaking, first principles calculations of thermal conductivity and mean free paths distribution, observation of coherent phonons in superlattices, explanation of phonon softening and low thermal conductivity in PbTe and other IV-VI materials, unification of conduction and radiation in the near-field regime, and phonon hydrodynamics in graphene and 2D materials have attracted much attention from the scientific community and highlighted in news. During the past decade, he concentrated on modeling electron and phonon transport in a variety of materials, especially thermoelectrics, which are used to convert heat to electricity Along with his collegaues, he has proposed for the first time a nano-diode made of n-p doped carbon nanotubes. With Prof. Yoshiyuki Kawazoe and Prof. Kaoru Ohno, he has authored a book called "COMPUTATIONAL MATERIALS SCIENCE FROM AB INTO TO MONTE CARLO" published by Springer in 1998 (1st Edition) and then 2018 (2nd Edition). He has published more than 230 papers with 10847 citations and h-index 48.

Abstract

In this talk equilibrium and non-equilibrium formalisms to treat anharmonic systems at high temperatures will be described. In equilibrium case, lattice dynamics at high-temperatures is described by an effective harmonic theory obtained from sampling of the phase space in the canonical ensemble. This could be done self-consistently based on a model anharmonic hamiltonian and is known as the self-consistent phonon theory. In the non-equilibrium case, while previous approaches used the Keldysh formalism, we have derived a simpler classical formalism based on the equation of motion method and Langevin thermostats attached to the central anharmonic device. In contrast to previous results, we find that the leading term which needs to be included is the quartic anharmonic term. Cubic terms are then a second-order correction to the latter, which can either be added perturbatively or self-consistently. Finally, our approach leads to a current-conserving approximation, which is not always guaranteed in non-linear models.

Registration is free.
Registration link: *https://tinyurl.com/29h9w6mk*
Zoom meeting details will be shared with the registered participants.

Conveners:
Dr. V.J.Surya and Dr.S. Yuvaraj
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