

Uncovering unconventional heat flow in semiconductors through predictive first-principles calculations

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ABSTRACT

Heat conduction in solids is traditionally described by the Fourier's law, which assumes diffusive transport. However, in materials with ultrahigh thermal conductivity (κ) at micro- to nanoscale length scales, this classical picture can break down, giving rise to unconventional heat transport regimes ranging from quasiballistic and ballistic transport to hydrodynamic (second sound) transport. Understanding and predicting these regimes is important for both fundamental physics and the thermal management of next-generation electronic and quantum devices. In this context, first-principles computations have played a pivotal role in discovering novel ultrahigh- κ materials. In my Ph.D. research, I have advanced this state-of-the-art first-principles approach to predict the materials and experimental conditions under which such unconventional heat flow regimes can be realized.

I am particularly interested in semiconductors, where heat is predominantly carried by the collective lattice vibrations called phonons. The transport of these heat carriers is governed by the Boltzmann transport equation (BTE), which is a fundamental microscopic equation for heat flow in these materials. In my research, I have established a direct correspondence between this microscopic description of heat carriers and the macroscopic equations for temperature dynamics, that are often used to describe unconventional, non-Fourier heat flow regimes. This one-to-one correspondence enabled us to identify the materials and the experimental conditions necessary to observe these non-Fourier heat flow regimes in an experiment. Further, I have developed a computationally-efficient low-rank solution of BTE, that remain accurate in regimes where the macroscopic equations break down, thus enabling a seamless exploration of Fourier and non-Fourier heat flows within the same first-principles computational framework.

Our results identify single-layer van der Waals materials are promising candidates for observing exotic transport regimes, such as hydrodynamic second sound, in which heat can propagate like a wave at speeds comparable to that of sound. This framework provides a predictive pathway for discovering materials that host such phenomena, extending beyond the limited set of experimental observations in the literature to date.

ABOUT THE SPEAKER

Nikhil Malviya is a PhD scholar in the Department of Mechanical Engineering at the Indian Institute of Science (IISc), Bangalore, working with Dr. Navaneetha Krishnan Ravichandran. He completed his B.Tech. in Mechanical Engineering from Motilal Nehru National Institute of Technology (MNNIT), Allahabad, in 2020 and thereafter joined IISc in October 2020. His research focuses on heat conduction in ultrahigh thermal conductivity materials at micro- to nano-length scales, where it challenges conventional laws.

