ME Seminar

Thermal Transport in Semiconductors and Metals from First-Principles

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ABSTRACT

The understanding of thermal transport physics is crucial for applications such as thermoelectric energy conversion, heat dissipation, and memory storage devices. In this talk, I will discuss our attempts to understand and predict the thermal transport physics in technologically relevant materials by using first-principles based density functional theory calculations, the Boltzmann transport equation, and more recently using machine learning techniques. We study the phonon thermal transport properties in (i) Conventional simple and compound semiconductors such as silicon and germanium, (ii) Semiconductor nanostructures (silicon nano-porous films) (iii) Two-dimensional semiconductor (phosphorene, graphene), and (iv) Metals (aluminum and gold). Our predicted values of thermal conductivities show excellent agreement with the experimentally measured values (wherever available) without the use of any fitting parameters.

ABOUT THE SPEAKER

Dr. Ankit Jain obtained his Bachelor degree in Mechanical Engineering from Indian Institute of Technology, Kanpur, India in 2011. After finishing his bachelors, he joined Ph.D. program in the mechanical engineering department at Carnegie Mellon University under the supervision of Prof. Alan McGaughey. After finishing his PhD in 2015, Dr. Jain worked with Prof. Edward Sargent from University of Toronto and Prof Jens Norskov from Stanford University as a postdoctoral fellow. In April 2019, Dr. Jain joined the mechanical engineering department at IIT Bombay where he is leading Materials Simulation Research Group on methods development for thermal transport, high-throughput materials discovery, and catalytic applications.

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