Abstract

Lattice thermal conductivity of solids from calculations

(Session 2, Oral)

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In this talk, we will discuss functional theory and recent advancements in lattice thermal transport in complex crystals and amorphous solids. Building on these advanced theories, we propose a practical method to discover simple crystalline solids with ultralow thermal conductivities at room temperature, and verify this protocal by finding simple crystal $AgTlI_2$ with ultralow thermal conductivity of 0.25 W/mK at room temperature. Additionally, below room temperature, we will explore the unusual glassy thermal conductivity in crystalline $Cs_3Bi_2I_6Cl_3$, providing a robust framework to understand its abnormal thermal transport mechanisms, considering both nuclear quantum effects and atomic disorder. This talk aims to offer a clear theoretical and experimental perspective on lattice thermal transport and its anomalies in solids.