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Theoretical Insight into Strongly Suppressed Thermal Conduction in Fully Dense Crystalline Solids

The thermal properties of materials are important for the development of various modern technologies. In particular, thermoelectric energy conversion and thermal barrier require materials with ultra-low thermal conductivity. Lattice vibration dominates heat transport in insulating solids; recent theoretical studies suggested that both propagation and diffuson-like behaviors of phonons can play a critical role when the phonon mean free path is close to the atomic distance. In this presentation, I will discuss abnormal thermal transport behaviors in complex argyrodite compounds and our theoretical insight into the phenomena. Based on the more in-depth understanding, we propose alternative principles to explore fully dense crystalline solids with ultra-low thermal conductivities. We performed our research based on the thermal transport unified theory, first-principles calculations of anharmonic lattice dynamics, and machine-learned interatomic potentials. This presentation will focus on discussing nonconventional phonon transport mechanisms in technologically important solids.

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