

Phonon engineering of chalcopyrite compound by unusual phase stabilization

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In the past century, the interdependence between electrical and thermal transport properties in inorganic solid compound has been studied in full swing. Thermoelectric (TE) technology has come out from high electrical energy transport with simultaneously softened phonon movement. CuFeS₂ has been highlighted for economical and toxic-free TE materials with decent electrical transport properties. Nevertheless, because of the diamond-like structure, the thermal energy is easily conducted inside the CuFeS₂ chalcopyrite and the energy conversion efficiency has not been improved.

Here we present a phonon engineering strategy for reducing lattice thermal conductivity of CuFeS₂-based materials by stabilizing high temperature phase. With locally stabilization of the high temperature phase, an atomic disorder between Cu and Fe site enhanced. It can weaken the heat transfer inside the chalcopyrite matrix, which results in ~60% decrease in lattice thermal conductivity of high temperature phase stabilized CuFeS₂ compared to that of pristine one.