Abstract Submitted
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First-principles study of anharmonic lattice dynamics and thermal conductivity of AgSbTe2 YI ZHANG, Department of Physics and Astronomy and High Pressure Science and Engineering Center, University of Nevada, Las Vegas, PAUL KENT, Computer Science and Mathematics Division, Oak Ridge National Laboratory, JIHUI YANG, Department of Materials Science and Engineering, University of Washington, CHANGFENG CHEN, Department of Physics and Astronomy and High Pressure Science and Engineering Center, University of Nevada, Las Vegas — We report on first-principles calculations of anharmonic lattice dynamics and thermal conductivity of AgSbTe2. We study the temperature dependence of phonon scattering and, in particular, examine the mechanism responsible for the low thermal conductivity of AgSbTe2, which holds the key to its potential thermoelectric applications. We perform systematic calculations and analysis to discuss the role of intrinsic anharmonic phonon-phonon scattering and strong phonon-nanodomain scattering in determining the phonon transport process in AgSbTe2.

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