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Thermodynamic Properties of Pb and Ag-Sb Based Chalcogenides: A First-Principles Study[1] YI ZHANG, University of Nevada, Las Vegas, XUEZHI KE, University of Nevada Las Vegas; East China Normal University, CHANGFENG CHEN, University of Nevada, Las Vegas, JIHUI YANG, General Motors, PAUL R. C. KENT, Oak Ridge National Lab — The Pb and Ag-Sb based chalcogenide compounds have received considerable interest for their potential applications in thermoelectric devices. Their low thermal conductivity plays a key role in producing the high figure of merit (ZT) that is critical for applications. We performed a series of first- principles calculations on several Pb and Ag-Sb based chalcogenide compounds to understand their lattice dynamics. The direct force method and density functional theory calculations were used to obtain the phonon dispersion and density of states. The phonon softening processes with the volume change were carefully evaluated. Moreover, we employed the quasiharmonic approximation to calculate the thermodynamic functions. The calculated results are in good agreement with available experimental data and provide insights for understanding the physical properties.

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