Abstract Submitted
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First-Principles Studies on Lattice Dynamical Properties of Zn_4Sb_3 Compounds[1] YI ZHANG, CHANGFENG CHEN, Physics Department and HiPSEC, University of Nevada, Las Vegas, JIHUI YANG, Electrochemical Energy Research Lab, GM R&D Center — The origin of extremely low lattice thermal conductivity in Zn_4Sb_3 compound has attracted great interests but remains not fully understood due to its complex crystal structure. We have performed extensive first-principles calculations on the lattice vibration modes and thermodynamics of Zn_4Sb_3 based on its experimental crystal structure. The low frequency modes and structural inhomogeneity that could be responsible for the low thermal conductivity have been discussed.

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