

Abstract Submitted  
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**First-Principles Studies on Lattice Dynamical Properties of  $\text{Zn}_4\text{Sb}_3$  Compounds**<sup>1</sup> 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  $\text{Zn}_4\text{Sb}_3$  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  $\text{Zn}_4\text{Sb}_3$  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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