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First-principles and experimental insights into the structural stability and thermoelectric properties of SnSb

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This study reports on the structural, electronic, dynamical, mechanical, thermodynamic, and thermoelectric properties of SnSb as a possible material for harvesting waste-heat energy. Complementary ab-initio density functional theory (DFT) and experimental studies have been carried-out to evaluate the thermoelectric performance of SnSb in the NaCl-type structure via the figure of merit, ZT. The computed ZT of 8.0 × 10⁻⁴ is an order of magnitude higher than the measured one, 5.03 × 10⁻⁵ at 300 K. The latter is limited by the measured total thermal conductivity of 76.84 Wm⁻¹K⁻¹ and the low power factor of 12.90 × 10⁻⁶ Wm⁻¹K⁻². Additionally, the elastic constants C_{11}, C_{12}, and C_{44} were computed but show disparity between the PBE and PBEsol approaches leading to deviations in the obtained Debye temperature $_D$ values. Furthermore, the computed $_D$ is overestimated when compared to the measured one of 162.83 K. The measured specific heat capacity, C_P, matches the computed one at low temperatures, while for $T >$ $_D$, there was a clear deviation as the measured one does not reach a constant of 3NR as expected near 300 K. Other properties such as the electronic, dynamical, mechanical and thermodynamic properties were determined computationally. Also, the effect of an applied field was investigated on the measured resistivity ρ and C_P, respectively.

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