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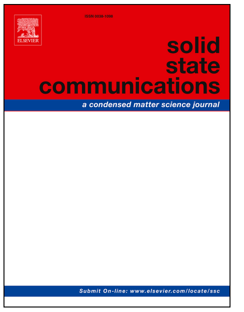

Thermoelectric properties of thin film topological insulators: A first-principles study

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Thermoelectric properties of thin film topological insulators: a first-principles study

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Abstract

The electronic and thermoelectric properties of Bi_2Te_3, Bi_2Se_3, and Sb_2Te_3 topological insulator thin films with thickness of 4~10 quintuple layers are analyzed using density functional theory and two-channel model combined with the Boltzmann transport equations. Our calculations show that the maximum figure of merit and the Seebeck coefficient are asymmetric for *n*- and *p*-type carriers, and the thickness dependence of the Seebeck coefficient exhibits different behavior upon variation in film thickness for these materials. We find that the band offset between the surface states and bulk band edges is responsible for the asymmetry and thickness dependence in *n*- and *p*- type carriers. The two-band model shows that the topological surface states serve as electronic leakage channels through conductivity modulation, degrading the thermoelectric property. We suggest that tuning the Dirac point by modifying surface chemistry to the band edges helps retain the enhancement of thermoelectric property from quantum confinement in thin film topological insulators.

Keywords

A. Three dimensional topological insulator; C. Thin films; D. Thermoelectric properties