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A first-principles study of thickness dependent thermoelectric power in topological insulating thin-films: Bi_2Te_3, Bi_2Se_3, and Sb_2Te_3
MYUNG-SOO LIM, Division of Advanced Materials Science, Pohang University of Science and Technology, SEUNG-HOON JHI, Department of Physics, Pohang University of Science and Technology — Three-dimensional topological insulator Bi_2Te_3, Bi_2Se_3 and Sb_2Te_3 are good thermoelectric materials. We study the semi-classical thermoelectric properties of this topological insulating thin films with the 4-10 quintuple-layer thickness using first-principles calculations and the two-channel model combined with the Boltzmann transport equations. We observe the thickness and material dependent Seebeck coefficients of n- and p-type doped films which is associated the bulk and surface gap, surface to bulk ratio and relative position of surface states with respect to bulk states.

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