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Maximizing the thermoelectric performance of topological insulator Bi_2Te_3 films in the few-quintuple layer regime HUIJUN LIU, JINGHUA LIANG, LONG CHENG, JIE ZHANG, Wuhan University, ZHENYU ZHANG, University of Science and Technology of China — Using first-principles calculations and Boltzmann theory, we explore the feasibility to maximize the thermoelectric figure of merit (ZT) of topological insulator Bi_2Te_3 films in the few-quintuple layer regime. We discover that the delicate competitions between the surface and bulk contributions, coupled with the overall quantum size effects, lead to a novel and generic non-monotonous dependence of ZT on the film thickness. In particular, when the system crosses into the topologically non-trivial regime upon increasing the film thickness, the much longer surface relaxation time associated with the robust nature of the topological surface states results in a maximal ZT value, which can be further optimized to ˜2.0 under physically realistic conditions. We also reveal the appealing potential of bridging the long-standing ZT asymmetry of p- and n-type Bi_2Te_3 systems. These findings help to establish intricate connections between the thermoelectric materials and topological insulators.

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