Abstract Submitted
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Enhancing the thermoelectric performance and bridging the p- and n-type carrier asymmetry of Bi_2Te_3 thin films *via* topological surface states[1] HUIJUN LIU, Wuhan University, ZHENYU ZHANG, University of Science and Technology of China — It has been recognized that some of the best thermoelectric materials are also topological insulators (TIs), yet whether these two classes of materials are inherently connected remains mysterious and conceptually perplexing. Here we combine first-principles calculations and Boltzmann theory to study the thermoelectric properties of Bi_2Te_3 thin films in the few quintuple layer regime, and demonstrate how the ZT values of such strong three-dimensional TIs can be tuned by both the film thickness and relaxation time of the topological surface states relative to the bulk states. We first show that when the surface and bulk states have comparable relaxation times, such films could actually have higher ZT values in the non-TI regime than those in the TI regime. Nevertheless, the very existence and robustness of the topological surface states in the TI regime offers unique new design strategies to not only significantly enhance their ZT values, but also potentially bridge the long-standing challenge of p- and n-type carrier asymmetry faced by the broad thermoelectric research and industrial communities.

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