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A comparative study of the tunable spin-orbit coupling in graphene proximity coupled to topological insulators ZHUONAN LIN, Wuhan University, WEI QIN, JIANG ZENG, ICQD, HFNL, University of Science and Technology of China, WEI CHEN, ICQD, HFNL, University of Science and Technology of China and Harvard University, PING CUI, ICQD, HFNL, University of Science and Technology of China, JUN-HYUNG CHO, Hanyang University, ZHENYU ZHANG, ICQD, HFNL, University of Science and Technology of China —
We present a comparative study of the electronic properties of the heterostructures consisting of a graphene sheet proximity coupled to the surfaces of three-dimensional topological insulators (TIs). Using density functional theory method, we first calculate the band structures of a single-layer graphene on the Bi_2Te_3 thin film. Counterintuitively, the spin-orbit coupling (SOC) can be barely induced in the graphene even though the intrinsic SOC strength of Bi_2Te_3 is stronger than that of Sb_2Te_3, which can readily introduce a giant SOC interaction into the graphene through proximity effect. In order to understand this exotic phenomenon, we next investigate the differences of the work functions and the charge transfers between the graphene and the TI substrates. It is found that the proximity-induced SOC in the graphene sheet can be enhanced by reducing the work function difference. These findings provide a simple work-function criterion for searching realistic materials that can be utilized as substrates to induce a large SOC gap in the graphene. Our criterion extends the posibities of experimental realization of quantum spin Hall state in graphene.

Zhuonan Lin
Wuhan Univ

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