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Ab initio study of epitaxial graphene on top of Sb_2Te_3 topological insulator KYUNG-HWAN JIN, Department of Physics, POSTECH, SEUNG-HOON JHI, Department of Physics and Division of Advanced Materials Science, POSTECH — Understanding topological phase as observed in Dirac materials such as graphene and topological insulator (TI) has been a central issue in the field of condensed matter physics. Graphene and TI exhibit unique 2D electronic structures that attract great attention for potential application to spintronic devices. Heterostructures of graphene and TI provide interesting platforms to explore exotic electronic and transport properties of Dirac materials. Electronic structures of graphene in contact with TI were investigated using first-principles methods and tight-binding models. The Dirac cones of graphene on top of TI surface show several interesting features including band-gap opening and band splitting. By fitting first-principles calculations to tight-binding models, we analyzed the origin of the changes in the Dirac cones. We found that both intrinsic and extrinsic spin-orbit couplings are enhanced significantly due to proximity to topological insulator Sb_2Te_3 and that graphene turns into quantum spin-Hall phase. Our results suggest that graphene is also useful as a probe of TI surface states.

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