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Strong Quantum Spin Hall Effect and Topological Phase Transition in Two-Dimensional Materials with Dirac Cones¹ YONGZHENG LUO, Department of Physics, National University of Singapore, LEI SHEN, Engineering Science Programme, National University of Singapore, YUAN PING FENG², Department of Physics, National University of Singapore — Spin-orbit coupling (SOC) can open a band gap in the 2D Dirac semi-metals for the application of the quantum spin hall effect (QSH), i.e., the two-dimensional (2D) topological insulators (TIs). The edge current of 2D TIs is topologically protected from backscattering, and thus hold great potential for applications in spintronics and quantum information. To find strong QSH states, the way of combining the effects of SOC and fundamental symmetries has drawn much more attention. Simultaneously, inspired by the development of graphene, seeking new 2D materials with Dirac cones as hosts of possible 2D TIs becomes more fashionable. Via the first-principles calculations with maximally localized Wannier functions, here, we propose a general way to produce 2D TIs with strong QSH states and demonstrate some non-trivial 2D quantum spin hall insulators by calculating the Z2 invariants and Berry curvature. Furthermore, a topological quantum phase transition between a non-trivial QSH phase and a trivial insulating/metallic phase can be realized by strain, and also, the SOC gap can be enhanced by strain. Thus our theoretical analysis can help searching large band gap 2D TIs.

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