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Edge-states engineering of bismuth bilayer nanoribbons using first principles calculation

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— Study of topological insulator (TI) is recently showing remarkable progress in both theory and experiment, particularly in finding three dimensional materials. Two dimensional TI (quantum spin Hall) materials, on the other hand, have comparatively fewer examples. As such, theoretical predictions of single Bi (111) bilayers to be TI draw great attention from experiment. We investigate the edge states of quantum spin-Hall phase Bi (111) bilayer nano-ribbons (BNRs) using first-principles calculations. In contrast to the case of unsaturated atomic edges, we observe very well-defined helical edge states with linear energy dispersion when the edge atoms are passivated by chemicals such as H, NO2 or -OH. Our calculations show that the Fermi velocity and spin texture of the edge states in the BNRs is very sensitive to the kind of chemicals. We demonstrate that BNRs can be used as spin-current valves to rectify the spin-polarized electric currents via the edge states by selective passivation. Further, we examine the electronic transport properties of BNR with impurities in particular configurations. Our results provide a practical way of utilizing two-dimensional topological insulator Bi bilayer for spintronic devices.

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