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Possible Gating on the Surface of a Weak Topological Insulator: $Bi_{14}Rh_3I_9$[1] MADHAV PRASAD GHIMIRE, MANUEL RICHTER, Leibniz Institute for Solid State and Materials Research, IFW Dresden, P.O. Box 270116, D-01171 Dresden, Germany — Recently synthesized $Bi_{14}Rh_3I_9$ was predicted to be a weak topological insulator. Scanning tunneling microscopy confirms this with a signatures of one-dimensional conducting states in the band gap at step edges of $[(Bi_4Rh)_3I]^{2+}$ (2DTI) surface layers. However, the surface-layer gap is found 0.25 eV below the Fermi level (E_F). Transport experiments are expected to be biased by intrinsic n-doping at the surface. Using density functional theory slab calculations we resolve this issue to shift E_F into the surface layer gap without losing its topological properties. We perform chemical modification on the surface of $Bi_{14}Rh_3I_9$: sparse layer of Iodine atoms is added onto the 2DTI surface. Investigation shows that deposition of one I atom per surface unit cell onto 2DTI surface opens a surface gap of 0.1 eV at E_F, if simultaneously one I atom is removed from the dorsal spacer layer. The same effect with reduced gap size (0.08 eV) is observed for adding/removing I atoms in two fold higher concentration. Comparing our results with the experiment [ACS Nano, 2016] we predict that Fermi level can be shifted to the surface gap by deposition of I atoms onto the 2DTI surface in an appropriate range of concentration.

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