Simultaneous Magnetic and Charge Doping of Topological Insulators with Carbon

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To enable many applications of topological insulators, it is necessary to open a surface energy gap and keep the Fermi energy inside the bulk gap. A two-step doping process, magnetic followed by charge or vice versa, is required to produce insulating massive surface states in topological insulators. Using first-principles calculations based on density funtional theory, we demonstrate here simultaneous magnetic and hole doping achieved with a single dopant, carbon, in Bi_2Se_3. Carbon substitution for Se (C_{Se}) results in an opening of a sizable surface Dirac gap (up to 85 meV), while the Fermi level (E_F) remains inside the bulk gap and close to the Dirac point at moderate doping concentrations. This *one-step* approach is possible because carbon doping simultaneously introduces localized spin moments and holes. The strong localization of 2*p* states of C_{Se} favors spontaneous spin polarization via a *p-p* interaction and formation of ordered magnetic moments mediated by the surface states. This dual function of carbon doping suggests a simple and effective way to realize insulating massive topological surface states.

Keywords: topological insulator, first-principles calculation, Bi_2Si_3, carbon-doping