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**Magnetic ordering and quantum anomalous Hall phase of Cr-doped topological insulators: First principles studies**[1] JEONGWOO KIM, Department of Physics and Astronomy, University of California, Irvine, SEUNG-HOON JHI, Department of Physics, Pohang University of Science and Technology, RUQIAN WU, Department of Physics and Astronomy, University of California, Irvine — Realization of transverse electric currents without external magnetic fields, so called the quantum anomalous Hall effect (QAHE), is achieved in Cr-doped topological insulating (Bi,Sb)2Te3 compounds. However, detailed mechanism of QAHE and magnetic ordering in topological insulators (TIs) is still unclear with several models in controversy. We study the origin of QAHE in magnetic impurity-doped TIs using first-principles calculations. We investigate a possibility of the quantum anomalous Hall phase in conventional three-dimensional topological insulators, such as Bi2Se3, Bi2Te3, and Sb2Te3. We find that Sb2Te3 is the most suitable compound for realizing QAHE, because it maintains insulating phase and relatively strong ferromagnetic ordering in a wide range of Cr doping while Bi2Se3 and Bi2Te3 become metallic even by a small amount of Cr doping. Contrary to previous predictions, the kinetic exchange is responsible for the magnetic phase of Cr-doped TIs and it induces spin-polarized valence and conduction bands in Sb2Te3. We also discuss the role of Bi doping in topological surfaces states of Cr-doped Sb2Te3, which leads to QAHE in (Bi,Sb)2Te3.

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