The role of native defects and magnetic dopants in topological insulators Bi_2Te_3 and Bi_2Se_3

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Magnetic doping is a way to add novel functionality to topological insulators [1], as well as a test of stability of topological properties. We calculate on ab initio level electronic structure of Bi2Te3 and Bi2Se3 doped by Mn at different possible positions in the lattice and also in the presence of native antisites. This provides for the first time a comprehensive map of possible behavior affecting strongly the bulk resistivity, carrier concentration and magnetism [2]. Density of states calculations reveal in which case the Fermi level lies at low conducting impurity Mn peak and which effects shift it. This allows us to tune the bulk resistivity, and also help to uncover the location of Mn atoms. Concentration dependence of resistivity exhibits significant difference between substitutional or interstitial Mn position, the resistivity for pure substitutional doping is significantly higher. Calculations indicate that at least two of the considered defects have to be present simultaneously in order to explain the observations, and the role of interstitials may be more important than expected. Exchange interactions between the Mn magnetic moments in bulk Mn-doped Bi2Se3 and Bi2Te3 have been calculated using ab initio methods. From these ferromagnetic Curie temperature and other magnetic magnetic properties are systematically studied by means of atomistic Monte Carlo simulations. Curie temperatures are shown to be significantly dependent on the concentration of Mn atoms in substitutional and interstitial positions. Theoretical results were compared to recent experimental studies [2].

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[2] K. Carva, J. Kudrnovsky, F. Maca, V. Drchal, I. Turek, P. Balaz, V. Tkac, V. Holy, V. Sechovsky, J. Honolka, *Phys. Rev. B* **93**, 214409 (2016).