

Electronic properties of chromium doped $\text{Bi}_2(\text{Se},\text{Te})_3$ topological insulators

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Three-dimensional topological insulators $(\text{Bi},\text{Sn})_2(\text{Se},\text{Te})_3$ have drawn a wide interest, because of their unusual physical properties, like symmetry protected surface states, and strong potential for applications in next-generation electronic, spintronic and quantum computation devices. Incorporation of magnetic impurities can lead to the merger between the symmetry protected surface states and the appearance of ferromagnetic order and thus provide a physical realization of the novel topological magneto-electric effect.

The aim of the presented work is to show the properties of Cr dopants in $\text{Bi}_2(\text{Se},\text{Te})_3$ and to explain their influence on the bulk and, most of all, on the surface states of host insulators. The calculations are performed in the framework of the density functional theory within relativistic variant of the local density approximation of exchange-correlation potential. Our results for bulk Bi_2Se_3 doped by Mn, Fe, Co and Ni have been presented in [1]. Here, the electronic structure of $\text{Bi}_2(\text{Se},\text{Te})_3:\text{Cr}$ is analyzed and shows that Cr occurs mainly in 3+ charge state, while the occupied Cr levels reside just below the valence band of Bi_2Se_3 .

References:

[1] A. Ptok, K. J. Karcia and A. Ciechan, J. Phys.: Condens. Matter **33**, 065501 (2021).

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