Persistence of symmetry-protected Dirac points at the surface of the topological crystalline insulator SnTe upon doping

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We investigate the effect of a non-magnetic donor impurity located at the surface of a topological crystalline insulator, SnTe [1]. Specifically, the changes on the surface states due to a Sb impurity atom are analyzed by means of first-principles simulations of pristine and impurity-doped SnTe. While semi-infinite and slab geometries are considered within the ab-initio approach, minimal and Green's function continuum models are also proposed with the same goal. We find that the Dirac cones are shifted down in energy upon doping; this shift strongly depends on the position of the impurity with respect to the surface. Moreover, the width of the impurity band shows an even-odd behavior by varying the impurity position. Comparing slab and semi-infinite geometries, we demonstrate that in the doped semi-infinite system the surface states remain gapless and their spin textures are unaltered. Besides its fundamental interest, tuning the Dirac cones of topological insulators can be of interest for transport and spintronic applications [2].

References

[1] O. Arroyo-Gascón, Y. Baba, J. I. Cerdá, O. de Abril, R. Martinez-Casado, F. Domínguez-Adame and L. Chico, Nanoscale, 14 (2022) 7151-7162
[2] J. Liu, T. Hsieh, P. Wei *et al.* Nature Materials 13 (2014) 178–183

Figures

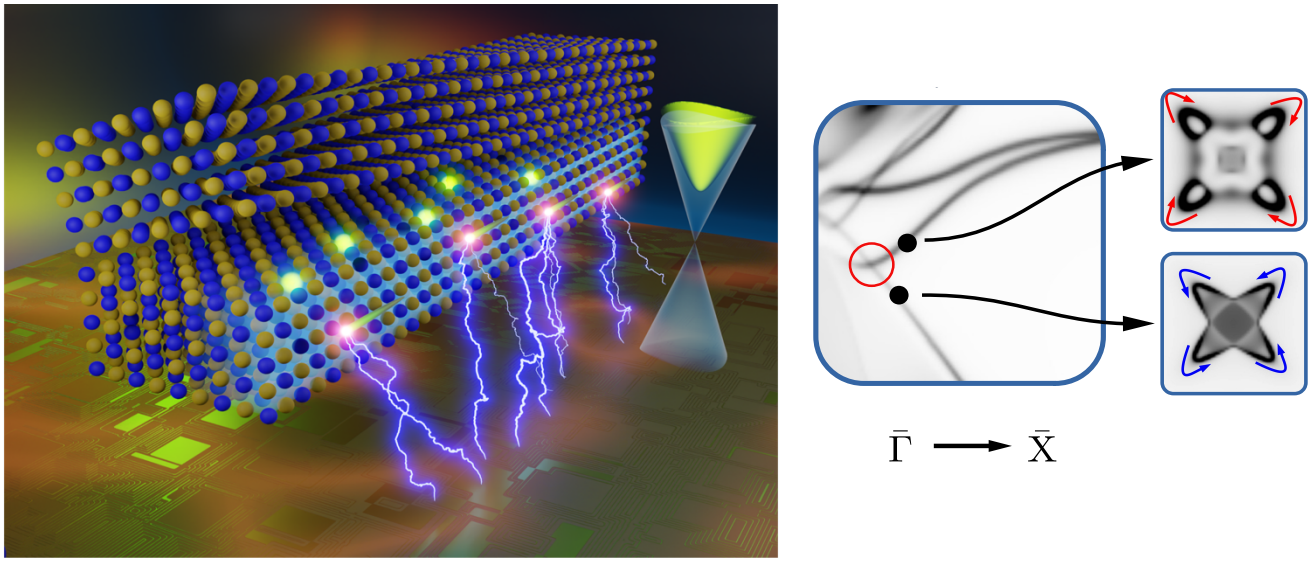

Figure 1: Left panel: Recreation of a SnTe slab. The Sb impurities and their contribution to the Dirac cone are highlighted in yellow. Central panel: projected density of states (PDOS(***k***,E)) maps of Sb-doped SnTe, with the Dirac cone circled in red. Right panel: PDOS(k_x,k_y,E) maps and spin textures above and below the Dirac point.