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

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We study the effect of a non-magnetic donor impurity located at the surface of the SnTe topological crystalline insulator [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. Both semi-infinite and slab geometries are considered within the ab-initio approach, and 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 position of the impurity. We compare slab and semi-infinite geometries, demonstrating 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. Martínez, F. Domínguez-Adame and L. Chico, arXiv:2108.06619 (2021).
[2] J. Liu, T. Hsieh, P. Wei *et al.* Nature Materials 13 (2014) 178–183.

## Figures

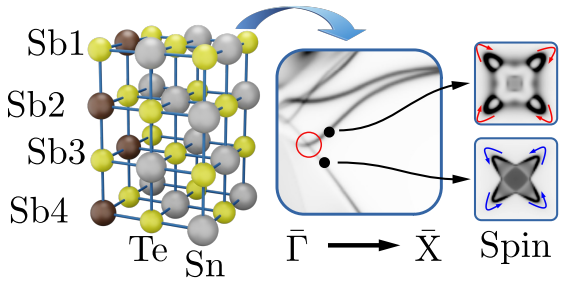


**Figure 1:** Left panel: SnTe slab unit cell. Sb impurities are highlighted in brown. Central panel: projected density of states (PDOS(***k***,E)) maps of Sb-doped SnTe. Right panel: PDOS($k_x$,$k_y$,$E$) maps and spin textures below and above the Dirac point.

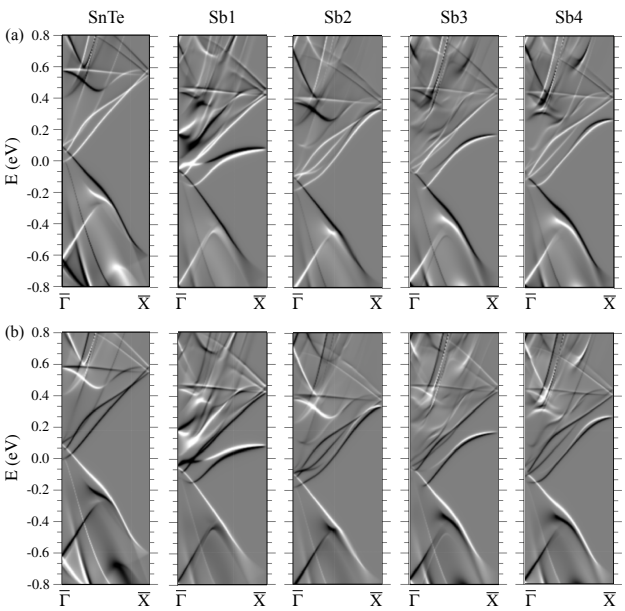


**Figure 2:** Magnetization maps (a) $M_x$(***k***,$E$) and (b) $M_y$(***k***,$E$) for the semi-infinite pristine and Sb-doped SnTe. White and black shades represent positive and negative $M_i$(***k***,$E$), respectively.