Topological *p–n* junctions based on stacking defects

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Topological insulators are natural candidates for developing new spintronic devices, where the correlation between the spin and momentum can be exploited for low dissipative spin transport protected against non-magnetic impurity scattering. Here, we propose a novel topological *p*−*n* junction (TPNJ) based on stacking defects in undoped Bi_2Se_3 thin films. We show that a realistic TPNJ can be built by matching two (0001) Bi_2Se_3 slabs with opposite arrangements of planar twin boundaries. Figure 1(a) shows a schematic representation of the proposed TPNJ. It consists of two semi-infinite two-dimensional (2D) films with buried twin boundaries (TBs) -not visible at the surface- in which the TB orientation is opposite on both slabs. We had recently shown, via density functional theory calculations, that self-doping of the surface Dirac cones of three-dimensional Bi dichalcogenides topological insulators can be achieved by inclusion of planar stacking defects -in the form of twin boundaries- inside the bulk crystal [1]. Total energy calculations reveal that the atomic structure of the proposed TPNJ is thermodynamically stable; the interface between the two different twin domains relaxes yielding a realistic geometry with dislocation defects in the hexagonal lattice of several quintuple layers of the slabs, and a smooth geometrical transition that retains the nearest-neighbors fcc-type topology throughout the defected layers -see Figure 1(b)-. In the 5QL thick junction shown in Figure 1(a) the bulk stacking sequence in odd QLs is preserved, while even QLs present a stacking mismatch between the left and right -as the one shown in Figure 1(b)- and therefore experience a large reconstruction at the interface.

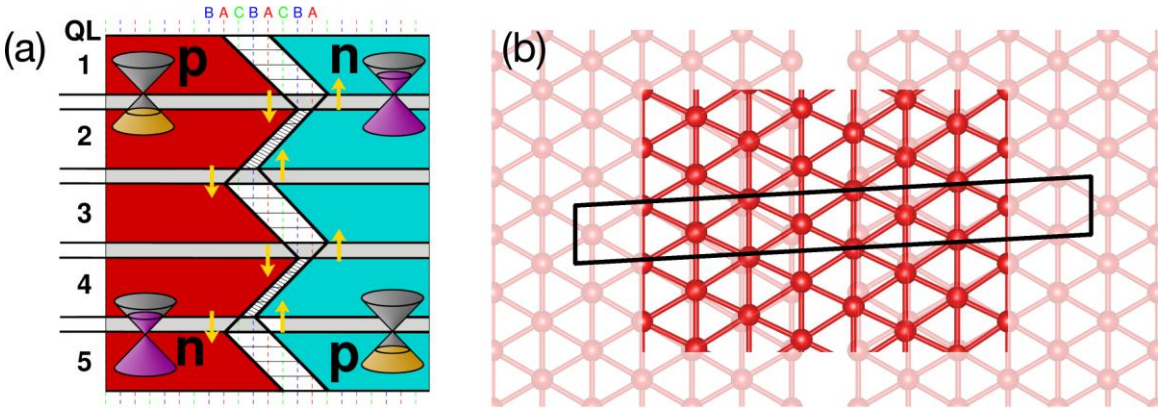

Figure 1: (a) Schematic view of the TPNJ. (b) Top view of the surfacemost Se layer before (semi-transparent) and after the atomic relaxation (solid).

The electronic, transport and magnetic properties of the TPNJ device have been calculated at the *ab initio* level. Our results confirm that indeed, a *p*−*n* junction is formed with a built-in potential as large as 350 meV and hence around the Fermi level the electronic transmission is determined by the topological surface states. They also prove the rectifying behavior of the device. Figure 2 presents the calculated total transmission probabilities, $T(k_y, E)$, around the Fermi level for the TPNJ (middle panel), together with

those corresponding to the left and right bulk-like source and drain subsystems in the absence of the interface (left and right panels, respectively). The system shows a quasi-ballistic transmittance in the *n*-*n* region and points to off-normal transmission probabilities in the *p*-*n* region larger than those anticipated with more simplified approaches. The $T(k_y, E)$ map shows a broad triangular feature centered at Γ whose intensity reduces with increasing $|k_y|$ although the transmission remains significant away from k_y=0. This indicates that off-normal incident electrons are also allowed to transmit. The calculations further reveal the evolution of the spin textures across the interface. We find that the magnetization of the carriers in the *p*–*n* region is not conserved and spin-flip occurs at the interface as long as the magnetization of the incoming electrons is not too large. Such a spin rotation process must be driven by the strong spin-orbit coupling present in the system, with spin torques arising from changes/rotations of the interface angular momenta of the atoms.

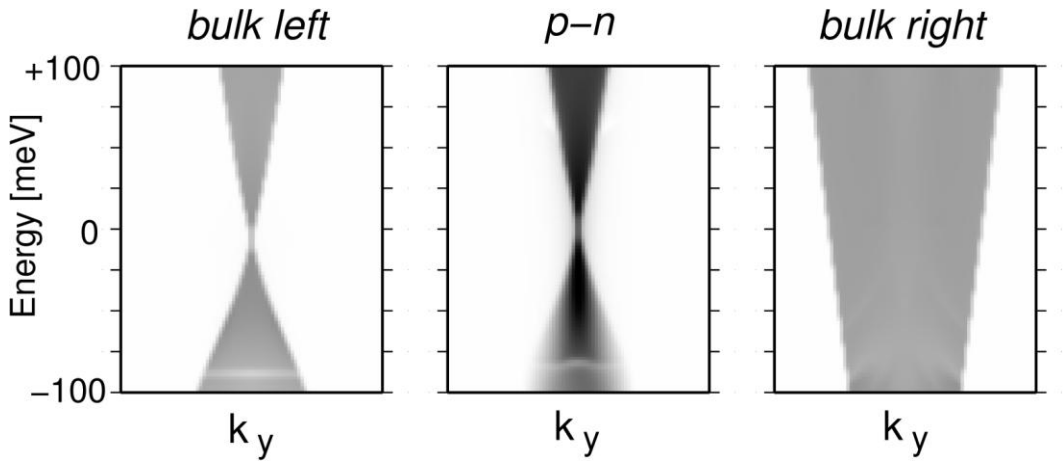

Figure 2: Transmission coefficient $T(ky,E)$ projected in the top QL. Left, middle and right panels correspond to the left bulk-like slab, the TPNJ and right bulk-like slab, respectively.

References

[1] H Aramberri, J.I. Cerdá, M.C. Muñoz, *Nano Letters* **15** (6), 3840-3844 (2015)
[2] H Aramberri, M. C. Muñoz, J. I. Cerdá, *Nano Research* **10** (5), 1784-1793 (2017)