Disorder-induced Randomization of Spin Polarization and Interfacially Protected Surface States in Three-dimensional Models of Topological Insulators

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Abstract

The growing interest on topological insulators (TI) relies on their fascinating electronic properties, namely, a non-trivial insulating bulk which guarantees the formation of highly robust Dirac-like states at the surface holding a chiral spin texture.**[1-3]** This new topological phase of condensed matter is governed by strong spin-orbit coupling and their surface states are protected against disorder preserving time-reversal symmetry (non-magnetic).

Here we use a three-dimensional model of TI on a diamond lattice, described by the Fu-Kane-Mele (FKM) Hamiltonian,**[4]** and show how Dirac cone characteristics can be tuned on opposite surfaces upon differentiation of atomic-scale surface terminations. In particular, when the outermost surface layers are removed, the number of Dirac cones in the surface Brillouin zone (SBZ) changes from three at the three equivalent M-points to a single one at Gamma. This result extends the applicability of the FKM model to real TI such as the frequently studied Bi2Se3, Bi2Te3 or Sb2Te3.

More interestingly, when opposite surfaces are geometrically differentiated by removing the outermost layer from only one surface, Dirac cones develop at the M-points in one surface and at the Gamma-point in the other and remain uncoupled and gapless down to few bulk layers (see Fig.1(b,e) for 11 and 3 layers thickness respectively).**[5,6]** Our findings are consistent with recent experimental observations by Bian *et al.***[7]** and open the way to controlled engineering of thin 3D-TI with highly robust chiral states.

Additionally, by introducing Anderson bulk disorder,**[8-11]** we investigate the changes in the spin texture with increasing disorder in the slab in order to determine the extent to which the topological protection of surface states is reduced. As disorder strength is increased, spin polarization becomes smaller and spread over a wider range of vector length, evidencing randomization of the spin texture fingerprint (see Fig. 2; blue and red arrows correspond to the clean and disordered cases respectively). Our findings suggest ways to analyze the bulk crystalline quality of TI by inspecting the spin texture features through spin-resolved ARPES experiments.

References

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Figures

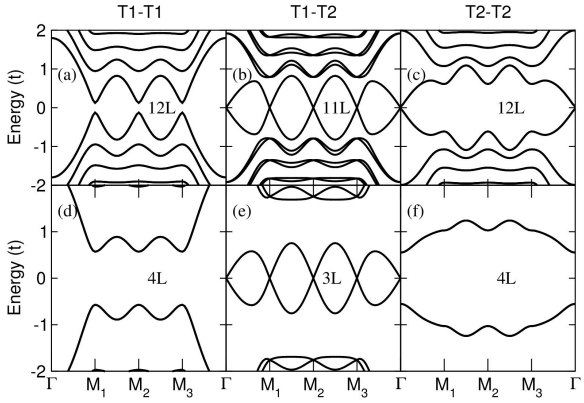

Figure 3. Band structure of slabs of various thicknesses (layers L) and surface terminations (T1 is the default termination and T2 is the one obtained by removing the outermost layer as explained in the text). When opposite surfaces are geometrically differentiated (b,e) the surface states remain gapless down to few bulk layers.

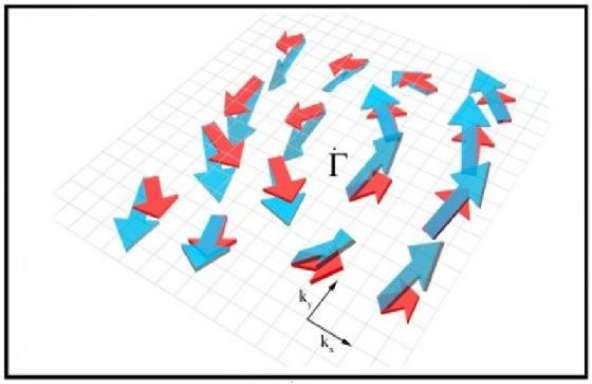

Figure 4. Spin texture of a T2-T2 slab (12 layers) in presence (red) and in absence (blue) of bulk Anderson disorder. The randomization of the spin texture in presence of bulk disorder is evident.