Dirac cones at topological/trivial semiconductor interface with atomic steps

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The family of IV-VI topological crystalline insulator materials feature band inversions located away from the Brillouin zone center. The resulting possibility of both valley interactions and mirror symmetry protection is responsible for generating Dirac points away from time reversal invariant momenta in interface states. Such degeneracies have been highlighted as a potential route towards a topological transistor, since they can be lifted by an applied electric field. Realizing such a device will require a detailed understanding of the intervalley physics responsible for generating the double Dirac cone. In addition, the operation of this or similar devices outside of ultra-high vacuum will require encapsulation, and the consequences of this for the topological interface state must be understood.

We address both topics for the case of 2D interface states, using angle resolved photoemission spectroscopy [1]. We examine bulk (Pb,Sn)Se (001) crystals overgrown with thin layers of PbSe, realizing topological/trivial heterostructures. We have shown that the topological interface state is preserved when encapsulated in a heterostructure and that observations of these buried interface states remain possible at depths of at least 8 ML. We demonstrate that the valley interaction which splits the two Dirac cones at each X point is extremely sensitive not only to PbSe layer thickness but also to atomic-scale details of the TCI-normal interface and heterostructure surface, exhibiting non-monotonic changes as PbSe deposition proceeds. This includes an apparent total collapse of the splitting for sub-monolayer coverage, while slightly more PbSe recovers it. This continues in an oscillatory fashion, although soon inelastic photoelectron scattering blurs the features of interest. For a large overlayer thickness we observe quantized PbSe states, which may reflect a novel confinement structure caused by the symmetry gap at the buried topological interface.

The detailed theoretical analysis supported by realistic tight binding model calculations has led to the conclusion that in the case of small number of PbSe layers the collapse of valley splitting depends mainly on the coverage of surface by a sufficiently dense array of terraces or steps. Terraces of the height of odd atomic layers cancel the valley interactions produced by surface and even-height regions. The overall effect is a cancellation of the valley splitting, dependent on the ratio of odd- to even-height regions on the surface.

Our model can also describe the case of wide terraces which exist for example at cleaved surface. When they are wider than 20nm the valley splitting is recovered and the odd-height steps define domain boundaries with additional 1D topological states reported recently by Sessi *et al.* [2].

[1] C. M. Polley, R. Buczko, A. Forsman, P. Dziawa, A. Szczerbakow, R. Rechciński, B. J. Kowalski, T. Story, M. Trzyna, M. Bianchi, A. GrubišićČabo, P. Hofmann, O. Tjernberg, and T. Balasubramanian, *ACS Nano* **12**, 617-626 (2018).

[2] P. Sessi, D. Di Sante, A. Szczerbakow, F. Glott, S. Wilfert, H. Schmidt, T. Bathon, P. Dziawa, M. Greiter, T. Neupert, G. Sangiovanni, T. Story, R. Thomale, M. Bode, *Science* **354**, 1269-1273 (2016)