Discovery of the intrinsic antiferromagnetic topological insulators: theory and experiment

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Using *ab initio* methods, we predict the van der Waals layered compound $MnBi_2Te_4$ (MBT) to be the first antiferromagnetic topological insulator (AFMTI) [1-3]. The interlayer AFM ordering makes MBT invariant with respect to the combination of the time-reversal (Θ) and primitive-lattice translation ($T_{1/2}$) symmetries, $S=\Theta T_{1/2}$, which gives rise to the Z_2 classification of AFM insulators, $Z_2 = 1$ for this material. The S-breaking (0001) surface of MBT exhibits a band gap in the topological surface state thus representing an ideal platform for the observation of the quantized magnetoelectric coupling and intrinsic axion insulator state. Our prediction is confirmed experimentally by means of structural, magnetic, and photoemission spectroscopy measurements [1]. In the 2D limit, MBT is expected to show a unique set of thickness-dependent magnetic and topological transitions, which drive it through FM and (un)compensated AFM phases, as well as quantum anomalous Hall (QAH) and zero plateau QAH states [4]. Thus, MBT is the first stoichiometric material predicted to realize the zero plateau QAH state intrinsically. This state was earlier predicted to host the axion insulator phase. The discovery of the first AFMTI opens a new field of magnetic TIs that focuses on intrinsically magnetic stoichiometric compounds [5-8]. Finally, apart from MBT itself, its FM building blocks can be used for creation of topological heterostructures [9-12].

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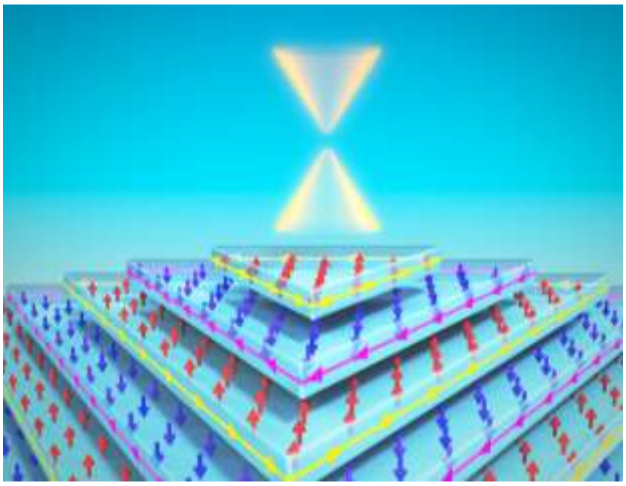

Figure: Artistic representation of the stepped surface of $MnBi_2Te_4$, and above, the characteristic electronic feature of an AFMTI, the so-called Dirac cone. The red and blue arrows represent the local magnetic moments of the Mn atoms, whose directions alternate from one terrace to the next (antiferromagnetic order). The yellow and pink lines and their respective arrows show the directions of propagation of the electric currents at the borders, which are opposite between neighbouring borders, which is known as Half-integer quantum Hall effect.