New Universal Type of Interface in the Magnetic Insulator/Topological Insulator Heterostructures

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Magnetic proximity effect at the interface between magnetic and topological insulators (MIs and TIs) is considered to have great potential in spintronics as, in principle, it allows realizing the quantum anomalous Hall and topological magneto-electric effects (QAHE and TME). Although an out-of-plane magnetization induced in a TI by the proximity effect was successfully probed in experiments, first-principles calculations reveal that a strong electrostatic potential mismatch at *abrupt* MI/TI interfaces creates harmful trivial states rendering both the QAHE and TME unfeasible in practice. Here, using density functional theory calculations, we resolve the latter problem by proposing a fundamentally new type of the interface between an MI film and a tetradymite-like TI [1, 2], which appears to be universal for binary magnetic insulators, as exemplified by MnSe/Bi_2Se_3, MnTe/Bi_2Te_3, and EuS/Bi_2Se_3. The fabrication of the proposed interface suggests a growth mechanism implying a sinking of the codeposited MI atoms into the outermost quintuple layer (QL) of the TI substrate and formation of the MnSe(Te) or EuS structure combined with few remnant atomic layers constituted the outermost QL of a TI surface: Se(Te)-Bi-Se(Te)-[MnSe(Te)]-Bi-Se(Te) or Se-Bi-Se-[EuS]-Bi-Se. Such a scenario is far more energetically favorable than that of the sharp interface formation and covalent type bonding to a TI. Strikingly, the realization of this scenario leads to a unique situation when the heterostructure's magnetic part, based on a material that intrinsically does not show van der Waals bonding (MnSe, MnTe, EuS, etc.), turns out to be van der Waals coupled to a TI substrate since the MI film is actually sandwiched between Se(Te)-Bi-Se(Te)- and -Bi-Se(Te) layers. The encapsulated magnetic film tends to adopt its bulk-like atomic structure starting already from a thickness of a few bilayers. Moreover, the total energy calculations also reveal the bulk-like magnetic ordering even for the relatively thin films inserted inside the TI QL. By adding more MI bilayers to the "grown-in" film, we have increased its thickness up to a couple of nanometers, finding each insertion to be very much energetically favorable. Altogether, this proves such systems to constitute a novel type of the MI/TI interface that provides a smooth MI-to-TI connection yielding the interface electronic structure essentially free of trivial states. These findings enable efficient engineering of the MI/TI interfaces with tailor-made properties and pave a way to realization of the QAHE and TME as well as their exotic consequences, such as image magnetic monopole or Majorana Fermions, on the basis of the MI/TI heterostructures.

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References

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