Magnetic order and electronic structure of lanthanide-containing thallium dichalcogenides

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One of the most promising approaches for realizing the quantum anomalous Hall effect is the magnetic extension of topological insulator [1]. To date, a number of promising systems have been proposed, based on topological insulator (TI) and magnetic thin films. The magnetic insulator in such a system has to satisfy a number of conditions. It has to have the same crystal structure as the TI, while its lattice parameter and work function should be close to those of the TI. In such a case, the heterostructure is guaranteed against appearance of harmful trivial interfacial states that could make the system spectrum gapless.

The thallium-based TIs $TlAX_2$ (*A* = Sb, Bi, *X* = Se, Te) family has been discovered in 2011. However, a suitable isostructural magnetic insulator to form a magnetic extension has not been reported so far. In this work, by means of *ab initio* calculations we have studied magnetic and electronic structure of lanthanide-containing thallium dichalcogenides $TlLnX_2$ (*Ln* = Gd, Eu, *X* = Se, Te) in order to check whether these materials are suitable to be a magnetic extension of the thallium-based TIs. Our results indicate that the intralayer FM ordering is favorable for $TlEuTe_2$, while for other three compounds a noncollinear antiferromagnetic 120° structure has the lowest energy. The gadolinium-based compounds were found to be semiconductors, while the europium compounds are metals, which, however, show a band gap in the conduction band.

Although the semiconducting systems studied here do not show desirable ferromagnetic order, the weak intralayer magnetic coupling theoretically makes it possible to control magnetic order by means of the external magnetic field. For example, the quantized Hall effect [2-3] has been measured in the $MnBi_2Te_4$ antiferromagnet that has been drive in the ferromagnetic state by the external magnetic field.

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References

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