Quantum Anomalous Hall effect and axion insulator phase in HgTe material class

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Dilute magnetic semiconductors have played a central role in the demonstrating and describing a strong and intricate sp-d exchange interactions, paving the way for the rise of magnetic topological insulators [1,2]. Recently, the exchange splittings of magneto-optical spectra in $Cd_{1-x}Mn_xTe$ and $Hg_{1-x}Mn_xTe$ have been described [3] and it has been demonstrated that superexchange dominates in magnetic topological insulators [4].

We study theoretically the interplay between magnetism and topology in HgTe-based systems in order to obtain the quantum anomalous Hall phase and the axion insulator phase.
To engineering the quantum anomalous Hall phase, we investigate the electronic and magnetic properties of the dilute magnetic semiconductors $Cd_{1-x}Cr_xTe$, $Hg_{1-x}Cr_xTe$, $Cd_{1-x}V_xTe$, $Hg_{1-x}V_xTe$ by using a density functional theory approach which goes beyond the standard functionals in order to correctly reproduce the topology and the band gap of these systems. We study the exchange couplings for all considered cases and we find that the coupling is ferromagnetic in case of doping with V, differently from the case of doping with Mn and Cr, where we find antiferromagnetic couplings. We conclude that the ferromagnetic coupling among V atoms in the insulating phase of topological HgTe can produce the quantum anomalous Hall phase[5].
To generate the axion insulator, we study the three-dimensional HgTe/MnTe superlattices stacked along the (001) axis. Our results show the evolution of the magnetic topological phases with respect to the magnetic configurations. An axion insulator phase is observed for the antiferromagnetic order with the out-of-plane Néel vector direction below a critical thickness of MnTe, which is the ground state amongst all magnetic configurations. Defining T as the time-reversal symmetry, this axion insulator phase is protected by a magnetic two-fold rotational symmetry $\mathbf{C_2 \cdot T}$. The axion insulator phase evolves into a trivial insulator as we increase the thickness of the magnetic layers. By switching the Néel vector direction into the ab plane, the system realizes different antiferromagnetic topological insulators depending on the thickness of MnTe. These phases feature gapless surface Dirac cones shifted away from high-symmetry points on surfaces perpendicular to the Néel vector direction of the magnetic layers[6].

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