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

G. Cuono[1], R. Islam[1], A Lau[1], S. Mardanya[2], T. R. Chang[2], B. Singh[3], C. M. Canali[4], T. Dietl[1] and *Carmine Autieri*[1]

[1]International Research Centre MagTop, Institute of Physics, Polish Academy of Sciences, Aleja Lotników 32/46, PL-02668 Warsaw, Poland

2Department of Physics, National Cheng Kung University, Tainan 70101, Taiwan

[3]Department of Condensed Matter Physics and Materials Science, Tata Institute of Fundamental Research, Colaba, Mumbai 400005, India

[4]Department of Physics and Electrical Engineering, Linnaeus University, Kalmar, Sweden

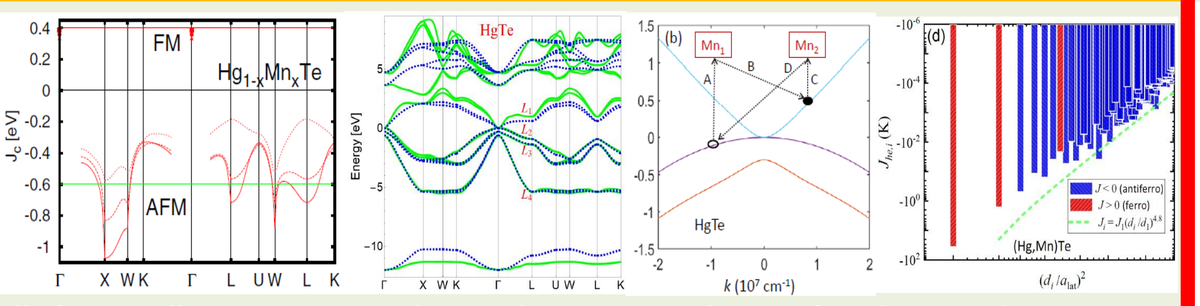
Email: autieri@magtop.ifpan.edu.pl

ABSTRACT

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]. Recently, the exchange splittings of magneto-optical spectra in $Cd_{1-x}MnxTe$ and $Hg_{1-x}MnxTe$ have been described [2] and it has been demonstrated that superexchange dominates in magnetic topological insulators[3]. 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.

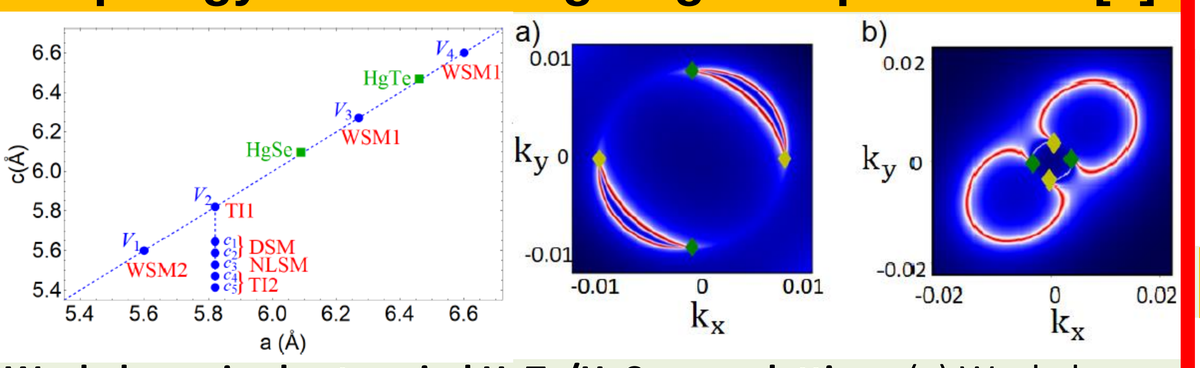
To engineering the quantum anomalous Hall phase, we investigate the electronic and magnetic properties of the dilute magnetic semiconductors $Cd_{1-x}Cr_xTe$, $Hg_{1-x}Cr_xTe$, $Cd_{1-x}VxTe$, $Hg_{1-x}V_xTe$ by using a density functional theory approach which goes beyond the standard functionals in 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[4]. To generate the axion insulator, we study the three-dimensional HgTe/MnTe superlattices stacked along the (001) axis. Previously, new topological phases have been predicted in non-magnetic HgTe-based superlattice [5]. 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].

Interplay between topology and magnetism[2,3]

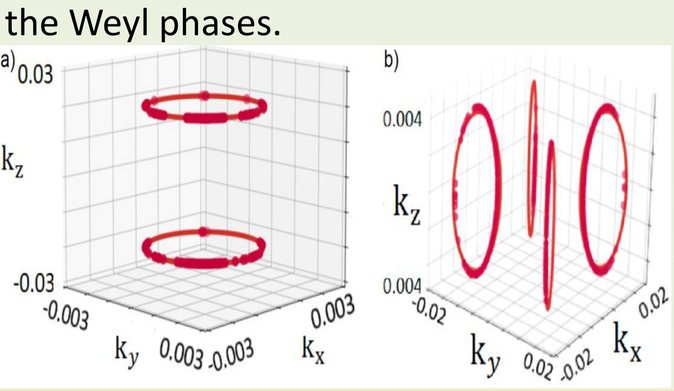


(left panel) Momentum dependent spin-splitting for the conduction band of HgTe doped with Mn. (central left panel) First principle band structure and minimal tight-binding model. (central right panel) Schematic interband mechanism of fourth order electron-hole contribution to magnetic exchange between two Mn ions. (right panel) Computed interband electron-hole contribution $J_{i,he}$ to the magnetic exchange. The superexchange mechanism dominates .

Topology in short-range HgTe superlattices[5]

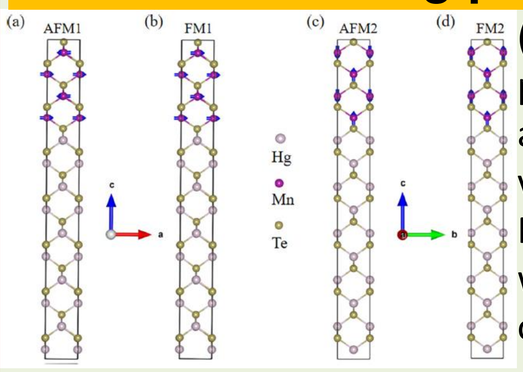


Weyl phases in short-period HgTe/HgSe superlattices. (a) Weyl phases WSM1 and (b) Weyl phases WSM2. Weyl points with chirality -2 are represented with yellow diamond markers. instead, the Weyl points with chirality +2 have green diamond markers. C_2T symmetry protects the Weyl phases.



Nodal lines in short-period HgTe-based superlattices. (a) Isoenergetic nodal-line in HgTe/CdTe and (b) non isoenergetic nodal-lines in HgTe/HgSe superlattice protected by mirror symmetry.

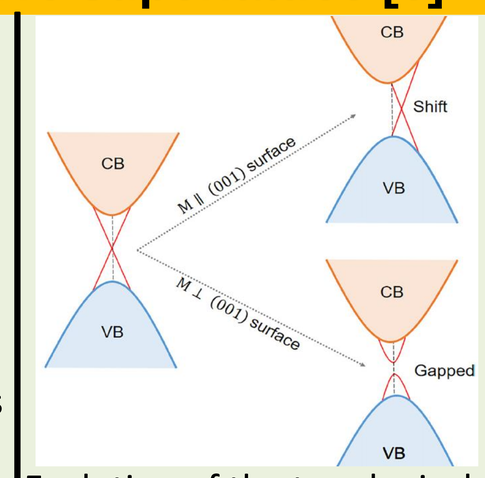
Axion insulating phase in HgTe/MnTe superlattice [6]



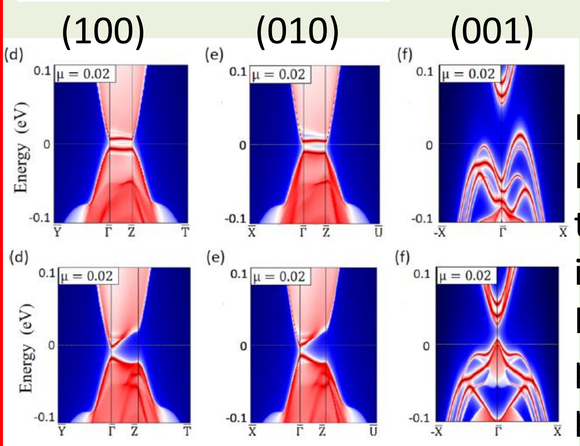
(a,c) Antiferromagnetic phases with in-plane and out of plane Néel vector. (b,d) Ferromagnetic phases with in-plane and out of plane Néel vector.

AFM1	AFM2	FM1	FM2
WATI/ SATI	NI/ AI	SM	MWSM

Different topological phases as a function of the magnetic order and Néel vector.

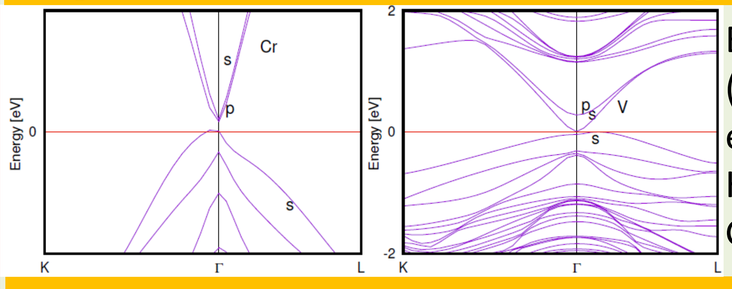


Evolution of the topological surface states as function of Néel vector orientation(**M**).



Increasing the thickness of the trivial phase MnTe, the AFM1 phase goes from a strong topological insulator to a weak topological insulator. Evidence from the TSS (not shown). Increasing the thickness of the MnTe, the AFM2 phase goes from the axion insulator phase (low panels) to the trivial insulating phase (top panels)

Quantum Anomalous Hall phase in V-doped HgTe [4]



Band structure of (a) $Hg_{0.875}Cr_{0:125}Te$ and (b) $Hg_{0.875}V_{0:125}Te$ with 32% of the exact exchange using the hybrid-functional. $Hg_{0.875}V_{0:125}Te$ is ferromagnetic in both GGA+U and hybrid-functional HSE06.

CONCLUSIONS

First principle modeling is a powerful tool to investigate topological materials and can be combined with tight-binding models. We can study electronic properties as topological invariants, surfaces states and Fermi arcs. We can investigate interplay between magnetism and topology.

Due to the robustness of the topology of HgTe, we predict several topological phases in HgTe-based systems and superlattices including nodal-line semimetal, quantum anomalous Hall and axion insulator phases.

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