Screening of $(MnBi_2Te_4)(Bi_2Te_3)_m$ family as axion insulators through electronic structure calculations

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Abstract

Due to close resemblance to Bi_2Te_3, the $(MnBi_2Te_4)(Bi_2Te_3)_m$ family was selected to be screened for its potential as axion insulators through electronic structure calculations to identify band gap and possible band inversion. Existing literature shows $MnBi_2Te_4$ (m=0) and $MnBi_8Te_{13}$ (m=3) ground states as an anti-ferromagnetic topological insulator state along with $MnBi_2Te_4$ hosting a quantized magnetoelectric effect. This study takes a computational approach to characterize the $(MnBi_2Te_4)(Bi_2Te_3)_m$ family to explore the effects of modified layer stacking and atomic substitution on its electronic structure.

Introduction and Background

Topological materials have been of recent interest in the field of materials by design due to their vast potential applications in spintronic and magnetoelectric devices. To date intrinsic axion insulators (AIs) have been discovered via doping existing topological insulators (TIs) with magnetic ions. With the presence of magnetic ions in AIs, magnetism breaks time-reversal symmetry which results in a larger and observable quantized magnetoelectric effect (QME). It is also notable that the quantum spin Hall effect is observable in axion insulators which is not the case for topological insulators. Continuing to identify AIs in the context of TIs, both share a band inversion and topologically protected surface states expected of an insulator.

Coh and Vanderbilt have made significant progress to identify promising materials that may give rise to isotropic magnetoelectric coupling.[1] The following properties are used to broadly screen material candidates: large spin-orbital coupling, magnetic ions present, and even number of d-orbital electrons. Such properties identify the $(MnBi_2Te_4)(Bi_2Te_3)_m$ family as promising materials. This family also has promise through being closely related to Bi_2Te_3, which shows topological properties and possible ME coupling with the addition of a magnetic ion. This study utilizes first principles electron structure calculations to screen the $(MnBi_2Te_4)(Bi_2Te_3)_m$ (m=0, 1, 2) family for its potential as axion insulators. With varying m-values, materials have different layering structures which may has potential for effective spin-orbital coupling to arise resulting in the desired band inversion.

Crystal Structure

Layering of $MnBi_2Te_4$ (m=0) closely resembles the structure of Bi_2Te_3 with the addition of magnetic ion Mn. Bi_2Te_3 is built of quintuple layers (5L) of Te-Bi-Te-Bi-Te that are separated by Te-Te gaps. To make $MnBi_2Te_4$, MnTe is inserted along with with a quintuple layer to form septuple layers (7L) of Te-Bi-Te-Mn-Te-Bi-Te that are separated by Te-Te gaps. The layering of higher analogs ($MnBi_4Te_7$ and $MnBi_6Te_{10}$) consist of alternating 7L and 5L layers. Reported crystal structures for many intermediates include Ge/Bi or Mn/Bi mixing which would cause computational issues. However, this is probably a stacking issue of 5L and 7L layers flipping such that identical layers are adjacent (5L-5L or 7L-7L) and not a mixed site issue.

The injection of a magnetic ion gives potential for large enough spin-orbital coupling to occur for QME. The structure of the $(MnBi_2Te_4)(Bi_2Te_3)_m$

family all fall within the R-3m space group which indicates that all materials hold the correct symmetry to host a large quantized magnetoelectric effect. Table 1 contains crystal parameters with rhombohedral axis for m = 0,1,2 of the $(MnBi_2Te_4)(Bi_2Te_3)_m$ family. The parameters began as .cif files with hexagonal axis which was converted to rhombohedral in VESTA, a 3-D crystal visualization program.

DFT calculations

Bulk band structures calculations were computed using Quantum Espresso being ran on the Maryland Advanced Research Computing Center (MARCC) Blue Crab cluster. For non-SOC bands calculations we utilized non-linear core corrected, scalar relativistic pseudopotentials. When making spin-orbital coupling calculations full-relativistic pseudopotentials were used. Calculations used a self-consistency convergence threshold of 1.0d-8 eV. To determine atomic positions, VESTA, a 3D structure modeling program, opened cif files which extracted the position per the desired unit cell and axis. Electronic structure calculations included spin-orbital coupling calculations for self-consistency. All calculations ran with a Monkhorst-Pack 4 x 4 x 4 k-point grid.

Table 1. Crystal Parameters of $(MnBi_2Te_4)(Bi_2Te_3)m$ family[2,3]

Compound	Space Group	a = b = c (Å)	$\alpha = \beta = \gamma$ (°)
$MnBi_2Te_4$	R-3m	13.86441	17.9831
$MnBi_4Te_7$	P-3m1	8.36392	30.6851
$MnBi_6Te_{10}$	R-3m	34.27440	7.3653

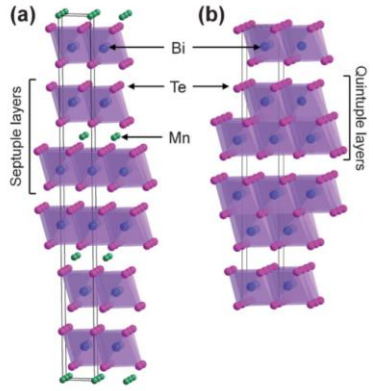

Figure 1. Crystal structures of (a) Bi_2MnTe_4 and (b) Bi_2Te_3 [5]

Results and Discussion

Electronic Structure calculations

Band calculations returned Fermi Energy calculations for $MnBi_2Te_4$ to be 2.0020 eV and 2.0614 eV with the latter factoring in spin-orbital coupling interactions. The band structure for $MnBi_2Te_4$ with SOC is displayed as figure 2. The non-SOC band plot is not displayed due to issues with plotting the k-points correctly. Literature states the importance of examining the band plot with spin-orbital coupling as the interactions may result in a band gap inversion not seen in calculations without SOC. The results show a narrow band gap which is indicative of a potential axion insulator.

Conclusions and Future Work

Future work includes expanding the calculations to the $(MnBi_2Te_4)(Bi_2Te_3)_m$ family for m = 2,3. We also hope to add topological surface calculations for a more through screening of the materials. There is also potential in replacing Mn with Pb as the magnetic ion. Screening the closely related $(PbBi_2Te_4)(Bi_2Te_3)_m$ family has promise for a large enough spin-orbital coupling that would result in the desired magnetoelectric effect for an axion insulator.

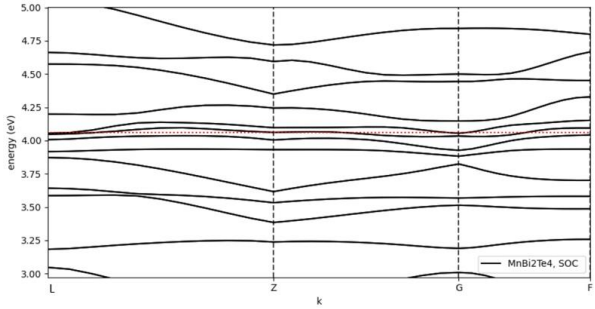

Figure 2. Band structure of $MnBi_2Te_4$ with spin-orbital coupling interactions

References

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