Ab initio study of magnetism in pristine and defected $MnBi_2Te_4$

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The magnetic material $MnBi_2Te_4$ (MBT) has garnered significant attention due to its exotic electronic behaviors. In its bulk form, MBT is an antiferromagnetic topological insulator[1], while in the ferromagnetic (FM) phase, MBT is predicted to transit into a Weyl semimetal.[2] In experimental samples, the presence of defects is known to influence its magnetic properties by inducing important modifications in the band structure. Indeed, defects such as the Mn_{Bi} and Bi_{Mn} antisites, can decrease the magnetic moment within each septuple layer, thereby reducing the total magnetization at low magnetic fields.[3] Theoretical investigations suggest that intermixing between these antisite defects can suppress the magnetic gap, thus influencing the electronic properties.[4] However, these preliminary works only focus on the antisite defects in MBT while other common structural defects are also observed experimentally. Our study aims to comprehensively explore using state-of-the-art ab intio techniques the impact of various defects on the electronic and magnetic properties of MBT. Atomistic models of MBT with different Mn-vacancy concentrations (as depicted in Fig. 1.a) were constructed. Mn-vacancy MBT is found to be most stable in the ferromagnetic phase, as illustrated in Fig. 1.b. The effect of Mn-enriched, Bi-enriched and intermixing defects in MBT are also investigated. The present theoretical study sheds light on the magnetic coupling mechanisms in MBT, providing a guideline for the experimental control of magnetism in $MnBi_2Te_4$.

References

[1] Li et al., Science Advances, **6** (2019) aaw5685.
[2] Zhang et al., Physical Review Letters, **20** (2019) 206401.
[3] Lai et al., (2021). Physical Review B, **18** (2021)184429.
[4] Tan et al., Physical Review Letters, **12** (2023) 126702.

Figures

(a) (b)

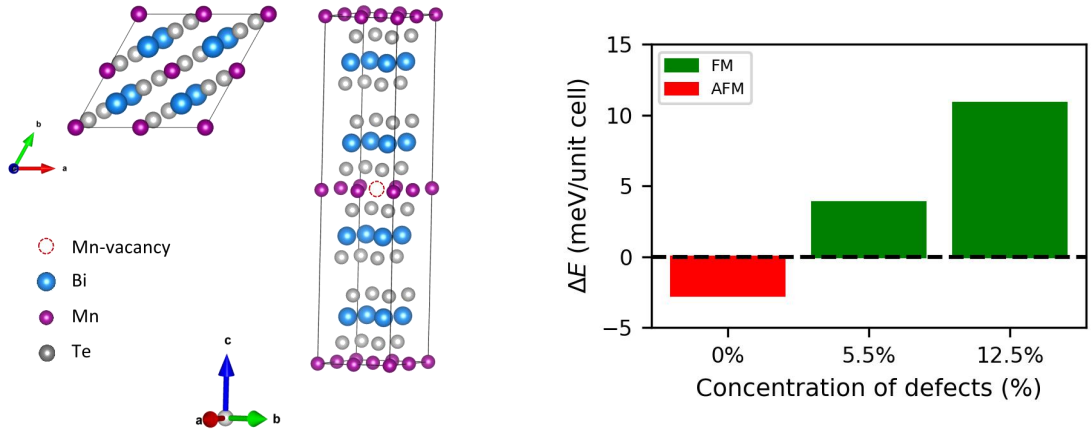

Figure 1: (a) Top and side view of the atomistic model of Mn-vacancy with 12.5% defect concentration. The defect locates in the middle of the Mn-layer. (b) *Ab intio* estimation of the magnetic interlayer coupling in the pristine and in the Mn-vacancy models.