Ab-initio studies of Mn-rich $MnBi_2Te_4$

Ana Fontes
Jiaqi Zhou, Jean-Christophe Charlier
Institute of Condensed Matter and Nanosciences (IMCN), Université catholique de Louvain, B-1348 Louvain-la-Neuve, Belgium
ana.pedrofontes@uclouvain.be

The magnetic topological material $MnBi_2Te_4$ (MBT) has attracted great attention due to its exotic behaviors [1]. Intrinsically, MBT presents the antiferromagnetic (AFM) coupling. By applying a strong magnetic field, it will be converted into a ferromagnetic (FM) phase where quantum anomalous Hall effect (QAHE) can be observed. Plenty of efforts have been devoted to facilitating the transition from AFM to FM. A new mechanism based on the intermixing of Mn and Bi sites has been proposed to realize the magnetic field-free transition [2]. Besides, it is reported that Mn-rich growing conditions and intermixing in $MnSb_2Te_4$ can also enhance the interlayer ferromagnetic coupling [3]. Motivated by these discoveries, we investigate the effect of increasing Mn concentration on MBT properties using *ab initio* calculations. Mn-rich atomic model has been built as Fig. 1, where Bi atoms are substituted by Mn atoms. Then we report the electronic and magnetic properties of Mn-rich MBT. With the interpretation of the magnetic coupling, this work can promote the practical applications of $MnBi_2Te_4$ in spintronic devices, including magnetic memory storage and quantum computation.

References

[1] Li et al., Science Advances **6** (2019) aaw5685.
[2] Tan et al., Physical Review Letters **12** (2023) 126702.
[3] Wimmer et al., Advanced Materials **42** (2021) 2102935.

Figures

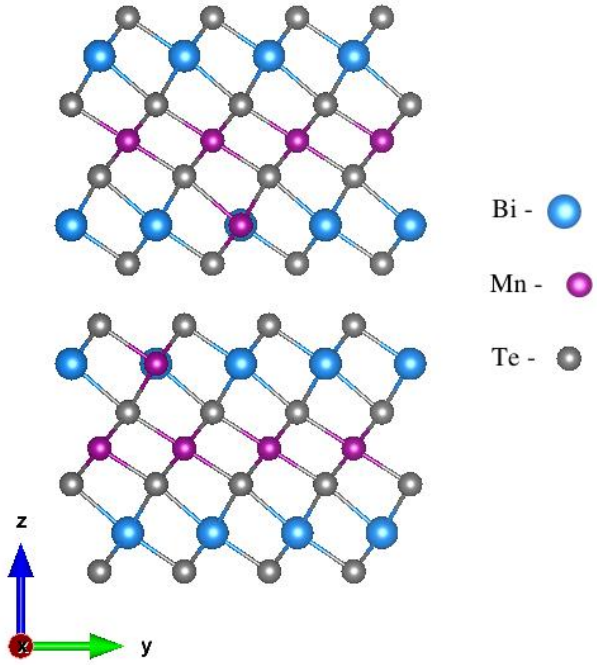

Figure 1: Side view (the yz plane) of atomic model of Mn-rich $MnBi_2Te_4$.