First-Principles Investigation of the Electronic, Magnetic, and Transport Properties of MnBi2Te4

Mirali Jafari,[1] Martin Gmitra,[2,3] and Anna Dyrdał[1]

[1] *Department of Mesoscopic Physics, ISQI, Faculty of Physics, Adam Mickiewicz University in Poznań, ul. Uniwersytetu Poznaskiego 2, 61-614 Poznań, Poland*

[2] *Institute of Physics, Faculty of Science, Pavol Jozef Šafárik University in Košice, Park Angelinum 9, 040 01 Košice, Slovakia*

[3] *Institute of Experimental Physics, Slovak Academy of Sciences, Watsonova 47, 040 01 Košice, Slovakia*

$MnBi_2Te_4$ is a material with unique electronic, magnetic, and transport properties that make it promising material for quantum computing and spintronics applications. We used the density functional theory to investigate its bulk and surface electronic states, and found that it is a topological insulator with a significant bandgap and a Dirac cone-like dispersion. The magnetic properties of this material arise from coupling between the magnetic moments of Mn atoms and non-magnetic Bi_2Te_4 layers, resulting in a high magnetic anisotropy with the easy-axis along the c-axis. We showed that an electric field can induce a splitting of the bandgap in the electronic structure, which could be useful for application in spin-based devices. However, the growth of high-quality $MnBi_2Te_4$ thin films remains a challenge, and further research is needed to uncover all their properties. [1-5]

References:

[1] D. Zhang, et al., Phys. Rev. Lett. 122 (2019) 206401.
[2] M. M. Otrokov, et al., Nature 576 (2019) 416-422.
[3] J. Jiang, et al., Phys. Rev. Mater. 2 (2018) 024201.
[4] Y. Li, et al., Phys. Rev. B 100 (2019) 134438.
[5] S. Patel, et al., Phys. Rev. B 106 (2022) 035125.

This work has been supported by the Norwegian Financial Mechanism 2014–2021 under the Polish-Norwegian Research Project NCN GRIEG "2Dtronics" no. 2019/34/H/ST3/00515.