Design of new topological materials

Carmine Autieri¹*

*Email presenter: autieri@magtop.ifpan.edu.pl

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

Materials belonging to SnTe materials class have been shown to be topological crystalline insulators. Thin films and nanowires of the SnTe materials class can produce new topological phases depending on the growth orientation, thickness and symmetries. I will review these new topological phases can range from the trivial phase at low thickness to the high-order topology in case of dislocations. Additionally, the Rashba effect can interplay with the topological properties in appropriate conditions.

In the second part of the talk, I will show how standard density functional theory overestimates the number of topological materials especially for magnetic topological insulators. Using accurate density functional theory, I will propose the design of two new magnetic topological systems to be synthesized as the axion insulator $EuIn_2Sb_2$ and the quantum anomalous Hall insulator (Hg,V)Te.