Group theoretic methods for semi-empirical electronic structure of topological insulators

Dimitri D. Vvedensky (CMTH), Jing, Zhang (EXSS), and Derek K. K. Lee (CMTH)

This project will examine the electronic structure of materials for topological insulators and valley electronics using semi-empirical modelling techniques. Topological insulators [1] are electronic materials that have a bulk band gap like an ordinary insulator but have protected conducting states on their surface in the sense that they are insensitive to scattering by impurities. These states are possible due to the combination of spin-orbit interactions and time-reversal symmetry. Such topological insulators may provide new routes to generating novel phases and particles, possibly finding uses in technological applications in spintronics and quantum computing.

There are two main theoretical tools that will be used: group theory, which will be applied to tight-binding theory, which is a compact way of describing the electronic structure of materials. In particular, the use of group theoretical method allows easy inclusion of three-centre interactions and spin degrees of freedom, which are frequently neglected in tight-binding schemes [2]. The objective is to investigate the importance of such interactions in more complex structures such as oxides or MoS$_2$.

The starting point of the project is the tight-binding method, including spin-orbit interactions and three-centre integrals, to which group theoretic methods are to determine the presence (or not) of topological states by the application of group theoretic methods. There are various materials to which these ideas can be applied, but the tight-binding calculations may need to be supplemented first-principles calculations. Once the presence of topological states has been established, the effect of these states on transport and optical properties can be investigated.

**Student skills required.** The student working on this project will need to have a thorough background in group theory. The tight-binding method and any first-principles calculations can be learned during the project.
