High-throughput simulations of topological materials

Maia G. Vergniory

1.Max Planck for the Chemical Physics of Solids, Nöthnitzer Str. 40, 01187 Dresden, Germany
2.Donostia International Physics Center, Paseo Manuel de Lardizabal, 20018 Donostia-San Sebastian, Spain

Maia.vergniory@cpfs.mpg.de

Since the theoretical proposal of the first 2D and 3D topological insulators (TIs) more than 15 years ago, solid-state realizations of topological materials have been discovered at a rapid pace. The recently developed theories of Topological Quantum Chemistry and Symmetry-Based Indicators (SIs), based on symmetry eigenvalues and irreducible representations have in particular facilitated high-throughput materials discovery and revealed that topological phases in band structures are more common than originally thought [1]. Indeed, over half of all of the known stoichiometric, solid-state, nonmagnetic materials are topological at the Fermi level, over 85% of the known stoichiometric materials host energetically isolated topological bands, and that just under 2/3 of the energetically isolated bands in known materials carry the stable topology of a TI or TCI. In this talk we will introduce topological electronic materials discovery in nonmagnetic and magnetic crystalline solids from the prediction based on TQC. We have also made all our results publicly and accessible through the Topological Materials Database (https://topologicalquantumchemistry.com/) [2].

References

[1] M.G. Vergniory, L. Elcoro, C. Felser, N. Regnault, B.A. Bernevig, Z. Wang , "A complete catalogue of High- Quality Topological Materials ", Nature 566, 480-485 (2019)

[2] All topological bands of all stoichiometric materials, Maia G Vergniory, Benjamin J Wieder, Luis Elcoro, Stuart SP Parkin, Claudia Felser, B Andrei Bernevig, Nicolas Regnault, Accepted in Science (2022), arXiv preprint arXiv:2105.09954

Figures

Figure 1: Homepage of the https://topologicalquantumchemistry.com