2D topological insulators

This section contains the results of the screening to search for 2D topological insulators (a.k.a. quantum spin Hall insulators or QSHIs). The screening is performed on a comprehensive database we recently created of 1825 monolayers that can be exfoliated from experimentally known compounds (N. Mounet et al, Nature Nanotechnology 13, 246 (2018), see also the 2D structures and layered materials discover section). Using density-functional and many-body perturbation theory simulations, we identify 13 monolayers that are candidates for QSHIs, including high-performing materials such as $AsCuLi_2$ and jacutingaite (Pt_2HgSe_3). We also identify monolayer Pd_2HgSe_3 as a novel Kane-Mele QSHI, and compare it with jacutingaite. Such a handful of promising materials are mechanically stable and exhibit Z_2 topological order, either unpertubed or driven by a small amount of strain. Such screening highlights a relative abundance of Z_2 topological order of around 1%, and provides an optimal set of candidates for experimental efforts.

Here, we provide for all the QSHI candidates the relaxed crystal structures of the monolayers, the electronic band structure obtained at the density-functional theory (PBE) level both with and without spin-orbit coupling, the phonon dispersions and some relevant information such as the space group, the inversion strength and more.

More details can be found in:

A. Marrazzo, M. Gibertini, D. Campi, N. Mounet, N. Marzari, Relative Abundance of Z_2 Topological Order in Exfoliable Two-Dimensional Insulators, Nano Lett. 2019, 19, 12, 8431-8440, doi:10.1021/acs.nanolett.9b02689.