TopoMat database

The database (version 0.1, 8-Aug-2018) contains 16705 unique entries, of which 4482 compounds show non-trivial Z2 indices. Each entry contains basic information about the materials, its crystal structure, Brillouin zone, calculated band structure, Wannier charge center plots (when available), and other data.

The crystal structures originate from ICSD [1] and COD [2] databases subject to the following pre-screening filters:

- 20 atoms or fewer in the unit cell;
- even number of electrons per unit cell;
- no rare-earth elements.

The first-principal calculations have been performed using the Quantum-ESPRESSO package [3] on experimental crystal structures without relaxation. Our computational methodology relies on the PBE exchange-correlations functional, pseudopotentials from the SSSP library [4], and take into account the spin-orbit coupling. The Z2 indices have been calculated using either the parity analysis for the centrosymmetric materials, or the Z2Pack methodology [5] for noncentrosymmetric crystal structures.

If you use this work, please cite the following publication in progress:
G. Autès, Q. S. Wu, N. Mounet & O. V. Yazyev, "TopoMat: a database of high-throughput first-principles calculations of topological materials", in preparation (2018).