**Towards ideal topological materials: Comprehensive database searches using symmetry indicators**

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Topological materials (TMs) showcase intriguing physical properties defying expectations based on conventional materials, and hold promise for the development of devices with new functionalities. While several theoretically proposed TMs have been experimentally confirmed, extensive experimental exploration of topological properties as well as applications in realistic devices have been held back due to the lack of excellent TMs in which interference from trivial Fermi surface states is minimized. We tackle this problem in the present work by applying our recently developed method of symmetry indicators to all non-magnetic compounds in the 230 space groups. An exhaustive database search reveals thousands of TM candidates. Of these, we highlight the excellent TMs, the 258 topological insulators and 165 topological crystalline insulators which have either noticeable full band gap or a considerable direct gap together with small trivial Fermi pockets. We also give a list of 489 topological semimetals with the band crossing points located near the Fermi level. All predictions obtained through standard generalized gradient approximation (GGA) calculations were cross-checked with the modified Becke-Johnson (MBJ) potential calculations, appropriate for narrow gap materials. With the electronic and optical behavior around the Fermi level dominated by the topologically non-trivial bands, these newly found TMs candidates open wide possibilities for realizing the promise of TMs in next-generation electronic devices.

1. Feng Tang, Hoi Chun Po, Ashvin Vishwanath, Xiangang Wan, arXiv:1807.09744 (2018).
2. Feng Tang, Hoi Chun Po, Ashvin Vishwanath, Xiangang Wan, arXiv:1806.04128 (2018).
3. Feng Tang, Hoi Chun Po, Ashvin Vishwanath, Xiangang Wan, arXiv:1805.07314 (2018).