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High-throughput search for topological insulators in two-dimensional materials ANTIMO MARRAZZO, MARCO GIBERTINI, NICOLAS MOUNET, DAVIDE CAMPI, NICOLA MARZARI, Theory and Simulation of Materials (THEOS) and National Centre for Computational Design and Discovery of Novel Materials (MARVEL), EPFL, Switzerland — Topological materials are a novel class of solids with outstanding properties protected by the interplay of topology and symmetry. Some of the phenomena that can be hosted in these materials, from dissipationless electron transport to spin filtering, could be very promising for many technological applications. Nevertheless, the rarity of materials exhibiting a stable, topologically non-trivial phase at room temperature hinders development. Here, we screen a comprehensive database we recently developed of about 1800 exfoliable 2D materials, computing topological invariants from first principles (DFT-PBE with spin-orbit coupling) to search for novel topological insulators and to estimate the relative abundance of promising candidates in two dimensions.

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