Discovering two-dimensional topological insulators from high-throughput computations -
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We have performed a computational screening of topological two-dimensional (2D) materials from the Computational 2D Materials Database (C2DB) employing density functional theory. A full ab initio scheme for calculating hybrid Wannier functions directly from the Kohn-Sham orbitals has been implemented and the method was used to extract $Z_2$ indices, Chern numbers, and mirror Chern numbers of 3331 2D systems including both experimentally known and hypothetical 2D materials. We have found a total of 48 quantum spin Hall insulators, seven quantum anomalous Hall insulators, and 21 crystalline topological insulators. Roughly 75% are predicted to be dynamically stable and one-third was known prior to the screening. The most interesting of the topological insulators are investigated in more detail. We show that the calculated topological indices of the quantum anomalous Hall insulators are highly sensitive to the approximation used for the exchange-correlation functional and reliable predictions of the topological properties of these materials thus require methods beyond density functional theory. We also performed GW calculations, which yield a gap of 0.65 eV for the quantum spin Hall insulator PdSe$_2$ in the MoS$_2$ crystal structure. This is significantly higher than any known 2D topological insulator and three times larger than the Kohn-Sham gap.

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