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Discovery of novel functional 2D materials via a 2D materials database JINBO PAN, HAOWEI PENG, JIE YU, JOHN PERDEW, QIMIN YAN, Temple Univ — Single-layer two-dimensional (2D) materials offer great new opportunities for the discovery and design of new functionalities in this compound space. In this work, we construct a comprehensive single-layer 2D materials database based on a data-driven approach. More than 1000 compounds with layered structures have been identified through a data-mining process in the ICSD material database, upon which single-layer structures are constructed. High-throughput computations based on density functional theory (DFT) with the PBE and newly developed SCAN functionals are performed to optimize the geometric structures. Electronic structures of these materials are evaluated using the PBE, SCAN, and HSE06 functionals. Key materials properties are stored in the database, which offers a great opportunity for the rational design of functional 2D materials for technical applications including solar fuel conversion, topological materials, electronics, and catalysis. As a showcase, we hope to present the discovery of novel 2D topological and energy materials. The work was supported as part of the Center for the Computational Design of Functional Layered Materials, an Energy Frontier Research Center funded by the U.S. Department of Energy, Office of Science.

Jinbo Pan
Temple Univ

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