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Construction of a 2D materials database and computational materials discovery of 2D photocatalysts

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Abstract - Single-layer two-dimensional (2D) materials have shown entirely different properties compared with their bulk counterparts, offering great new opportunities for the discovery and design of new functionalities in this largely unexplored compound space. In this work, we construct a comprehensive single-layer 2D materials database based on a stable and efficient data-mining approach. Around 1000 compounds with layered structures have been identified through the data-mining process utilizing the ICSD crystallographic materials database, upon which single-layer structures are constructed. As a showcase of the potential usage of our newly constructed 2D database, we focus on the computational discovery of 2D materials for solar water splitting, which is regarded as a clean, environmentally friendly, and renewable strategy to generate hydrogen gas as chemical fuels. A computational screening workflow is designed and high-throughput computations based on density functional theory with PBE and HSE functional are performed. We identified more than 50 promising candidates as photoanodes and photocathodes for solar water splitting with thermodynamic stability, suitable band gaps, and optimal band edge energies. The computational predictions provide a promising materials test set for future experimental investigations.