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Discovery of Novel Perovskites for Solar Thermochemical Water Splitting from High-Throughput First-Principles Calculations ANTOINE EMERY, CHRIS WOLVERTON, Northwestern Univ — Among the several possible routes of hydrogen synthesis, thermochemical water splitting (TWS) cycles is a promising method for large scale production of hydrogen. The choice of metal oxide used in a TWS cycle is critical since it governs the rate and efficiency of the gas splitting process. In this work, we present a high-throughput density functional theory (HT-DFT) study of ABO_3 perovskite compounds to screen for thermodynamically favorable two-step thermochemical water splitting materials. We demonstrate the use of two screens, based on thermodynamic stability and oxygen vacancy formation energy, on 5,329 different compositions to predict 139 stable potential candidate materials for water splitting applications. Several of these compounds have not been experimentally explored yet and present promising avenues for further research. Additionally, the large dataset of compounds and stability in our possession allowed us to revisit the structural maps for perovskites. This study shows the benefit of using first-principles calculations to efficiently screen an exhaustively large number of compounds at once. It provides a baseline for further studies involving more detailed exploration of a restricted number of those compounds.

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