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High-throughput discovery of electrochemically stable photocatalysts for oxygen evolution. JIE YU, JCAP, Lawrence Berkeley National Laboratory, QIMIN YAN, WEI CHEN, ANUBHAV JAIN, Lawrence Berkeley National Laboratory, JOHN GREGOIRE, JCAP, California Institute of Technology, JEFFREY NEATON, Molecular Foundry, Lawrence Berkeley National Laboratory, KRISTIN PERSSON, EETD, Lawrence Berkeley National Laboratory — Widespread use of artificial photosynthesis hinges upon development of photocatalysts and light absorbers with excellent electrochemical stability in aqueous solution. The poor stability of most semiconductors in the highly oxidizing environment of a solar fuels photoanode has been a key factor limiting the use of many candidates light absorbers. We assess the stability of candidate transition metal oxides (TMOs) in alkaline aqueous environments from calculated Pourbaix diagrams. Our analysis reveals interesting trends in the electrochemical stability of TMOs containing elements which have not traditionally been explored for photocatalysts. Utilizing the Pourbaix diagram analysis as the first screen-layer in a high-throughput workflow that incorporates automating density functional theory and hybrid functional calculations, we screen for electrochemically stable TMO compounds with low band gaps and optimal band edge energies. Applying our new data-driven approach, we successfully identify several new TMOs with promising band gaps and edges that are predicted to resist corrosion under aqueous conditions relevant to solar water splitting. Materials synthesis and electrochemical measurements confirm several predictions and demonstrate the utility of computational screening for identifying new solar fuels materials.

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