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First-principles data-driven discovery of transition metal oxides for artificial photosynthesis

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We develop a first-principles data-driven approach for rapid identification of transition metal oxide (TMO) light absorbers and photocatalysts for artificial photosynthesis using the Materials Project. Initially focusing on Cr, V, and Mn-based ternary TMOs in the database, we design a broadly-applicable multiple-layer screening workflow automating density functional theory (DFT) and hybrid functional calculations of bulk and surface electronic and magnetic structures. We further assess the electrochemical stability of TMOs in aqueous environments from computed Pourbaix diagrams. Several promising earth-abundant low band-gap TMO compounds with desirable band edge energies and electrochemical stability are identified by our computational efforts and then synergistically evaluated using high-throughput synthesis and photoelectrochemical screening techniques by our experimental collaborators at Caltech. Our joint theory-experiment effort has successfully identified new earth-abundant copper and manganese vanadate complex oxides that meet highly demanding requirements for photoanodes, substantially expanding the known space of such materials. By integrating theory and experiment, we validate our approach and develop important new insights into structure-property relationships for TMOs for oxygen evolution photocatalysts, paving the way for use of first-principles data-driven techniques in future applications. This work is supported by the Materials Project Predictive Modeling Center and the Joint Center for Artificial Photosynthesis through the U.S. Department of Energy, Office of Basic Energy Sciences, Materials Sciences and Engineering Division, under Contract No. DE-AC02-05CH11231. Computational resources also provided by the Department of Energy through the National Energy Supercomputing Center.