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Discovery of earth abundant light absorbers for solar water splitting: $Mn_2V_2O_7$ and beyond[1] QIMIN YAN, Moelcular Foundry, Lawrence Berkeley National Laboratory, PAWL F. NEWHOUSE, California Institute of Technology, GUO LI, JIE YU, WEI CHEN, KRISTIN PERSSON, Lawrence Berkeley National Laboratory, JOHN GREGOIRE, California Institute of Technology, JEFFREY NEATON, Lawrence Berkeley National Laboratory — Utilizing a first-principles data driven discovery approach with high-throughput computations and machine learning techniques, we screen for transition metal oxide (TMO) compounds with low band gaps and optimal band edges for solar water splitting applications. Combining the computational screening with the high-throughput experimental synthesis efforts, we identify the complex oxide β-$Mn_2V_2O_7$ as exhibiting a band gap and band edges that are near optimal for photocatalytic water splitting. Experiments, corroborated by theory, indicate that β-$Mn_2V_2O_7$ has a near-direct band gap near 1.8 eV. Our calculations further reveal a valence band maximum composed of mixed O-p/Mn-d states, and a conduction band maximum of V d-character, leading to dipole-allowed direct transitions at the band edges. Photoelectrochemical measurements indicate appreciable photocurrent from $Mn_2V_2O_7$ samples, corroborating our predictions. We further discuss design principles for guiding the discovery of more promising metal oxides with optimal band energetics for solar fuels applications.

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