Abstract Submitted
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First-principles data-driven discovery of new low-band-gap oxides for solar energy capture and conversion[1] QIMIN YAN, Molecular Foundry, Lawrence Berkeley National Lab, WEI CHEN, ANUBHAV JAIN, KRISTIN PERSSON, Lawrence Berkeley National Lab, JEFFERY B. NEATON, Physics Department, UC Berkeley; Molecular Foundry, Lawrence Berkeley National Lab — We develop first-principles data driven discovery approach to explore experimentally-known oxide compounds with low band gaps. Cr-based oxide compounds comprise a nice test bed for assessing high throughput discovery of light absorbers and photocatalysts. An interesting subclass with promising band gaps, this Cr oxide testbed spans a range of electronic and magnetic properties; predicting trends across such a range can challenge for standard density functional theory and many-body perturbation theory. We focus on this set and implement a broadly-applicable high-throughput workflow for calculation of band gaps, adsorption spectra, and band edges, initially using semi-local and hybrid functionals. We develop best practices for analysis of these data, and successfully identify several promising new compounds for solar energy capture and conversion applications, which we then apply more rigorous many-body perturbation theory including GW method and beyond to further study their optical and electronic properties.

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