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First Principles Study of the Electronic Properties of Biaxially Strained Strontium Titanate ROBERT BERGER, Molecular Foundry, Lawrence Berkeley National Lab, CRAIG FENNIE, School of Applied and Engineering Physics, Cornell University, JEFFREY NEATON, Molecular Foundry, Lawrence Berkeley National Lab — Strontium titanate (STO) is one of a handful of materials that can be used to convert solar photons into hydrogen fuel. However, its band gap (3.1 eV) is not well matched to the solar spectrum, reducing its potential as an efficient photocatalyst. Through the growth of epitaxial thin films of STO on lattice mismatched substrates, experimentalists can now tune STO through a large structural parameter space and potentially optimize its electronic properties for photocatalysis. In this work, the effect of biaxial strain on the band structure of STO is explored using DFT and many-body perturbation theory within the GW approximation. In these calculations, in-plane lattice parameters are fixed, and all other structural parameters are relaxed. Changes in band gaps and band edge energies are investigated for strains within 5 percent of the cubic lattice parameter, and compared with experimental results. This work is supported by DOE through the Energy Materials Center, an EFRC at Cornell University.

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