

Abstract Submitted
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Tuning the electronic structure of $(\text{SrTiO}_3)_n/(\text{SrFeO}_{3-x})_m$ superlattices¹ ROBERT BERGER, Lawrence Berkeley National Laboratory, DANIEL BROBERG, University of Texas, CAROLINA ADAMO, Stanford University, SHAWN SALLIS, NICHOLAS QUACKENBUSH, LOUIS PIPER, Binghamton University, CRAIG FENNIE, DARRELL SCHLOM, Cornell University, JEFFREY NEATON, Lawrence Berkeley National Laboratory — SrTiO_3 and other d^0 perovskite-derived compounds are of interest as possible solar water-splitting catalysts, due to their band-edge energies and stability in water. To optimize their ability to absorb and convert solar energy, it is desirable to understand how to tune the electronic structure and band gap of these compounds. One controllable way to experimentally tune the crystal structure, and consequently the electronic structure, of these compounds is through the growth of epitaxially layered superlattices. Past computational work has studied the interleaving of SrTiO_3 and SrFeO_3 , in which the $d^4 \text{Fe}^{4+}$ atoms result in metallic electronic structure. However, the synthesis of related compounds suggests that oxygen vacancies in these superlattices would likely reduce some or all of the Fe^{4+} to Fe^{3+} (d^5), which could once again open a tunable band gap. We use density functional theory and beyond to study the energetics of oxygen vacancy patterns in $(\text{SrTiO}_3)_n/(\text{SrFeO}_{3-x})_m$, and the possibility of favorably tuning the electronic structure and band gap of these superlattices via changes in layering, oxygen vacancy concentration, and biaxial strain. Our results are thoroughly discussed in the context of recent experiments.

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