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Optical Properties of Epitaxial Sr-Ti-O Compounds from First Principles[1] ROBERT BERGER, JEFFREY NEATON, Molecular Foundry, Lawrence Berkeley National Laboratory — $SrTiO_3$ is a representative of the property-rich perovskite family, and a material whose ability to convert solar photons to H_2 fuel would be more efficient if its wide optical bandgap (3.25 eV) better matched the solar spectrum. The Sr- and Ti-based Ruddlesden-Popper (RP) phases, $Sr_{n+1}Ti_nO_{3n+1}$, are structural modifications of $SrTiO_3$ with potentially useful electronic properties. While bulk growth is limited to $n < 4$ and $n = \infty$ ($SrTiO_3$), thin films of larger finite n structures have been grown epitaxially. In optical experiments, bandgaps of these films decrease monotonically with increasing n.[2] In density functional theory (DFT), however, the $n = \infty$ gap is larger than those for finite $n > 3$. This disagreement could stem from limitations in both experiment and theory. We explore this issue in depth using DFT, many-body perturbation theory, and tight-binding techniques.

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[2]C.-H. Lee et al., to be published.

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