First-principles band-gap engineering of $SrTiO_3$ via biaxial strain

Robert F. Berger[1], Craig J. Fennie[2], Darrell G. Schlom[3], and Jeffrey B. Neaton[1]

[1]*Molecular Foundry, Lawrence Berkeley National Laboratory*

[2]*School of Applied and Engineering Physics, Cornell University*

[3]*Department of Materials Science and Engineering, Cornell University*

$SrTiO_3$ 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 band gap (3.25 eV) better matched the solar spectrum. For both reasons, there is interest in modifying the crystal structure of $SrTiO_3$ to tune its electronic structure and band gap. Varying biaxial strain and temperature have been shown in past experiment and theory to modify the $SrTiO_3$ crystal structure via ferroic distortions.

In this work, density-functional theory (DFT) within the local-density approximation (LDA) is used to study the effects of biaxial strain and temperature on the band gap of $SrTiO_3$. In-plane lattice parameters are constrained to values within $\pm 4\%$ of the optimized cubic lattice parameter, and all other structural parameters are allowed to relax. Room-temperature structures of strained $SrTiO_3$ are constructed using a Landau-Ginzburg-Devonshire model. While DFT-LDA is known to underestimate band gaps compared to experiment, the validity of DFT-LDA band gap trends is confirmed using many-body perturbation theory within the GW approximation. We show that experimentally achievable conditions can be expected to tune the gap of $SrTiO_3$ by 10–20%. General symmetry arguments are used to rationalize the observed trends in band gap vs. strain and structural distortion, suggesting that similar trends hold across the perovskite family.

This work is supported as part of the Energy Materials Center at Cornell (EMC^2), an Energy Frontier Research Center funded by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences under Award Number DE-SC0001086.