Modeling Piezoelectricity in Improper Ferroelectrics

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Piezoelectric materials are key components of many important technologies, and discovering materials with improved piezoelectric responses is a major goal of materials science. In particular, finding new mechanisms for piezoelectricity which allow for high piezoelectric coefficients, especially in lead-free materials, could have great technological impact. While piezoelectric coefficients can be calculated directly with standard electronic structure codes, accurate modeling of the contributions to piezoelectric responses, and in particular the complicated interplay between atomic relaxations and strain, is needed in order to understand and explore new mechanisms for piezoelectric response. In this work, we present our model for the piezoelectric response in $Ca_3Ti_2O_7$, an improper ferroelectric which we find has large piezoelectric coefficients. We expand the energy in terms of strain and a small number of important atomic displacements, and then minimize over the remaining degrees of freedom, allowing our model to accurately capture the piezoelectric response with a minimal number of degrees of freedom.

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