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First Principles Study of Piezoelectricty in Improper Ferroelectrics KEVIN GARRITY, KARIN RABE, Rutgers University — 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. Recently, there has been a renewed interest in improper ferroelectrics, which are materials where a non-zero polarization is induced indirectly by the coupling of the polar distortion to non-polar unstable modes, frequently oxygen octahedral rotations. This mechanism for creating a polarization may also offer the possibility of increased coupling to strain, leading to high piezoelectric coefficients. Here, we use first principles density functional theory to investigate the mechanism of the piezoelectric response of $Ca_3Ti_2O_7$, an improper ferroelectric which we find to have large piezoelectric coefficients.

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