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Current-density implementation for calculating flexoelectric coefficients[1] CYRUS E. DREYER, Department of Physics and Astronomy, Rutgers University, MASSIMILIANO STENGEL, ICREA, 08010 Barcelona, Spain and ICMAB-CSIC, DAVID VANDERBILT, Department of Physics and Astronomy, Rutgers University — The flexoelectric (FxE) effect, where polarization is induced by a strain gradient, is universal in all insulators. As devices shrink to the micro and nano scale, large strain gradients can occur, and therefore the FxE effect can play a significant role in their electrical and mechanical properties; also, the FxE effect can be exploited for novel device design paradigms such as piezoelectric "meta-materials" constructed from nonpiezoelectric constituents, or mechanical switching of ferroelectric polarization. One of the crucial limitations to understanding and exploiting the FxE effect is the lack of an efficient first-principles methodology to calculate all of the components of the bulk FxE tensor; the transverse and shear components in particular are problematic. In this work we develop such a methodology based on density functional theory to calculate the full bulk, clamped-ion FxE tensor from a single unit cell by calculating the current-density response to the adiabatic displacement of atoms from a long wavelength acoustic phonon. We benchmark our methodology on simple systems of isolated nobel gas atoms, and apply it to calculate the clamped-ion flexoelectric constants for a variety of technologically important cubic materials.

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