Beyond Piezoelectrics: First-Principles Theory and Calculation of Flexoelectricity

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Flexoelectricity, which is the linear response of polarization to a strain gradient, can have a significant effect on the functional properties of dielectric nanostructures. Despite growing experimental interest, there have been relatively few theoretical studies of flexoelectricity, especially in the context of first-principles calculations. Previous theories have tended to focus either on the lattice or the electronic contribution, and have involved some approximations or limitations. Here we develop a general and unified first-principles theory of the piezoelectric and flexoelectric tensors, formulated in such a way that the tensor elements can be computed directly in the context of density-functional calculations. We demonstrate a supercell method for calculating the flexoelectric coefficients using first-principles methods, including lattice and electronic contributions. In order to obtain the longitudinal elements of the flexoelectric tensor, we carry out calculations on supercells extended along different orientations, taking special care to carry out conversions between objects calculated under fixed $\mathcal{E}$ or fixed D electric boundary conditions in different parts of the procedure. In this way, the longitudinal elements of both the electronic and lattice contributions to the flexoelectric tensor are determined.