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First-principles calculations of flexoelectric coefficients JIAWANG HONG, DAVID VANDERBILT, Rutgers University — Flexoelectricity, which is the linear response of polarization to a strain gradient, can have a significant effect on the functional properties of dielectric thin films, superlattices and nanostructures. Despite growing experimental interest, there have been relatively few theoretical studies of flexoelectricity, especially in the context of first-principles calculations. In this talk, we present a complete theory of both the electronic (or “frozen-ion”)¹ and lattice contributions to flexoelectricity, and demonstrate a supercell method for calculating the flexoelectric coefficients using first-principles density-functional methods. Results are presented for cubic materials including CsCl and SrTiO₃. In order to obtain all the elements of the flexoelectric tensor, transverse as well as longitudinal, we carry out calculations on supercells extended along different orientations (e.g., [110] as well as [100]), taking special care to carry out conversions between objects calculated under fixed E or fixed D electric boundary conditions in different parts of the procedure. In this way, all the elements of both the electronic and lattice contributions to the flexoelectric tensor are determined.

¹J. Hong and D. Vanderbilt, Phys. Rev. B, **84** 180101(R) (2011).

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