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First-principles theory of flexoelectricity

DAVID VANDERBILT, Rutgers University

Flexoelectricity is the linear response of polarization to a strain gradient. Because strain gradients break inversion symmetry, flexoelectricity occurs in all insulating crystals. The flexoelectric effect is negligible on conventional length scales, but it can become very strong at the nanoscale where large strain gradients can significantly affect the functional properties of dielectric thin films and superlattices. Previous theories have tended to focus either on the lattice [1-3] or the electronic (i.e., frozen-ion) [4-5] contribution, and have involved some approximations or limitations. Here we develop a general first-principles theory of the flexoelectric tensor, formulated in such a way that the tensor elements can be computed directly in the context of density-functional calculations. Special attention will be paid to several subtleties, including surface contributions, pseudopotential dependence, the calculation of transverse components, fixed E vs. fixed D boundary conditions, and a degree of non-uniqueness that is present for some strain gradients. We introduce several practical supercell-based methods for calculating the flexoelectric coefficients from first principles, and demonstrate them by computing the coefficients for a variety of insulating materials.(Work done in collaboration with Jiawang Hong. Supported by ONR N00014-12-1-1035.)

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