

Abstract Submitted
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First Principles Study of Flexoelectricity JIAWANG HONG, DAVID VANDERBILT, Rutgers University — Flexoelectricity is the linear response of polarization to a strain gradient. Because strain gradients break inversion symmetry, flexoelectricity allows for charge to be extracted from deformations even in materials that are not piezoelectric. The flexoelectric effect is negligible on conventional length scales, but it becomes very strong at the nanoscale where large strain gradients can significantly affect the functional properties of dielectric thin films and superlattices. We present first-principles calculations of flexoelectric effects in non-piezoelectric materials by introducing the strain gradient artificially in a slab geometry and obtain the flexoelectric coefficients. Furthermore, we model the results in terms of quantities, such as dynamical charges and higher¹ multipole moments that can be computed in the bulk, bringing us closer to a full theory of flexoelectricity.

¹R. Resta, Phys. Rev. Lett. **105**, 127601 (2010).

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