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Flexoelectricity from density-functional perturbation theory

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Flexoelectricity describes the electric polarization that is linearly induced by a strain gradient, and is being intensely investigated as a tantalizing new route to converting mechanical stimulation into electrical signals and vice versa. While several breakthrough experiments have been reported in the past few years, progress on the theoretical front has been comparatively slow. The main difficulty with calculating the flexoelectric response of a material is the inherent breakdown of translational periodicity that a strain gradient entails, which at first sight questions the very applicability of traditional plane-wave pseudopotential methods.
In this talk I will show how these obstacles can be overcome by combining density-functional perturbation theory with generalized coordinate transformations [1,2], gaining access to the full microscopic response (in terms of electronic charge density, polarization and atomic displacements) of a crystal or nanostructure to an arbitrary deformation field. As a practical demonstration, I will present results on the full flexoelectric response of SrTiO3, including atomic relaxations and surface effects. [3] I will show that, upon bending a SrTiO3 slab, one obtains a positive voltage if the crystal lattice is terminated by a TiO2 layer, a negative voltage if the termination is of the SrO type. This points to a dramatic dependence of the flexoelectric effect on the details of the surface: an atomically thin termination layer can affect the magnitude, and even the sign, of the response of a macroscopically thick object.

[1] M. Stengel, Phys. Rev. B 88, 174106 (2013).
[2] M. Stengel, Nature Communications 4, 2693 (2013).
[3] M. Stengel, Phys. Rev. B 90, 201112(R) (2014).

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