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Flexoelectricity via coordinate transformations

MASSIMILIANO STENGEL, Institut de Ciencia de Materials de Barcelona (ICMAB-CSIC), Campus UAB, 08193 Bellaterra, Spain

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 [1]. While several breakthough experiments have been reported in the past few years, progress on the theoretical front has been comparatively slow, especially in the context of first-principles electronic-structure theory. 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 [2,3], 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 a $SrTiO_3$ film, including atomic relaxations and surface effects.

[1] P. Zubko, G. Catalan, and A. K. Tagantsev, Annu. Rev. Mater. Res. **43**, 387-421 (2013).
[2] M. Stengel, Phys. Rev. B, in press. (arXiv:1306.4240).
[3] M. Stengel, Nature Communications **4**, 2693 (2013).