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Flexoelectricity via coordinate transformations
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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 [1]. While several breakthrough 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 wave-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.