O.27 Calculating the flexoelectric tensor with ABINIT

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The first-principles theory of flexoelectricity, describing the macroscopic polarization produced by a strain gradient, has made impressive progress since the pioneering works of Resta and Hong et al. in 2010 [1,2]. The main difficulty in dealing with the flexoelectric effect, i.e., the breakdown of translational symmetry, has been overcome by reformulating the problem in terms of long-wavelength acoustic phonons. As of early 2020, a complete implementation of the bulk flexoelectric tensor is fully integrated in the latest release of the ABINIT package [3], which is now publicly available. Additional surface contributions, that are relevant to the flexural deformation of a finite (quasi-two-dimensional) sample have also been understood, and can be accessed as a by-product of the main linear-response calculation [4].

In this presentation, I will recap the underlying theoretical formalism of the implementation, which is based on an analytical long-wave extension of density-functional perturbation theory (DFPT) [5]. The latter provides, in close analogy to the third-order non-linear response functions module, the intermediate-level spatial-dispersion quantities that are necessary to build the bulk flexoelectric tensor and related materials properties. Then, I will illustrate the performance of the implementation on two markedly different systems, bulk perovskite oxides and two-dimensional materials.

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[1] Resta, PRL **105**, 127601 (2010).

[2] Hong *et al.*, JPCM **22**, 112201 (2010).

[3] Romero *et al.*, JCP **152**, 124102 (2020).

[4] Springolo, Royo and Stengel, arXiv:2010.08470.

[5] Royo and Stengel, PRX **9**, 021050 (2019).