Current density at finite *q* for clamped-ion flexoelectricity

Cyrus E. Dreyer[1,2], Andrea Schiaffino[3], Massimiliano Stengel[3,4], David Vanderbilt[5]

1. Department of Physics and Astronomy, Stony Brook University, Stony Brook, New York 11794-3800, USA
2. Center for Computational Quantum Physics, Flatiron Institute, 162 5th Avenue, New York, NY 10010
3. Institut de Ciència de Materials de Barcelona (ICMAB-CSIC), Campus UAB, Bellaterra, Spain.
4. ICREA-Institució Catalana de Recerca i Estudis Avançats, Barcelona, Spain
5. Physics and Astronomy, Rutgers University, Piscataway, NJ, USA

Current density is a fundamental quantum mechanical observable and is used in first-principles calculations of physical properties including magnetic and dielectric susceptibility, NMR chemical shifts, and EPR *g* tensors. In addition, the current density resulting from an atomic-displacement perturbation gives clamped-ion electromechanical couplings such as piezoelectricity and flexoelectricity (polarization induced by a strain gradient). We have recently developed a density-functional perturbation theory implementation to efficiently calculate flexoelectric coefficients from the current-density response to the adiabatic displacement of atoms from a long wavelength acoustic phonon [1]. In this context, determining the current is complicated because of the nonuniform (i.e., finite wavevector **q**) nature of the perturbation, and the presence of nonlocal pseudopotential operators. In this talk I will outline our methodology, including recent developments [2] combining it with the recently-developed "metric wave" approach [3].

[1] C. E. Dreyer, M. Stengel, D. Vanderbilt, Phys. Rev. B 98, 075153 (2018).
[2] A. Schiaffino, C. E. Dreyer, D.Vanderbilt, and M. Stengel, Phys. Rev. B 99, 085107 (2019).
[3] M. Stengel and D. Vanderbilt, Phys. Rev. B 98, 125133 (2018)