Abstract Submitted
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Lifshitz invariants from ab initio lattice dynamics[1] ANDREA SCHIAFFINO, MASSIMILIANO STENGEL, ICMAB-CSIC — The interaction between different order parameters is vital to explain the emergence of new functionalities (hybrid improper ferroelectricity, magnetoelectricity) in multiferroic systems. While considerable theoretical efforts have been directed in the past at studying couplings (e.g. trilinear or biquadratic) that occur in a homogeneous sample, recent research has revealed an increasing number of cases where the interesting physics emerges from inhomogeneities in some order parameter (e.g. flexoelectricity, domain walls), rather than the uniform bulk phase itself. These are usually described in phenomenological theories via symmetry-allowed gradient-mediated terms, the so-called Lifshitz invariants. Here I will present a general method to calculate such couplings ab initio, within the framework of density-functional perturbation theory. I will start with a brief overview on the most challenging aspects of these calculations, i.e. how to deal with the breakdown of the translational symmetry, and with the unusual electrostatic effects that occur in such a regime. Next, I will demonstrate this strategy in practice by presenting calculations of the most relevant gradient coefficients involving strain, octahedral tilts and polarization in ferroelastic $SrTiO_3$.

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