

Abstract Submitted
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Magnetoelectricity in BiFeO₃ films - first-principles-based computations and phenomenology¹ SERGEY PROSANDEEV, University of Arkansas, IGOR KORNEV, Ecole Centrale Paris, LAURENT BELLAICHE, University of Arkansas, UNIVERSITY OF ARKANSAS TEAM, ECOLE CENTRALE PARIS TEAM — A first-principles-based effective Hamiltonian is used to compute linear and quadratic magnetoelectric (ME) coefficients in epitaxial (001) BiFeO₃ thin films. Its predictions are analyzed within a phenomenological model that provides analytical expressions of the ME coefficients in terms of polarization, as well as, dielectric and magnetic susceptibilities. Main discoveries are: (i) the quadratic ME coefficient is dramatically enhanced by increasing the magnitude of the compressive strain within the Cc phase, as similar to the previously reported enhancement of the linear ME coefficient in these films; (ii) the enhancements of the linear and quadratic ME coefficients have the same macroscopic origin, namely an increase in the dielectric permittivity; and (iii) the relative contribution of *two* different free-energy terms on the total linear ME coefficient is extracted from the simulations. The analytical expressions also help in understanding other ME effects.

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