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Effective Hamiltonian modeling of ferroelectric ultra-thin films

INNA PONOMAREVA, IVAN NAUMOV, IGOR KORNEV, HUAXIANG FU, LAURENT BELLAICHE, Physics Department, University of Arkansas, Fayetteville, Arkansas 72701, USA — We have further extended first principles Hamiltonian approaches [1,2] that are applicable to the bulk systems (i.e., 3D systems periodically repeated in all three Cartesian directions) to study ferroelectric properties of ultra-thin films. The main feature of our new approach is that we treat the dipole-dipole interactions for the systems with 2D periodicity *exactly*, based on the symmetrized Green's function $\mathcal{G}(\mathbf{r}', \mathbf{r})$ of the Laplace equation. Although essentially microscopic, our model nevertheless accurately reproduces macroscopic characteristics such as depolarization and Lorentz fields in the limit of thick films. Within this approach, the finite-temperature behavior of different ferroelectric ultra-thin films have been simulated under different boundary conditions. Our results (1) are compared with those obtained in the framework of a 3D-like approach [3] that uses thick vacuum gaps between the periodic replicas of the films within an atomistic Hamiltonian, (2) provide a deep microscopic understanding of ferroelectric thin films. This work is supported by NSF grants DMR-0404335 and DMR-9983678 and by ONR grants N 00014-01-1-0365, N 00014-04-1-0413 and N 00014-01-1-0600. [1] Zhong *et al*, Phys. Rev. Lett. **73**, 1861 (1994); Phys. Rev. B **52**, 6301 (1995). [2] L. Bellaiche *et al*, Phys. Rev. Lett. **84**, 5427 (2000). [3] I. Kornev *et al*, Phys. Rev. Lett. **93**, 196104 (2004).

L. Bellaiche
Physics Department, University of Arkansas
Fayetteville, Arkansas 72701, USA

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