Developments in the effective-Hamiltonian simulation of phase transitions

Jorge Íñiguez*
Department of Physics and Astronomy, Rutgers University, Piscataway, New Jersey 08854-8019

In a seminal paper, Zhong, Vanderbilt and Rabe [1] showed that it was possible to simulate the phase-transition sequence of a ferroelectric perovskite such as $BaTiO_3$ by computing the statistical mechanics of a first-principles derived effective Hamiltonian. In this talk we summarize recent methodological developments associated with this approach. We will (i) present an efficient method for the direct computation of the Devonshire-Landau free energy [2] and (ii) discuss how an external pressure can properly be included in effective-Hamiltonian based simulations. We will illustrate our work with results for $BaTiO_3$.

---

* The co-authors of this work(s) are Alberto García, J. M. Pérez-Mato S. Ivantchev and David Vanderbilt.

[1] W. Zhong, D. Vanderbilt and K. M. Rabe, Phys. Rev. Lett. **73**, 1861 (1994); Phys. Rev. **B52**, 6301 (1995).
[2] Jorge Íñiguez, S. Ivantchev, J. M. Perez-Mato and Alberto García, Phys. Rev. **B 63**, 144103 (2001).