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Fully-atomistic first-princples approach to the temperature-dependent lattice-dynamical properties of perovskite oxides MATHIAS LJUNGBERG, JACEK WOJDEL, JORGE INIGUEZ, ICMAB-CSIC — We present a methodology for the parametrization of effective Hamiltonians for ferroelectric perovskites that provides a fully atomistic description of the materials. The parameters in our effective models are obtained from first-principles calculations; no experimental input is used. The potential energy surface is represented by a truncated Taylor expansion around the ideal cubic perovskite structure, and is, up to second order, exactly equivalent to the first-principles computed one. Higher order terms are determined by fitting to the first-principles energetics and phonon dispersion relations of the relevant low-symmetry phases. By treating all structural degrees of freedom explicitly, our models allow us to investigate the competition between the soft modes that drive the ferroelectric phase transitions in these materials and other, secondary modes. We will show that such an interaction is of significant importance in the prototypical ferroelectric compound PbTiO3; our method's ability to capture it constitutes a considerable improvement upon earlier approaches. We will also report on our current work to extend this methodology to treat inhomogeneous materials, as e.g. superlattices.

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