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All-atom effective models for first-principles simulations of the temperature-dependent behavior of complex ferroelectric oxides[1] JORGE INIGUEZ, JACEK C. WOJDEL, ICMAB-CSIC, PATRICK HERMET, PHILIPPE GHOSEZ, University of Liege, ZEILA ZANOLLI, ICMAB-CSIC and University of Liege — Since its introduction in the 90's, the first-principles effective-Hamiltonian method has been successfully used to simulate temperature-driven phenomena in increasingly complex ferroelectrics, from classic compound $BaTiO_3$ to multiferroic $BiFeO_3$. Currently, the emergence of nano-structured materials – e.g., in the form of ultra-thin films or short-period superlattices – poses new challenges to the simulations, and the development of predictive models seems to require a reconsideration of the traditional approach. Of particular interest are cases in which novel interfacial effects determine the behavior, as in the $PbTiO_3$-$SrTiO_3$ superlattices of Bousquet *et al.* [Nature **452**, 7188 (2008)]. In such situations a large number of structural distortions may become active, and it may be difficult to decide which ones need to be included in the model. In order to tackle these difficulties, we are extending the first-principles effective-Hamiltonian method so as to retain a full atomistic description of the material, thus removing the so-called *local mode* approximation. I will describe our new approach and show preliminary results for $PbTiO_3$.

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Jorge Iniguez
ICMAB-CSIC

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