First-Principles Study of $BaTiO_3$ Ultra-Thin Films

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Ferroelectric thin films present an interest for various technological applications. As it is well known, the ferroelectric behavior of such films is strongly influenced by the electrical and mechanical boundary conditions. I will present recent DFT first-principles results concerning the ferroelectric behavior of $BaTiO_3$ ultra-thin films in contact with two $SrRuO_3$ metallic electrodes. I will compare the results with what is obtained for free slabs and for $BaO/BaTiO_3/BaO$ heterostructures. I will also discuss how the information accessible from these calculations can be used in the construction of an effective hamiltonian suitable for the study of the ferroelectric phase transition of thin films in temperature.

This work has been done in collaboration with Magali Zimmer.