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**Comparative study of the properties of BaTiO<sub>3</sub> and PbTiO<sub>3</sub> using DFT (LDA, GGA), HF and hybrid (B3LYP) functionals** D. I. BILC, P. HERMET, PH. GHOSEZ, Departement de Physique, Universite de Liege, 4000 Liege, BELGIUM, J. INIGUEZ, Institut de Ciencia de Materials de Barcelona, 08193 Bellaterra, SPAIN — The study of ferroelectrics (FE) requires to be able to reproduce accurately not only the structure but also in some cases their energy gap  $E_g$ . DFT underestimates  $E_g$  of a typical FE by a factor of about two, while hybrid Hartree Fock (HF)-DFT functionals such as B3LYP are known to give improved values for  $E_g$ . Therefore, we performed B3LYP and HF study of BaTiO<sub>3</sub> and PbTiO<sub>3</sub> and compared our results to those of LDA and GGA. For the cubic phase, B3LYP gives very good agreement with the experimental lattice constants and  $E_g$ . For the tetragonal FE phase, if the atomic positions are relaxed at the experimental lattice constants then LDA, GGA and B3LYP give comparable results for the atomic distortions. However, full relaxation of the tetragonal phase using B3LYP gives a supertetragonality comparable to GGA. We performed hybrid calculations for different values of the three Becke's parameters and found that the supertetragonality is introduced by the non-local part of the Becke GGA exchange. This suggests that a hybrid functional generated from a better GGA<sup>1</sup> might provide simultaneously better structural and electronic properties of FE. 1. Z. G. Wu, and R. E. Cohen, PRB **73**, 235116, (2006).

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