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A new hybrid exchange-correlation functional for accurate prediction of the electronic and structural properties of ferroelectric oxide bulks and nanostructures D.I. BILC, Université de Liège, Belgium, R. SHALTAF, Université Catholique de Louvain, Belgium, J. ÍÑIGUEZ, Institut de Ciencia de Materials de Barcelona, Spain, PH. GHOSEZ, Université de Liège, Belgium — We report a systematic comparison of various DFT and hybrid exchange-correlation functionals for the prediction of the electronic and structural properties of prototypical ferroelectric oxides. We find that some, although not all, usual DFT functionals predict the structure with acceptable accuracy, but always underestimate the electronic band gaps. Conversely, common hybrids yield an improved description of the band gaps, but overestimate the volume and atomic distortions associated to ferroelectricity, giving rise to an unacceptably large c/a ratio for the tetragonal phases of BaTiO_3 and PbTiO_3 . This *super-tetragonality* is found to be induced mainly by the GGA exchange energy. We thus propose an alternative hybrid functional, B1-WC, that mixes exact exchange following the B1 scheme with the recently improved GGA proposed by Wu and Cohen. This B1-WC renders accurate description of both the structural and electronic properties of typical ferroelectric oxide at the bulk level. The case of Pt/BaTiO_3 heterostructures is also considered and a comparison of the of B1-WC and LDA results for atomic relaxation and electronic band alignment at the interface is presented.

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