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Structural and Ferroelectric Properties of Prototypical Ferroelectric Materials: Comparative first-principles investigations YUBO ZHANG, JIANWEI SUN, University of Texas at El Paso, JOHN PERDEW, XIFAN WU, Temple University — Ferroelectricity originates from the breaking of spatial inversion symmetry, and spontaneous polarization is determined by the amplitude of the polar structural distortion. Although the density functional theory has been widely used for studying ferroelectric properties, an accurate quantitative prediction of the distortion is rather challenging and is to a great extent limited by the reliability of the adopted exchange-correlation functionals. For the most studied perovskites, the local density approximation (LDA) seems to be more reliable than the generalized gradient approximation (GGA). However, the cell volumes are usually strongly underestimated by the LDA. The B1-WC hybrid functional systematically improves the calculated ferroelectric properties, but its application is restricted to small systems because of the expensive computational effort. The recently developed strongly constrained and appropriately normed (SCAN) meta-GGA is accurate for geometries and energies of diversely-bonded materials. Here, we show that the SCAN is a universally accurate approach for predicting the structural and electric properties of several prototypical ferroelectric materials. The SCAN is comparable or more accurate than the B1-WC hybrid functional but with much cheaper computational cost.

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