Abstract Submitted
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First-principles study of charged vacancies in PbTiO3[1] YANPENG YAO, HUAXIANG FU, University of Arkansas — First-principles calculations within local density approximation (LDA) are performed to study the vacancy formation energies for charged vacancies in $PbTiO_3$. Within the constraint of thermodynamic limit, the chemical potential and Fermi energy dependence of the vacancy formation energy, as well as the transition energy levels, are studied. We found that: (i)the Formation energy of V_O^{2+} is much lower than that of the neutral oxygen vacancy, irrespective of μ_O; (ii) Under oxygen rich condition, the main defect is V_{Pb}^{2-}; (iii) When oxygen is deficient, either V_{Pb}^{2-} or V_O^{2+} can form, depending on the Fermi energy level; (iv) At certain condition, both V_{Pb}^{2-} and V_O^{2+} have similar formation energy, and can coexist.

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