First-principles study of charged vacancies in PbTiO₃

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 PbTiO₃. 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 \( \mu_O \); (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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