

Abstract Submitted
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First-principles calculations of structural energetics of Pb-O di-vacancies in PbTiO₃ and their role in up-down asymmetry of thin films.

O. PAZ, S. P. BECKMAN, D. VANDERBILT, K. M. RABE, Rutgers University — Defects have been proposed as an important influence on the performance of technologically relevant ferroelectric (FE) materials, even at low concentrations. In PbTiO₃, $V_{\text{Pb}}-V_{\text{O}}$ vacancy pairs (VPs) are neutral defects, with a local electric dipole moment that can couple to the bulk polarization. To investigate the role that these defects might play in imprint behavior (i.e., a history-dependent up-down asymmetry), we carried out first-principles supercell calculations of VPs in PbTiO₃. While previous works considered a cubic host,^{1,2} we study the tetragonal FE case for periodic arrays of 1st, 2nd and 3rd-neighbor VPs at densities as low as 3%. Our lowest energy VP is a 2nd-neighbor one oriented so as to break the bulk symmetry between the up and down polarization states. Other VP arrangements are higher in energy by at least 0.2 eV. Atomic relaxation is of particular importance in lowering the energy of the 2nd below that of the 1st-neighbor VP. Berry-phase polarization calculations reveal that the total polarization is only slightly modified for VPs whose dipoles are aligned with the polarization, but is significantly suppressed by antialigned VPs.

¹S. Pöykkö and D. J. Chadi, Appl. Phys. Lett. **76**, 499 (2000).

²E. Cockayne and B. P. Burton, Phys. Rev. B **69**, 144116 (2004).

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