Supporting Information

Multiferroic Grain Boundaries in Oxygen-Deficient Ferroelectric Lead Titanate

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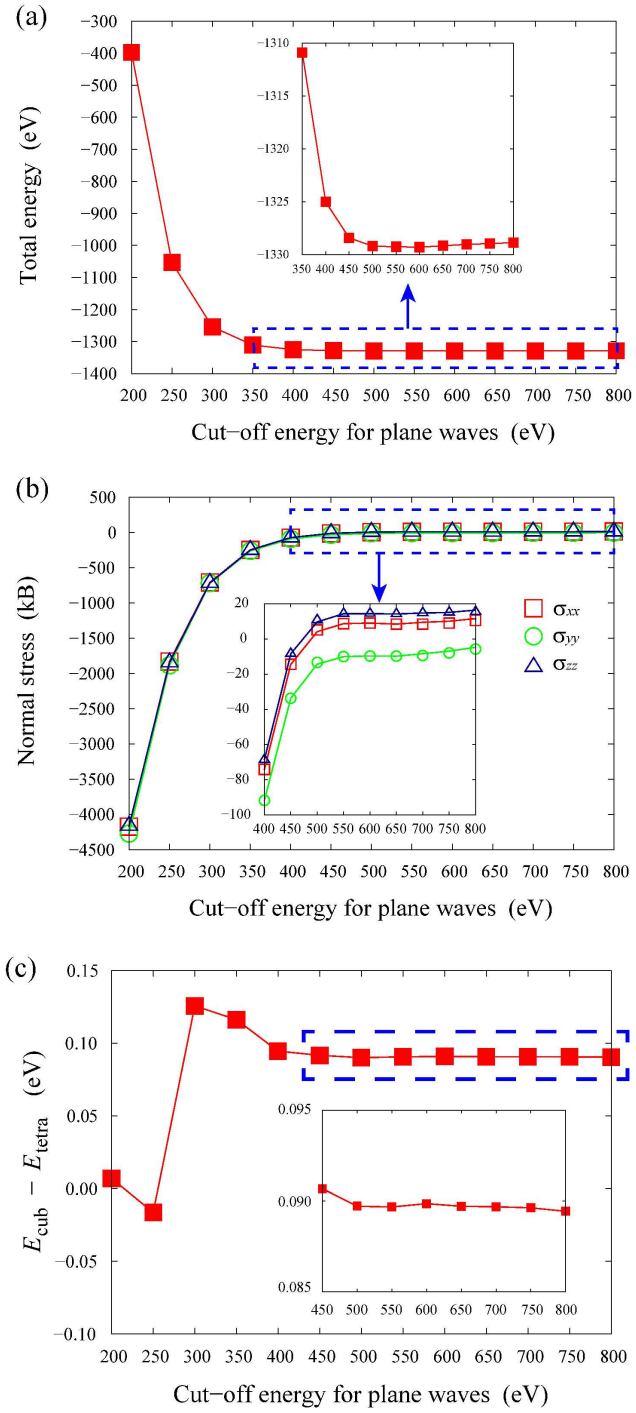
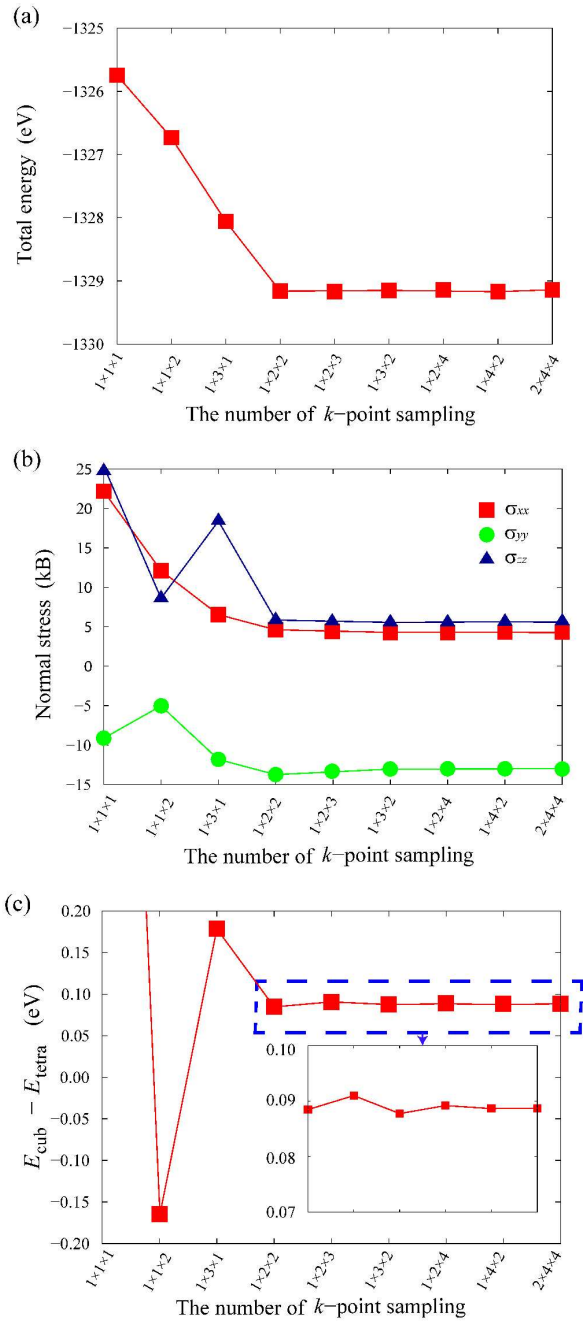
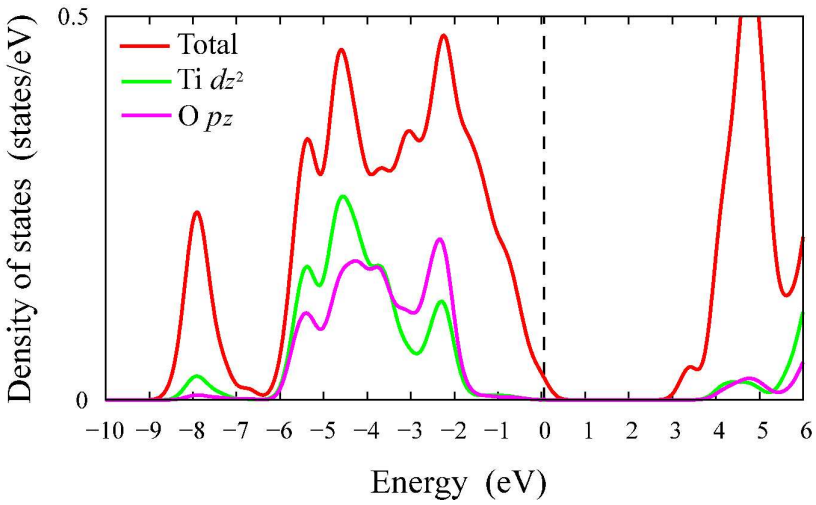


Supporting Figure S1. (a) Total energy and (b) stresses for the simulation supercell used in the present study, and (c) the energy difference between paraelectric and ferroelectric phases as a function of cut-off energy of plane waves. Both the total energy and stresses sufficiently converges when the cut-off energy is equal to or more than 500 eV.



Supporting Figure S2. (a) Total energy and (b) stresses for the simulation supercell used in the present study, and (c) the energy difference between paraelectric and ferroelectric phases as a function of number of k-points. Both the total energy and stresses sufficiently converges when the *k*-point mesh is equal to or denser than 1×2×2. The half reduction is used for the exact exchange portion of the exchange-correlation functional when the mesh division number is even, but the effect of this treatment does not appreciably change the results, e.g., less than 0.01 eV for the total energy.



Supporting Figure S3. Total and atom-resolved angular-momentum-projected density of states (DOS) for ferroelectric $PbTiO_3$ bulk. The projected DOS of Ti d_{z^2} and O1 p_z orbitals are overlapped from the energy levels of −6 eV to −2 eV, which indicates the hybridization of these orbitals in $PbTiO_3$. The vertical dashed line indicates the Fermi level.