Erratum: Ferroelectricity in ultrathin perovskite films [Phys. Rev. B 72, 020101(R) (2005)]

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We have performed calculations at both the theoretical (3.86 Å) and the experimental (3.905 Å) in-plane lattice parameters. We have only reported the rumplings for the experimental in-plane lattice constant, which are about 30% less than those for the theoretical lattice constant. Because the *a* parameter of ferroelectric tetragonal PbTiO₃ is known experimentally to lattice match to cubic SrTiO₃ (common growth substrate), the use of the theoretical in-plane lattice parameter of 3.86 Å (stress-free theoretical conditions) probably best models experiments where PbTiO₃ is freestanding or grown on a bulk SrTiO₃ substrate.

The rumpling parameters in Fig. 1 were transposed—the order from top to bottom should be reversed. The text in the second sentence of the second paragraph on page 2 should read as "As Fig. 1 illustrates, an upward pointing polarization leads to an enhancement of the relative displacements at the top interface, and a reduction at the bottom interface, relative to the interior layers." The next sentence, "This observation is in agreement with previous DFT calculations with external fields.¹²" should be replaced with "This observation differs from a previous DFT calculation with external fields¹² and can be understood from the interfacial chemical bonding mechanism presented below." The main results and the conclusion of the paper are unaffected by the correction.