Supplementary Material for: On the possibility that $PbZrO_3$ not be antiferroelectric

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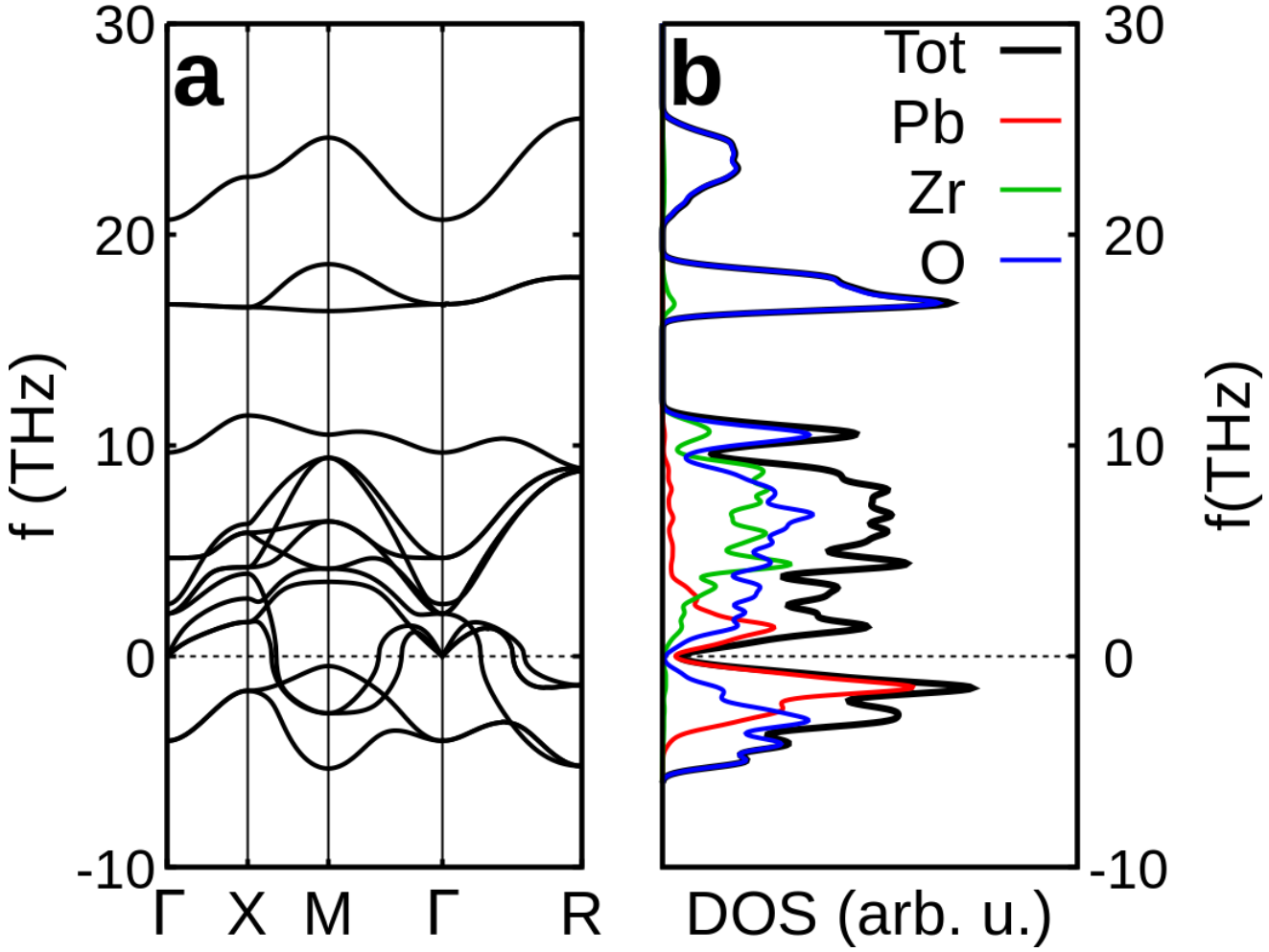
Supplementary Movie 1. Condensation of mode R_4^+ of the FiE state of $PbZrO_3$.
Supplementary Movie 2. Condensation of mode Σ_2 of the FiE state of $PbZrO_3$.
Supplementary Movie 3. Condensation of mode Γ_4^- of the FiE state of $PbZrO_3$.

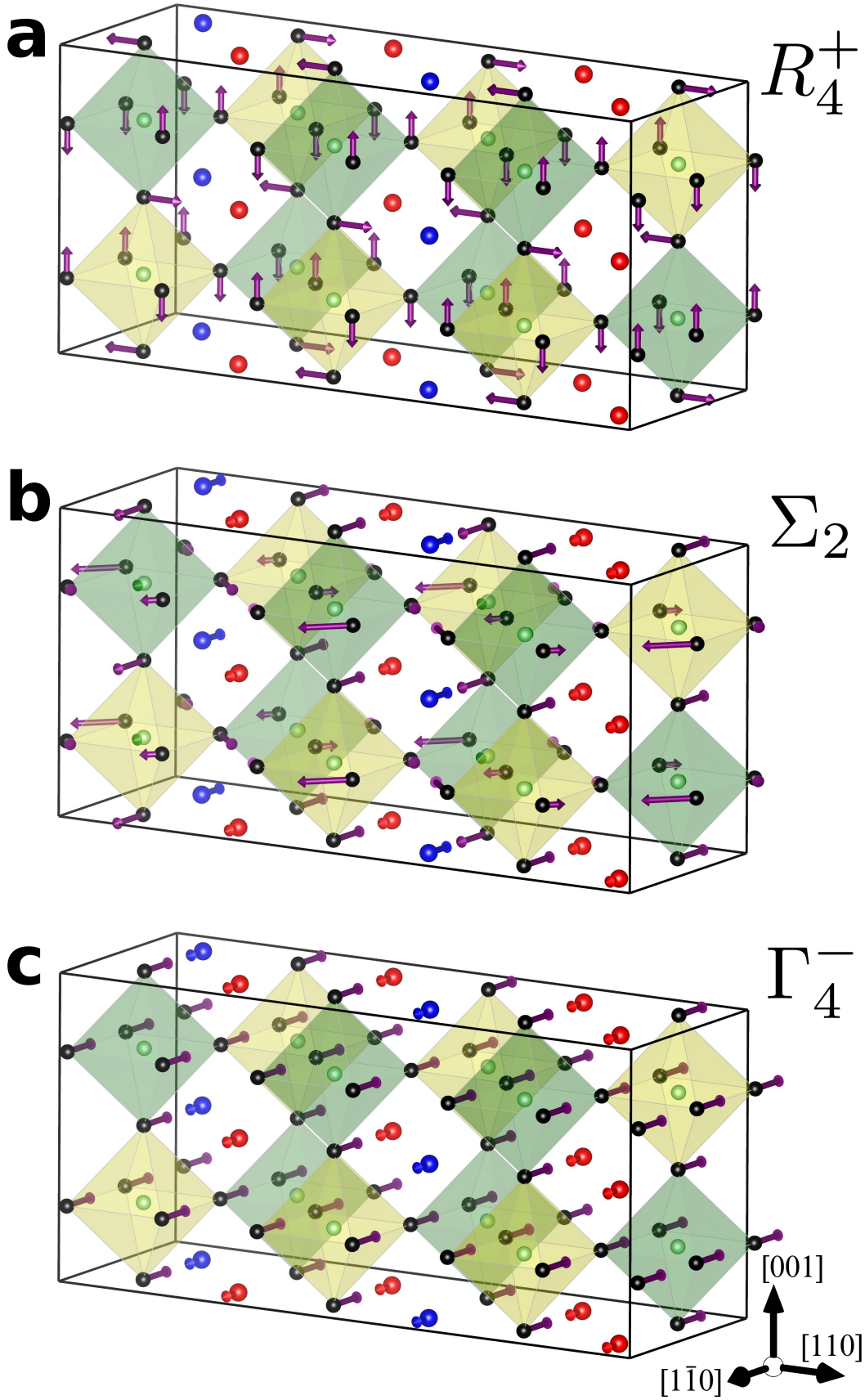


Supplementary Figure 1. Phonon dispersion (a) and phonon density of states (DOS) (b) of the $PbZrO_3$ in the cubic perovskite phase. Large instabilities associated to Pb and O distortions span the whole Brillouin zone and represent a large portion of the DOS.

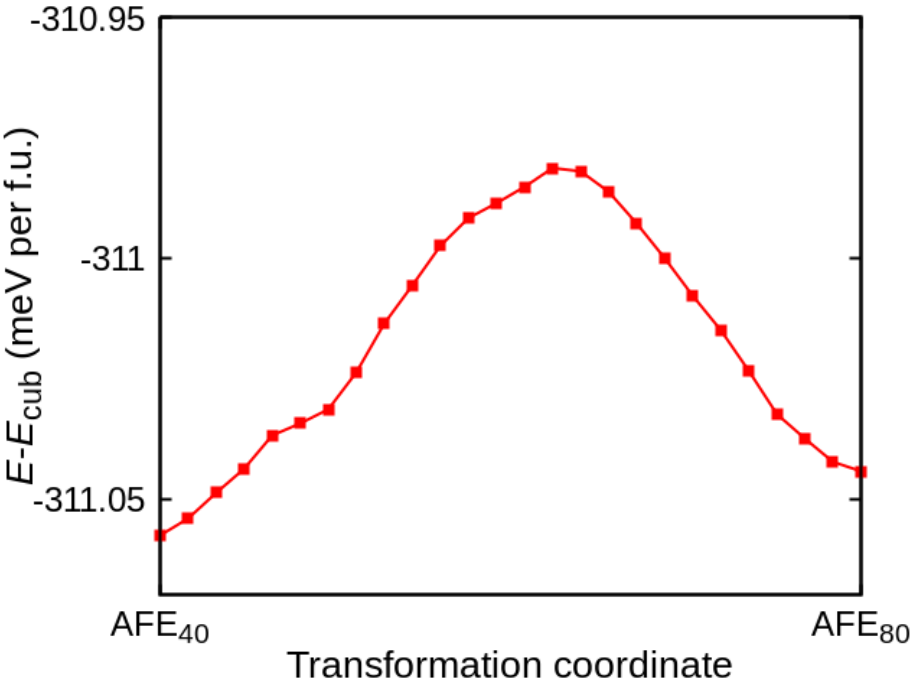
$PbZrO_3$ *Ima*2; a=8.186 Å; b=17.639 Å; c=5.861 Å

Atom	Wyckoff pos.	x	y	z
Pb	4b	0.25000	0.66817	0.71223
Pb	4b	0.25000	0.16782	0.20026
Pb	4b	0.25000	0.00355	0.79090
Zr	8c	0.99986	0.66635	0.23930
Zr	4a	0.00000	0.00000	0.25564
O	4b	0.25000	0.85125	0.79741
O	8c	0.52515	0.23882	0.03876
O	4b	0.25000	0.18836	0.77287
O	4b	0.25000	0.97546	0.20611
O	8c	0.02513	0.08749	0.48474
O	8c	0.54703	0.57921	0.48449

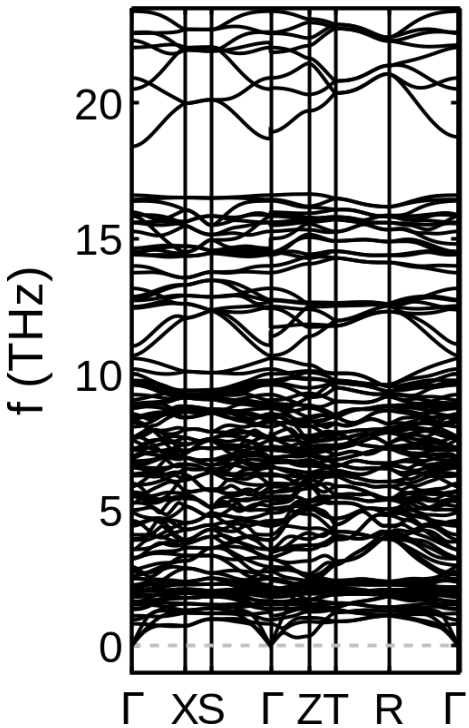
Supplementary Table I. Wyckoff positions of the FiE state of $PbZrO_3$ optimized with PBEsol (see main text).



Supplementary Figure 2. Atomic displacements associated to the three most relevant distortions in the FiE phase of $PbZrO_3$. The cubic perovskite structure is taken as the parent phase. O and Zr atoms are colored in black and green, respectively. The Pb atoms that undergo an upward (downward) distortion are colored in red (blue). The displacements associated to the R_4^+, Σ_2, and Γ_4^- modes are displayed in a, b, and c, respectively. The arrow sizes are proportional to the associated atomic displacements. The arrows in a, b and c have been respectively scaled by a factor of 1.0, 4.0, and 5.0 for visualization purposes.



Supplementary Figure 3. Energy profile along the interpolated path between the AFE_{40} and AFE_{80} phases as obtained with SCAN. Both phases appear as minima of the energy, with a small barrier in between.



Supplementary Figure 4. Phonons of the AFE_{40} phase as obtained with SCAN. The structure presents no instabilities.