Abstract Submitted
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Trilinear couplings and the multi-mode anti-ferroelectric transition of $PbZrO_3$: a first-principles investigation[1] JORGE INIGUEZ[2], ICMAB-CSIC, MASSIMILIANO STENGEL, ICREA and ICMAB-CSIC, SERGEY PROSANDEEV, LAURENT BELLAICHE, University of Arkansas — We have studied ab initio the phase transition in $PbZrO_3$, a perovskite oxide usually presented as the prototypic anti-ferroelectric material. Our work reveals the crucial role that anti-ferrodistortive modes–involving concerted rotations of the oxygen octahedra in the structure–play in the transformation, as they select the observed anti-ferroelectric phase, among competing structural variants, via a cooperative trilinear coupling. The resulting picture is that of a complex transition whose multi-mode character is essential to its very occurrence, and poses the provocative question of whether such an intricate behavior can be taken as representative of anti-ferroelectricity in perovskite oxides.

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