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The Origin of Uni-axial Negative Thermal Expansion in a Layered Perovskite[1] CHRIS ABLITT, Imperial College London, SARAH CRADDOCK, MARK SENN, University of Oxford, ARASH MOSTOFI, NICHOLAS BRISTOWE, Imperial College London — Using first-principles calculations within the quasi-harmonic approximation (QHA), we explain the origin of experimentally observed uni-axial negative thermal expansion (NTE) in a layered perovskite: the Ruddlesden–Popper (RP) oxide Ca_2MnO_4, which has anti-ferromagnetic ordering at low temperatures and is closely related to $Ca_3Mn_2O_7$, which exhibits hybrid improper ferroelectricity and uni-axial NTE in competing phases. Dynamic tilts of MnO_6 octahedra, common in many complex oxides, drive the expansion of the a axis and contraction of the c axis of the tetragonal NTE phase. We find that ferroelastic RP phases with a frozen octahedral rotation are unusually compliant to particular combinations of strains along different axes. The atomic mechanism responsible is characteristic of the perovskite/rock-salt interfaces present in the RP structure. We show that the contribution from this anisotropic elasticity must be taken into account in order to accurately predict NTE over the temperature range observed in experiment. A similar compliance to cooperative strains is found in other systems with uni-axial NTE. The development of this mechanistic understanding of NTE in complex oxides may pave the way for designing tunable multifunctional materials.

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