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Negative Thermal Expansion in the Homologous Series of Ruddlesden-Popper Calcium Titanate NATHAN KOOCHEER, LIANG-FENG HUANG, JAMES RONDINELLI, Northwestern University — Recently, it was predicted that the hybrid-improper ferroelectric compound $\text{Ca}_3\text{Ti}_2\text{O}_7$ ($n = 2$) with the layered Ruddlesden-Popper (RP) structure ($A_{n+1}B_n\text{O}_{3n+1}$) exhibits a pressure-tunable negative thermal expansion (NTE) [Huang *et al.*, Phys. Rev. Lett. **117**, 115901 (2016)]. The NTE is proposed to arise from the quasi-two-dimensional nature of an acoustic mode and strong Ti–O bonding. Here, the effect of layer thickness n on the NTE and thermodynamic properties of the homologous titanates is investigated using the self-consistent quasi-harmonic approximation (SC-QHA) method implemented within density functional theory. We show a significant dependence of the lattice dynamical modes with n , and compare our results and associated microscopic underpinnings of the NTE responses to that proposed for $\text{Ca}_3\text{Ti}_2\text{O}_7$ ($n = 2$). We conclude by describing a model for the anharmonic lattice properties in terms of layer dimensionality.

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