Competing structural instabilities in Ti-based layered-perovskite-oxide superlattices[1] SERGE NAKHMANSON, Argonne National Lab — Utilizing first-principles computational techniques, we have mapped out structural instabilities in the Ruddlesden-Popper homologous oxide superlattice families with a general chemical formula $A_{n-1}A'_2Ti_nO_{3n+1}$, A = Sr, Ba, Pb (perovskite-type block) and A' = Sr (rocksalt-type block), for $n = 1$–5. Our calculations show that each superlattice family has a unique set of "instability footprints" — including the ferroelectric, antiferroelectric and antiferrodistortive types — which may or may not have a strong coupling to epitaxial strain. Furthermore, the existence and strength of structural instabilities within each particular family change dramatically with an increasing number of perovskite-type layers n, granting us wide flexibility to fine-tune the properties of these materials for various device applications or, e.g., for integration into composites with magnetic Ru- or Mn-based layered-perovskite-oxide compounds.

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