

Abstract Submitted
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A unified view of the substitution-dependent antiferrodistortive phase transition in SrTiO₃ ERIC MCCALLA, JEFF WALTER, CHRIS LEIGHTON, University of Minnesota — The cubic-to-tetragonal antiferrodistortive transition at 105 K in the most widely studied perovskite, SrTiO₃, is perhaps the preeminent example of a second-order structural phase transition. Extensive investigations since the 1960's have tracked the softening of the phonon mode associated with this transition, and the interplay with incipient ferroelectricity and superconductivity. Lesser known is that modest ionic substitutions vary the transition temperature (T_a) over a remarkable range in SrTiO₃, from 0 K to above ambient, the trends being difficult to understand based on simple ionic radii or tolerance factor ideas. In addition to providing new data on the thermodynamics of the transition *via* specific heat, we present here the first quantitative rationalization of the trends in T_a with substitution in SrTiO₃. We emphasize the importance of ionic valence mismatch, using bond valence concepts to establish a new parameter, $\langle \varepsilon^4 \rangle$, exhibiting a universal linear dependence with T_a for all known substitutions. This provides the first unified view of the substituent-dependent T_a in SrTiO₃, deepens our understanding of the phase transition (including a theoretical maximum in the rate of T_a suppression), and demonstrates predictive power *via* a simply computed parameter.

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