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Structural investigations and the effect of strain on lead based double perovskites BRIAN ABBETT, CRAIG J. FENNIE, School of Applied and Engineering Physics, Cornell University — The $A_2BB'O_6$ double perovskite structure, in which the B and B' ions are ordered (typically in a rocksalt configuration), provides a versatile platform to realize new properties such as multiferroicity. In particular, compounds with a lone-pair cation on the A-site, such as A=Pb^{2+}, and magnetic B=Co, Mn, and diamagnetic B'= Te, Mo, W, Re, cations have been investigated experimentally, but as of yet none have been found to display ferroelectricity, although several are known to be antiferroelectric. Here we present a first-principles study of the structural and dielectric properties of this family of compounds. We resolve any conflicting reports in the literature as to the ground state structure of compounds and predict the ground state structure when no structural data is available. Additionally, we investigate the effect of epitaxial strain on the structural and magnetic properties.

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