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Magnetoelectric coupling in layered perovskites from first principles TURAN BIROL, CRAIG J. FENNIE, School of Applied and Engineering Physics, Cornell University — The rational design of a multiferroic with a large polarization and a strong coupling between the polarization and the magnetization remains a challenge. Recognizing the limitations of bulk materials, we attempt to design a strongly coupled multiferroic by focusing on artificial layered materials. In particular, strained Sr-Ti-O layered perovskites have recently been shown to have ferroelectric lattice instabilities that can be controlled by altering the effective dimensionality of the layered system. We use a combination of density-functional theory and group theoretical methods to investigate the interplay of magnetization with ferroelectricity when a layer of magnetic transition metal ions are introduced into this highly tunable dielectric superlattice.

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