Modeling functional piezoelectricity in perovskite superlattices with competing instabilities CHARLES SWARTZ, XIFAN WU, Temple University — Multi-component Perovskite Superlattices (SLs) of the form ABO_3, provide a very promising avenue for the design of materials with multifunctional properties. Furthermore the interfaces of such multi-component SLs are home to competing anti-ferrodistortive and ferroelectric instabilities which can produce unexpected functionalities. However, at present first principles calculations exceeding more than 10 units cells, are particularly costly as they scale with the valence electrons as N^3. We present a first-principles modeling technique that allows us to accurately model the piezoelectric strains of paraelectric/ferroelectric SLs, $BaTiO_3/CaTiO_3$ and $PbTiO_3/SrTiO_3$, under a fixed displacement field. The model is based on a maximally localized wannier center layer polarization technique, as well as a truncated cluster expansion, that makes use of the fact that such PE/FE SLs have been shown to have highly localized ionic and electronic interface effects. The prediction of the piezoelectricity for a SL of an arbitrary stacking sequence will be demonstrated. We also use our model to conduct a systemic study of the interface effects on piezoelectric response in the above SLs paying special attention to a strong non-linear effect observed in Bulk $SrTiO_3$.

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