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Structure and Properties Across a Strain-induced Ferri-to-ferroelectric Transition JAMES RONDINELLI, Drexel University, GAOYANG GOU, Xi' an Jiaotong University, China — We identify a first-order, isosymmetric transition between a ferrielectric (FiE) and ferroelectric (FE) state in *A*-site ordered $LaScO_3/BiScO_3$ and $LaInO_3/BiInO_3$ superlattices using density functional calculations. Such a previously unreported ferroic transition is driven by the easy switching of cation displacements without changing the overall polarization direction or crystallographic symmetry. Epitaxial strains less than 2% are predicted to be sufficient to transverse the phase boundary, across which we capture a $\sim$5X increase in electric polarization. In a fashion similar to Pb-based perovskite ceramics with a morphotropic phase boundary (MPB), we predict an electromechanical response up to 102 pC/N in the vicinity of the FiE-FE phase boundary in multidomain materials. The structural origin of the unanticipated piezoelectric enhancement is explained.

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