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Predicting polarization enhancement in multicomponent ferroelectric superlattices SERGE NAKHMANSON, Rutgers University, KARIN RABE, DAVID VANDERBILT — We use ab initio calculations as an input to develop a one-dimensional chain model of the local polarization in epitaxial short-period $CaTiO_3/SrTiO_3/BaTiO_3$ superlattices grown on a $SrTiO_3$ substrate. The model is then combined with a genetic algorithm optimization technique to predict the arrangement of individual $CaTiO_3$, $SrTiO_3$ and $BaTiO_3$ layers in a superlattice that would simultaneously have the highest possible polarization and a low in-plane lattice constant mismatch with the substrate. This modelling procedure can be applied to a wide range of layered perovskite-oxide nanostructures providing guidance for experimental development of nanoelectromechanical devices with substantially improved polar properties.

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