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Enhanced piezoelectricity in PbTiO<sub>3</sub>/BaTiO<sub>3</sub> superlattices VALENTINO R. COOPER, Oak Ridge National Laboratory, KARIN M. RABE, Rutgers University — Short period ferroelectric/ferroelectric PbTiO<sub>3</sub> (PTO)/BaTiO<sub>3</sub> (BTO) superlattices are studied using density functional theory. Contrary to the trends in paraelectric/ferroelectric superlattices the polarization remains nearly constant for PTO concentrations below 50%. In addition, a significant decrease in the c/a ratio below the PTO values is observed. We predict an enhancement in the  $d_{33}$  piezoelectric coefficient peaking at ~75% PTO concentration due to the different polarization-strain coupling in PTO and BTO layers. Further analysis with a superlattice effective Hamiltonian reveals that these trends are bulk properties which are a consequence of the reduced P brought about by the polarization saturation in the BTO layers.

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