Abstract Submitted
for the MAR10 Meeting of
The American Physical Society

Novel interface effect in $CaTiO_3/BaTiO_3$ superlattices XIFAN WU, Princeton University, KARIN M. RABE, DAVID VANDERBILT, Rutgers University — Interfaces are a key focus for tuning the functionality of short-period superlattices. Previous work has shown that an increased density of interfaces normally tends to suppress the ferroelectricity in ferroelectric superlattices, but this is not always the case. Here, we show how suppression of rotational distortions at interfaces can enhance ferroelectricity. We carry out first-principles calculations for $CaTiO_3/BaTiO_3$ superlattices with epitaxial strain favoring the development of a spontaneous polarization along the [001] (out-of-plane) direction, and consider octahedral rotations as well as ferroelectric distortions. The calculations are done as a function of electric displacement field, and both a macroscopic and a local electrostatic analysis is carried out. We find that strong octahedral rotations occur for TiO_6 octahedra sandwiched between CaO layers on both sides, but are strongly suppressed if either neighboring layer is a BaO layer. Due to the resulting enhancement of the ferroelectric instability in these layers, we find that overall the ferroelectric instability of the superlattice is enhanced by the interface. Thus, short-period superlattices in this system have a higher polarization ferroelectricity than longer-period ones of the same average composition, contrary to the general expectation.

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Date submitted: 04 Jan 2010 Electronic form version 1.4