Abstract Submitted
for the MAR09 Meeting of
The American Physical Society

Local polarization discontinuities in perovskite superlattices via compensating heterointerfaces EAMONN MURRAY, DAVID VANDERBILT, Rutgers University — Using first-principles methods, we investigate an approach to the production of multicomponent perovskite superlattices with discontinuities in the layer polarizations. The recent paper of Wu and Vanderbilt[1] demonstrated how 180° domain walls could be formed in a perovskite superlattice through chemical substitution of atoms in the layer at the domain boundary. We examine an alternative approach in which large discontinuities in the local polarization are induced by constructing superlattices out of II-IV and I-V perovskite constituents. The "polar discontinuities" at the heterointerfaces provide compositional charges that approximately cancel the polarization bound charges, thereby allowing stable polarized regions to form. We illustrate the concept via first-principles calculations on $KNbO_3/SrTiO_3$ superlattices. We also show how the Wannier-based definition of layer polarization described by Wu *et al.*[2] may appropriately be applied to a system containing non-neutral layers, and use this to quantitatively examine the local variations in polarization in the $KNbO_3/SrTiO_3$ system.

[1]X. Wu and D. Vanderbilt, Phys. Rev. B. **73**, 020103(R) (2006).
[2]X. Wu *et al.*, Phys. Rev. Lett. **97**, 107602 (2006).

Eamonn Murray
Rutgers University

Date submitted: 19 Nov 2008 Electronic form version 1.4