Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

First-principles study of charge-order-driven ferroelectricity in $LaVO_3/SrVO_3$ superlattices[1] SE YOUNG PARK, Rutgers University, ANIL KUMAR, Los Alamos National Laboratory, KARIN RABE, Rutgers University — We investigate the structure and electronic properties of the 1:1 superlattice composed of $LaVO_3$ and $SrVO_3$ using the density functional theory plus U (DFT+U) method. We find two low-energy antiferromagnetic Mott-insulating phases with distinct charge ordering patterns. In one of these phases, spontaneous polarization normal to the interface is nonzero due to a layered charge-ordering. The polarization calculated by the Berry phase method is 32 $\mu C/cm^2$; we have identified a possible switching path on which the system remains insulating. When fully relaxed, the energy per 5-atom-unit-cell of the polar state is only 3 meV higher than the non-polar state and we find that the energy difference can be reduced to zero by tensile strain. This suggests that that the polar state could be induced by applied electric field, and, depending on the switching process, a ferroelectric hysteresis loop could be observed.

[1]Support: ONR N00014-11-0666

Se Young Park
Rutgers Univ

Date submitted: 06 Nov 2015 Electronic form version 1.4