Abstract Submitted
for the MAR15 Meeting of
The American Physical Society

Epitaxial-strain-induced insulating phase in 1:1 $SrCrO_3$/$SrTiO_3$ superlattices: A first-principles study YUANJUN ZHOU, KARIN RABE, Rutgers University — Using first principles calculations, we studied the structure and electronic properties of the 1:1 superlattice combining the magnetic metallic oxide $SrCrO_3$ and the band insulator $SrTiO_3$. We determined the epitaxial-strain dependent ground-state structures of the superlattice using the "stacking" method. An insulating polar ground state is found when the tensile strain is greater than 2.2%. The insulating character of this phase is related to the $d^1_{xy}d^1_{yz}d^0_{xz}$ orbital ordering of the Cr t_{2g} electrons. Specifically, the 1:1 periodic superlattice structure eliminates the Cr-O-Cr bonds in the direction normal to the interface, which reduces the hopping of 3d electrons in this direction. The band widths of d_{yz} and d_{xz} for Cr are thus significantly reduced, enhancing the effect of the in-plane polar distortions in the $SrCrO_3$ layer responsible for opening the the band gap. The elucidation of this mechanism opens an new approach to band engineering, encouraging further investigations on related metallic/dielectric superlattice systems.

Yuanjun Zhou
Rutgers University

Date submitted: 13 Nov 2014 Electronic form version 1.4