Abstract Submitted
for the MAR15 Meeting of
The American Physical Society

**Interfacial intermixing in $\delta$-doped oxide superlattices**[1] VALENTINO R. COOPER, MSTD, Oak Ridge National Laboratory, HOULONG L. ZHUANG, P. GANESH, CNMS, Oak Ridge National Laboratory, HAIXUAN XU, Department of Materials Science and Engineering, The University of Tennessee, P. R. C. KENT, CNMS and CSMD, Oak Ridge National Laboratory — First principles studies of the interfaces between dissimilar insulating oxides have been fundamental in understanding both the origin of emergent interfacial phenomena and ways to control conduction pathways and charge carrier densities. However, these calculations often assume sharp interfaces; neglecting the effects of interfacial cation intermixing. Using density functional theory, we examine the effect of $A$-site interfacial intermixing on the stability and electronic structure of oxide $\delta$-doped heterointerfaces. We find that the dominant effect of interfacial intermixing is the reduction in carrier densities of the 2DEG states at the interface. Our previous work suggest that this reduction in carrier density (i.e. fractional $\delta$-doping) may lead to enhancements in electron mobilities. These results offer a plausible explanation for the deviations in carrier mobilities and densities measured in different experimental samples. Furthermore, our calculations show that intermixing above 1/4 concentration is unstable relative to a clean interface; thus having implications for large scale production, where experimental growth techniques, such as chemical vapor deposition, may be a viable alternative.

[1]Support from LDRD of ORNL (VRC, HZ, PG, PRCK) and (HX) JDRD of UT and UT/ORNL JIAM. This research used resources of NERSC.

Valentino R. Cooper
Materials Science and Technology Division, Oak Ridge National Laboratory

Date submitted: 12 Nov 2014 Electronic form version 1.4