Abstract Submitted
for the MAR11 Meeting of
The American Physical Society

First Principles Study of Resonant Phonon Coupling across the LSMO / STO Interface KEVIN F. GARRITY, YARON SEGAL, CARLOS A.F. VAZ, JASON D. HOFFMAN, FRED J. WALKER, CHARLES A. AHN, SOHRAB ISMAIL-BEIGI, Yale University — Epitaxial interfaces permit dynamical modification of the properties of a thin film via coupling to the substrate. In particular, the coupling of phonons between two materials allows one to manipulate the atomic structure and vibrational modes near an interface. We use first principles density functional theory (DFT) to study the octahedral oxygen rotations at and across an interface between $La_xSr_{(1-x)}MnO_3$ (LSMO) and $SrTiO_3$. By performing finite temperature Monte Carlo sampling on a classical potential built to reproduce our DFT energetics, we demonstrate that as the $SrTiO_3$ is driven through the phase transition where its octahedral rotations become frozen in place, phonons from the $SrTiO_3$ couple into the interfacial LSMO. These couplings can then modify the LSMO transport properties, as observed in our experiments. The decay length of the phonon coupling into the LSMO agrees with our experimental determinations on this system. We demonstrate that the observed changes in resistance are not due to static changes in the LSMO structure, confirming the phonon coupling.

Kevin F. Garrity
Yale University

Date submitted: 29 Dec 2010 Electronic form version 1.4