Abstract Submitted
for the MAR13 Meeting of
The American Physical Society

Controlling the density of electrons in the 2DEG at complex oxide interfaces[1] CHRIS VAN DE WALLE, LARS BJAALIE, LUKE GORDON, ANDERSON JANOTTI, Materials Department, University of California, Santa Barbara — The formation of a two-dimensional electron gas (2DEG) at the interface between two insulators, $SrTiO_3$ (STO) and $LaAlO_3$ (LAO), has sparked huge interest in oxide electronics. In spite of almost a decade of research, the mechanisms that determine the density of this 2DEG have not yet been unravelled. The polar discontinuity at the STO/LAO interface can in principle sustain an electron density of $3.3\text{x}10^{14}\,\text{cm}^{-2}$ (0.5 electrons per unit cell). However, experimentally observed densities are more than an order of magnitude lower. Using a combination of first-principles and Schrödinger-Poisson simulations we investigate the origin of the electrons in the 2DEG at the STO/LAO interface. We analyze the asymmetric nature of the heterostructures, i.e., the inability to form a second LAO/STO interface that is a mirror image of the first, and the effects of passivation of the LAO surface. Our results apply to oxide interfaces in general, and explain why the $SrTiO_3/GdTiO_3$ interface has been found to exhibit the full density of 0.5 electrons per unit cell.

[1]This work has been supported by the ARO and NSF.

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Date submitted: 09 Nov 2012 Electronic form version 1.4