

Abstract Submitted
for the MAR15 Meeting of
The American Physical Society

Surface charging in $\text{LaAlO}_3/\text{SrTiO}_3$ heterostructures¹ KARTHIK KRISHNASWAMY, CYRUS E. DREYER, ANDERSON JANOTTI, CHRIS G. VAN DE WALLE, University of California, Santa Barbara — The two-dimensional electron gas (2DEG) observed at the interface between LaAlO_3 (LAO) and SrTiO_3 (STO) is known to depend on its proximity to the LAO surface (thickness of LAO) and the conditions to which the surface is exposed. It has been proposed that electrons from the 2DEG can leak to surface states, resulting in a charged surface. Using first-principles calculations, we determine the electronic structure of the LAO surface and the coupling between the surface of LAO and the interface 2DEG. We develop a methodology for treating charged dielectric surfaces and apply it to LAO. This allows for the determination of the 2DEG density as well as the stable surface terminations and reconstructions of LAO on STO as a function of LAO thickness, under any given experimental conditions. Under oxygen-rich conditions, we find an increase in critical thickness required to form the 2DEG, and under hydrogen-rich environment the critical thickness decreases.

¹This work was supported by the LEAST Center (SRC/DARPA) and by ARO.

Karthik Krishnaswamy
Univ of California - Santa Barbara

Date submitted: 13 Nov 2014

Electronic form version 1.4