Abstract Submitted
for the MAR09 Meeting of
The American Physical Society

Oxygen vacancy, charge doping, and polarization screening in
LaAlO$_3$/SrTiO$_3$ interface$^1$ YUN LI, JAEJUN YU, Seoul National University —
A high mobility electron gas has been observed in the $n$-type (TiO$_2$)/(LaO) interface
between two insulators: non-polar SrTiO$_3$ (STO) and polar LaAlO$_3$ (LAO) and the
mechanism of conductivity and dimensionality of electron gas at the interface have
been intensively investigated in various experiments. There are two mechanisms
suggested for the observed conductivity at the interface: electronic reconstruction
and oxygen vacancy. We carried out density-functional-theory calculations to in-
vestigate the distribution of electron carriers for the $n$-type LAO/STO interfaces
with and without oxygen vacancy. When no oxygen vacancy is present, the criti-
cal thickness of LAO film for conducting interface was found to be consistent with
experiments. The induced carrier density at the interface without oxygen vacancy
turns out to be an order of magnitude smaller than the one expected from the elec-
tronic reconstruction. This implies that the lattice polarization takes a significant
role in charge screening. On the other hand, when oxygen vacancies are present, the
vacancy-induced states are found to affect the carrier doping as well as the screening
of polar electric field of LAO film. From the results, we propose that the upper limit
of carrier doping should be 0.375 electrons per unit cell.

$^1$Supported by BK21 FPRD, KOSEF, and KISTI.

Jaejun Yu
Seoul National University

Date submitted: 18 Nov 2008

Electronic form version 1.4