A First Principle Study of LaAlO$_3$/SrTiO$_3$
Heterointerfaces

Hanghui Chen$^1$ and Sohrab Ismail-Beigi$^{1,2}$

$^1$Department of Physics, Yale University, New Haven, Connecticut, 06511, USA
$^2$Department of Applied Physics, Yale University, New Haven, Connecticut, 06511, USA

In order to understand the origin of the intriguing high-mobility quasi two dimensional electron gas formed at LaAlO$_3$/SrTiO$_3$(001) heterointerfaces, we carry out first principle calculations on the electronic structure and properties of complementary interfaces. The intrinsic polar properties are investigated and the average electronic potential increase by each LaAlO$_3$ layer is calculated, which can account for the recent observed fact that the heterointerfaces are not metallic until the number of LaAlO$_3$ layers reaches a critical thickness. When the interface becomes metallic, the spatial distributions of mobile electrons and holes reveal a fundamental asymmetry between the n-type and p-type interfaces. A large cation-cation hopping matrix element which only exists at the n-type interface turns out to be the key reason for this asymmetry.