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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 investigate the distribution of electron carriers for the n-type LAO/STO interfaces with and without oxygen vacancy. When no oxygen vacancy is present, the critical 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 electronic 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.

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