A First Principle Study of $LaAlO_3/SrTiO_3$ Heterointerfaces

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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.