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A First Principle Study of the $LaAlO_3/SrTiO_3$ Heterointerface HANGHUI CHEN, Department of Physics, Yale University, SOHRAB ISMAIL-BEIGI, Department of Applied Physics, Yale University — In order to understand the origin of the intriguing high mobility quasi two dimensional electron gas formed at the $LaAlO_3/SrTiO_3(001)$ heterointerface, we carry out first principle calculations on the electronic structures and properties of complementary interface. 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 experiment fact that the heterointerface is not metallic until the number of $LaAlO_3$ layers reaches a critical value. We also study the effects of different surface terminations of $SrTiO_3$ which surprisingly turn out to influence the electronic structure of the interface and so far have not been focused on in experiments.

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