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Structural Effect of $LaAlO_3/SrTiO_3$ Interface on Electronic Properties: Ab-initio Calculations

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At the interface between two perovskite oxides, observation of two dimensional electron gases (2DEG) was reported. Although $LaAlO_3$ (LAO) and $SrTiO_3$ (STO) are two conventional non-magnetic and insulating materials with wide band gaps, from superconducting to magnetism variety of physical phenomena are leaded by high charge density and high mobility of the 2DEG. In recent years, many theoretical studies have been concentrated to explain the conducting/insulating properties at the interfaces.

In this study, the constriction of unit cells, the movements of each atoms and charge density have been calculated to explain the electrical properties of p-type and n-type interfaces. In particular, quantitative analysis of structural change and charge density induced by different LAO layer thickness.

The LAO/STO structure was modeled for two types; 3 unit cells of LAO on 4 unit cells of STO and 4 unit cells of LAO on 4 unit cells of STO. The $LaAlO_3$ layers built on the $SrTiO_3$ were compressed while $SrTiO_3$ layers were expanded. The oxygen atoms moved to n-type interface and these displacements could contribute the conductivity of n-type interface. The charge density of TiO_2 in 4 unit cells LAO system was higher than the one of TiO_2 in 3 unit cells LAO system.