

Complex oxide interfaces

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The formation of a two-dimensional electron gas (2DEG) at the interface between two insulators, SrTiO₃ (STO) and LaAlO₃ (LAO), has sparked huge interest in oxide electronics. In spite of almost a decade of research, the mechanisms that determine the density of this 2DEG have not yet been unravelled. The polar discontinuity at the STO/LAO interface can in principle sustain an electron density of $3.3 \times 10^{14} \text{ cm}^{-2}$ (0.5 electrons per unit cell). However, experimentally observed densities are more than an order of magnitude lower.

We have investigated the issue using first-principles calculations based on DFT+ U , as well as using a hybrid functional. We have analyzed the nature of the heterostructures, in particular whether it is possible or not to form a second LAO/STO interface that does not act as a sink for electrons.¹ The effects of different terminations of the LAO surface are examined.

Our results apply to oxide interfaces in general, and explain why the SrTiO₃/GdTiO₃(GTO) interface has been found to exhibit the full density of 0.5 electrons per unit cell.² We have also investigated the effects of strain on the band structure of STO,³ with the goal of guiding strain engineering to enhance the mobility in the 2DEG. Explicit first-principles calculations for both STO/LAO and STO/GTO heterostructures will be discussed.

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