Complex oxide interfaces

Chris G. Van de Walle

Materials Department, University of California
Santa Barbara, CA 93106-5050, USA

The formation of a two-dimensional electron gas (2DEG) at the interface between two insulators, $SrTiO_3$ (STO) and $LaAlO_3$ (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 3.3×10^{14} 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 $SrTiO_3$/$GdTiO_3$(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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