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Electronic Reconstruction at oxide interfaces: from an electron-hole bilayer to a spin-polarized 2DEG
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The origin of conductivity at the interface between the band insulators LaAlO_3 and SrTiO_3 has been subject of continued interest and debate. Density functional theory calculations can provide not only insight into the underlying mechanisms but also allow one to identify further parameters to tune the electronic reconstruction in this system in view of device applications. In particular, the potential build up induced by the polarity of the LaAlO_3 film is found to be counteracted by a strong lattice polarization in the LaAlO_3 film. The latter allows the system to remain insulating for the first several LaAlO_3 layers before a crossover to an electronic reconstruction takes place at around 4-5 monolayers (ML). We demonstrate that, owing to a dispersive surface state, an additional SrTiO_3 capping layer can trigger the insulator-to-metal transition already at two ML of LaAlO_3 . As a result, two spatially separated sheets of carriers emerge: electrons at the interface and holes at the surface that are only 1 nm apart and can be used to study excitonic phenomena. Furthermore, we explore the effect of a metallic contact layer on top of the LaAlO_3 film which not only eliminates the potential build up but turns out to be a promising way to enhance the carrier concentration and possibly to realize a spin-polarized electron gas at the interface. Work in collaboration with W.E. Pickett, K. Otte, V. Ruiz López.