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Role of surface defects on the formation of the 2-dimensional electron gas at polar interfaces[1] EMILIO ARTACHO, Nanogune and DIPC, San Sebastián, Spain; Ikerbasque, Bilbao, Spain and Cavendish Lab. University of Cambridge, UK., PABLO AGUADO-PUENTE, CIC nanoGUNE and DIPC, San Sebastián, Spain — The discovery of a 2-dimensional electron gas (2DEG) at the interface between two insulators, $LaAlO_3$ and $SrTiO_3$, has fuelled a great research activity on this and similar systems in the last years. The electronic reconstruction model, typically invoked to explain the formation of the 2DEG, while being intuitive and successful on predicting fundamental aspects of this phenomenon like the critical thickness of $LaAlO_3$, fails to explain many other experimental observations. Oxygen vacancies, on the other hand, are known to dramatically affect the physical behaviour of this system, but their role at the atomic level is far from well understood. Here we perform ab initio simulations in order to assess whether the formation of oxygen vacancies at the surface of the polar material can account for various recent experimental results that defy the current theoretical understanding of these interfaces. We simulate $SrTiO_3/LaAlO_3$ slabs with various concentrations of surface oxygen vacancies and analyze the role of the defects on the formation of the metallic interface, their electrostatic coupling with the 2DEG and the interplay with the different instabilities of the materials involved.

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