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One-Dimensional Electron Gas at the Steps of a LaAlO3-SrTiO3 Interface[1]

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Thin films of $LaAlO_3$ (LAO) epitaxially grown on $SrTiO_3$ (STO) substrates give rise to a two-dimensional electron gas that has spurred lots of interest and activity, given its application possibilities (if, for instance, coupled to any of the many interesting effects displayed by perovskite materials as LAO and STO), and the fundamental questions it poses. The gas originates as a consequence of the polarisation discontinuity at the interface: Although both materials are centrosymmetric, one (STO) belongs to the category of such insulators with zero bulk dielectric polarisation, while LAO is a member of the family that displays half a polarisation quantum along its $\langle 001 \rangle$ direction. The lattice of polarisation values associated to each material allows the prediction of the different polarisation discontinuities for different interface directions. This includes vicinal interfaces, which would be expected to display a structure of terraces of lower index interfaces separated by steps. This enables predicting the effect of steps in the electrostatics across these films, and the possibility of charge carriers being attracted to them. Large-scale first-principles calculations based on density functional theory were performed to substantiate such predictions, allowing to expect the formation of one-dimensional electron gases associated to steps at well-chosen interfaces of the two materials. Such gases should prove to be of fundamental interest since they are expected to show highly correlated electron carriers. The polarisation analysis and the results of the calculations will be presented along related and supporting results.

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