Density-Functional Study of the Two-Dimensional Electron Gas at the Perovskite Titanate Interface

RANJIT NANDA, ZORAN POPOVIC, SUNITA THULASI, SASHI SATPATHY, University of Missouri — Oxide superlattices and microstructures hold the promise for creating a new class of devices with unprecedented functionalities. Density-functional studies\(^1\) of the recently fabricated, lattice-matched perovskite titanates\(^2\) \((\text{SrTiO}_3)_n/(\text{LaTiO}_3)_m\) reveal a classic wedge-shaped potential well for the monolayer structure, originating from the Coulomb potential of a charged La sheet. The potential in turn confines the electrons in the Airy-function-localized states. This resulting two-dimensional electron gas may be described in terms of the simplified jellium model\(^3\) and it describes reasonably well the observed charge modulation of the Ti atoms near the interface. Concerning magnetism, it is suppressed for the monolayer LaTiO\(_3\) structure, while in structures with a thicker LaTiO\(_3\) part, bulk antiferromagnetism is recovered, with a narrow transition region separating the magnetic LaTiO\(_3\) and the non-magnetic SrTiO\(_3\).

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