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Density-Functional Study of the Two-Dimensional Electron Gas at the Perovskite Titanate Interface[1] 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] $(SrTiO_3)_n/(LaTiO_3)_m$ 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 $SrTiO_3$. 1. Z. S. Popovic and S. Satpathy, Phys. Rev. Lett. 94, 176805 (2005) 2. A. Ohtomo et al., Nature 419, 378 (2002) 3. S. Thulasi and S. Satpathy, Phys. Rev. B (2006)

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