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First-principles modeling of titanate/ruthenate superlattices[1]

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The possibility to create highly confined two-dimensional electron gases (2DEG) at oxide interfaces has generated much excitement during the last few years. The most widely studied system is the 2DEG formed at the LaO/TiO_2 polar interface between $LaAlO_3$ and $SrTiO_3$, where the polar catastrophe at the interface has been invoked as the driving force. More recently, partial or complete delta doping of the Sr or Ti cations at a single layer of a $SrTiO_3$ matrix has also been used to generate 2DEG. Following this recipe, we report first principles characterization of the structural and electronic properties of $(SrTiO_3)_5/(SrRuO_3)_1$ superlattices, where all the Ti of a given layer have been replaced by Ru. We show that the system exhibits a spin-polarized two-dimensional electron gas extremely confined to the $4d$ orbitals of Ru in the $SrRuO_3$ layer, a fact that is independent of the level of correlation included in the simulations. For hybrid functionals or LDA+U, every interface in the superlattice behaves as minority-spin half-metal ferromagnet, with a magnetic moment of $\mu = 2.0\ \mu_B/SrRuO_3$ unit. The shape of the electronic density of states, half metallicity and magnetism are explained in terms of a simplified tight-binding model, considering only the t_{2g} orbitals plus (i) the bi-dimensionality of the system, and (ii) strong electron correlations. Possible applications are discussed, from their eventual role in thermoelectric applications to the possible tuning of ferromagnetic properties of the 2DEG with the polarization of the dielectric. Work done in collaboration with P. García, M. Verissimo-Alves, D. I. Bilc, and Ph. Ghosez.

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