

Highly-confined spin-polarized two-dimensional electron gas in SrTiO₃/SrRuO₃ superlattices

P. Garcia-Fernandez¹, M. Verissimo-Alves¹, D.I. Bilc², P. Ghosez² and J. Junquera¹

¹Departamento de Ciencias de la Tierra y Física de la Materia Condensada, Universidad de Cantabria, Cantabria Campus Internacional, Avenida de los Castros s/n, 39005, Santander, Spain

²Physique Theorique des Materiaux, Universite de Liege, Allee du 6 aout 17 (B5), B-4000, Sart Tilman, Belgium

garcia@unican.es

We report first principles characterization of the structural and electronic properties of (SrTiO₃)₅/(SrRuO₃)₁ superlattices. We show that the system exhibits a spin-polarized two-dimensional electron gas extremely confined to the 4*d* orbitals of Ru in the SrRuO₃ layer. Every interface in the superlattice behaves as minority-spin half-metal ferromagnet, with a magnetic moment of $\mu = 2.0 \mu_B/\text{SrRuO}_3$ 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. As a result we find that the half-filled degenerate Ru(dxz,dyz) bands participating at the Fermi energy have strong bonds only along one-direction and so display characteristics of even lower dimensionality. Finally we study the consequences of this particular electronic structure over the transport properties, particularly thermoelectric ones, by using Boltzmann's transport theory.