Orbital and electronic reconstructions at surfaces and interfaces of transition metal oxides

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Electron occupancy of 3d-orbitals of transition metal is determined by the total number of electrons in the 3d shell and by the energies of the five 3d orbitals. At free surfaces or interfaces between dissimilar oxides in epitaxial heterostructures, there is an inherent breaking of symmetry that may produce changes of electronic orbitals positions and subsequently, promote charge redistribution that may ultimately lead to emerging properties. It has been shown, for instance, that interface-mediated tensile strain acting on the 3d-orbitals of regular octahedrally-coordinated metal ions, such as $3d^4$-Mn^{3+}, breaks the degeneracy of x^2-y^2 and $3z^2$-r^2 states favoring electron filling of in-plane x^2-y^2 orbitals subsequently determining the orbital and magnetic ordering. It has also been shown, that at the interface between robust band insulators, such as $LaAlO_3$ and $SrTiO_3$, there is a charge transfer towards the empty Ti-3d orbitals leading to the formation of 2D electron system of high mobility and even superconducting behavior.

In this presentation we will report on recent results addressing the physics affecting to electronic occupancy at free surfaces of oxides and the electronic reconstructions occurring at the interfaces of uncommon (110) and (111) planes of $SrTiO_3$ and several large band gap oxides.

We will first address the free surfaces of transition oxide thin films. It will be show that the symmetry breaking at the free surfaces of transition metal oxides produces a preferential occupation of out-of-plane $3z^2$-r^2 that add or combine with any existing strain effect to determine the electronic properties of these surfaces. Therefore, from catalytic activity to surface magnetic anisotropy, surface properties can be tailored at wish.

Next, we will address the occurrence of electronic reconstructions at the interface between (110) and (111) $SrTiO_3$ single crystals and several oxides. It will be show that, under the appropriate conditions, a highly mobile 2D gas can be obtained. Interestingly enough, this achievement does not require crystalline interfaces but amorphous capping layer can also be used [2]. These findings may not only contribute to disclose the ultimate origin of these charge redistribution but also to pave the way to integrate these oxides on silicon platforms.

[1] D. Pesquera, G. Herranz, A. Barla, E. Pellegrin, F. Bondino, E. Magnano, F. Sánchez, J. Fontcuberta, Nat. Commun. 3, 1189 (2012)

[2] G. Herranz, F. Sánchez, N. Dix, M. Scigaj & J. Fontcuberta, Scientific Reports 2, 758 (2012)