Electronic properties of oxide interfaces: the effect of oxygen vacancies and cation intermixing

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Thin films of $LaAlO_3$ (LAO) grown over $SrTiO_3$ (STO) in the (001) direction present a two dimensional electron gas in one of the possible interfaces. In some cases, this system also shows ferromagnetism and superconductivity.
On the other hand, thin films of TiO_2 in the anatase structure grown over both LAO and STO present room temperature ferromagnetism, sometimes even without magnetic impurities.

The interfaces TiO_2/LaO and TiO_2/AlO_2 are the same in both systems although the total crystallographic structure of the slabs is different. In both cases the former interface is the lowest in energy when there are no defects but if the interface has oxygen vacancies, the electrostatic force increases the cohesion and makes them comparable.

Our ab-initio calculations show that the TiO_2/AlO_2 interface with vacancies can be either insulating or metallic, depending on the optimum stacking for each heterostructure. In fact, the ground state can have the interfacial Ti atoms located either at hollow or bridge sites of the AlO_2 surface plane and this geometrical property is what determines the electronic character of the interface. In addition, cation inter-diffusion along with oxygen vacancies, increases the size of the band gap in the insulating case or even opens up a gap in the metallic one.