Electronic properties of a 2D electron gas at the interface between complex transition metal oxides

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For the paradigmatic oxide heterostructure with $LaAlO_3$ (LAO) thin films grown on $SrTiO_3$ (STO) substrates, distinct electronic phases have been extensively characterized at the LAO/STO interface: for LAO films with more than three layers and LaO termination towards the TiO_2 interface, a metallic state is formed in the STO layers next to the interface which becomes superconducting below a temperature scale of 300 mK [1, 2]. Strikingly, the superconducting state coexists with a magnetic state possibly formed in patches of an inhomogeneous interface state. The magnetism appears to be stable up to the room temperature but its origin has not been settled. It may be well related to oxygen vacancies which lead to an orbital reconstruction of nearby Ti-sites and generate a local triplet state [3].

In our work by means of *ab-initio* calculations within GGA+*U* approach we performed a systematic variation of the values of the Coulomb parameters applied to the Ti 3*d* and La 4*f* orbitals [4]. We put previous suggestions to include a large value for the La 4*f* states into perspective in order to shift levels to the higher energy and avoid spurious mixing of La 5*d* and 4*f* states. Our calculations provide deeper insight into the band gap landscape in the space spanned by these Coulomb parameters and the resulting complex interference effects. In addition, we identify important correlations between the local Coulomb interaction within the La 4*f* shell, the band gap, and the atomic displacements at the interface.

We demonstrated an impact of electron-donor defects (H-adatom, O-vacancy and also H-adatom+O-vacancy) in different concentration and located in different layers of LAO and STO slabs separately and in the heterostructure on the structural and electronic properties. We have shown that surface adsorbates shift the Fermi-level to the higher energy, which leads to a insulator-metal transition in a STO slab and in the LAO/STO heterostructure with three LAO overlayers, whereas a LAO slab undergoes a transition from semiconductor to insulator state. We addressed the defect profiles through the entire heterostructure and reconsider orbital reconstruction of the Ti 3*d* states.

As a continuation of the study of complex oxides we extended our research to pairs of manganites and ferroelectric compounds.

References

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