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Ab initio study of TiO₂/LaAlO₃ interfaces

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Abstract – We calculate the electronic structure and magnetism of the interface between two non-magnetic oxides: TiO₂ anatase and LaAlO₃ (LAO), concentrating on the role played by structural relaxation and oxygen vacancies. LAO has a layered structure along the epitaxial (001) direction with alternating LaO and AlO₂ planes. Using Density Functional Theory, we search for magnetic solutions, as magnetism has been unexpectedly found in undoped TiO₂ films grown on LAO. Our results show that the interface LaO/TiO₂ is favored compared to the AlO₂/TiO₂ one when there are no oxygen vacancies whereas the contrary happens when there are oxygen vacancies. In both cases, the cohesive energy is of the same order of magnitude but only the AlO₂/TiO₂ interface has stable magnetic solutions, depending on the vacancy location and structure.

Room-temperature ferromagnetism has been observed in both doped and undoped insulating oxide thin films such as TiO₂, ZnO and HfO₂ grown over other oxides or semiconductors [1,2]. This magnetic order can be weak and the determination of its intrinsic character may require complementary, independent and careful techniques to be probed. Many authors have attributed an important role to oxygen vacancies and other defects to produce this magnetic ordering [2], but the effect of the substrate or the interface has not been taken into account in the interpretations. In this work we explore the possibility of observing magnetism at the interface formed when a simple oxide such as anatase TiO₂ grows epitaxially on LAO. As it is not clear if the substrate surface is mostly composed of LaO or AlO₂ planes, we consider both possibilities. The existence of oxygen vacancies is related to the finding of Ti⁺³ and Ti⁺² ions in these films by XPS experiments [3] and a larger vacancy concentration has been found to increase the magnitude of the magnetization [2].

As in previous work on bulk oxides [4], we have used the Wien2k code to model the TiO₂/LAO interface. We do this by performing calculations for superlattices ...TiO₂/LAO/ TiO₂/LAO... for the different types of interfaces. The total energies of the relaxed structures indicate that oxygen vacancies at the TiO₂ plane are preferred compared to those at any of the LAO planes. Magnetic solutions are stable for some oxygen deficient interfaces, depending on their structure and vacancy concentration. Our calculations show that the position of atoms close to the interface is critical: not only first but also further neighbors determine if an interface will be magnetic or not.

References

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