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Oxygen vacancies and magnetism at titanate interfaces[1]

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Breaking the translation or inversion symmetry at surfaces and interfaces may lead to the formation of new charge, spin and orbital electronic states which are different than the bulk states. The emergence of these states is particularly relevant for oxides where the balance of competing interactions and the resulting stable electronic phase crucially depend on the local oxidation state near the interface. A prominent example is the interface of $LaAlO_3$/$SrTiO_3$ (LAO/STO), which exhibits a two-dimensional electron liquid state in the structures with $LaAlO_3$-layers more than 4uc thick, and undergoes a transition into a superconducting state below 0.2 K. Depending on growth conditions LAO/STO has also been found to display pronounced magnetotransport effects indicating the existence of local moments. Recently, even a coexistence of ferromagnetism and superconductivity has been reported, possibly due to an electronic phase separation within the interface. We analyze the magnetic state at the LAO/STO interface within density functional theory and provide evidence that it is caused by the spin polarization of Ti 3d interface electrons. The magnetic state depends strongly on the oxidation state of the interfaces. We show that oxygen vacancies at titanate interfaces induce a complex multiorbital reconstruction which involves a lowering of the local symmetry and an inversion of t_{2g} and e_g orbitals resulting in the occupation of the e_g orbitals of Ti atoms neighboring the O vacancy. In contrast to stoichiometric nonmagnetic interfaces of $LaAlO_3$ and $SrTiO_3$, the vacancy-induced orbital reconstruction at LAO/STO interfaces generates a two-dimensional interface magnetic state not observed in bulk $SrTiO_3$. We demonstrate that oxygen vacancies in the TiO_2 interface layer enhance the tendency for ferromagetism considerably. This allows for the notion that areas with increased density of oxygen vacancies produce ferromagnetic puddles and account for the previous observation of a superparamagnetic behavior in the superconducting state. Using generalized gradient approximation (LSDA) with intra-atomic Coulomb repulsion (GGA+U), we find that this magnetic state is common for titanate surfaces and interfaces.

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