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Correlation driven charge order at $LaAlO_3/SrTiO_3$ and $LaTiO_3/SrTiO_3$ Interfaces

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Correlated behavior at complex oxide interfaces offers additional degrees of freedom to compensate charge imbalance not available *e.g.* in polar semiconductor heterostructures. This can result in electronic, charge and magnetic phases that do not exist in the bulk and offers new possibilities for device applications. For instance, the interfaces of LaTiO3 and SrTiO3 [1] as well as LaAlO3 and SrTiO3 [2] show metallic conductivity, although the respective bulk materials are Mott (LTO) and band insulating (STO, LAO). Here we present the results of material-specific correlated band theory (LDA+U) employing the FP-LAPW code in the WIEN2k implementation for a variety of (n,m) multilayers containing n LTO (or LAO) and m STO-layers. To explore the relaxation length towards bulk behavior n and m is varied between 1 and 9. We find that charge mismatch at the LTO/STO IF is accommodated by the formation of a charge and orbitally ordered (CO/OO) layer with a checkerboard arrangement of Ti^{3+} and Ti^{4+} and an antiferromagnetic coupling of the Ti^{3+}-spins [3]. Lattice relaxations lead to the observed conducting behavior. An analogous diluted layer of Ti^{3+}spins is obtained for the n-type LAO/STO interface, although the corresponding bulk materials are nonmagnetic. For a structurally ideal p-type LAO/STO IF the measured insulating behavior can only be understood by a charge disproportionation on the oxygen sublattice and the formation of a CO/OO magnetic OPπ hole. Alternatively, charge compensation by oxygen vacancies and the formation of a charge conjugate F-center is considered. [1] A. Ohtomo, and H.Y. Hwang, Nature **423**, 378 (2002). [2] A. Ohtomo, D.A. Muller, J.L. Grazul, and H.Y. Hwang, Nature **419**, 378 (2002). [3] R. Pentcheva and W.E. Pickett, cond-mat/0608212. [4] R. Pentcheva and W.E. Pickett, Phys. Rev. B **74**, 035112 (2006).