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Stabilization mechanisms at $LaXO_3/SrTiO_3$ (X=Ti, Al, V) Heterointerfaces[1] R. PENTCHEVA, University of Munich, W. PICKETT, University of California Davis — Multivalent transition metal ions that are being incorporated into oxide heterointerfaces offer more degrees of freedom to compensate the charge imbalance at the interface than is the case for conventional semiconductor interfaces. Density-functional theory calculations including a Hubbard U (LDA+U) have shown that a charge and orbitally ordered layer of Ti^{3+} and Ti^{4+} is formed at the interface (IF) between the Mott and the band insulator $LaTiO_3$ (d^1) and $SrTiO_3$ (d^0) [Phys. Rev. Lett. 99, 016802 (2007)] as well as between the two band insulators $LaAlO_3$ and $SrTiO_3$ [Phys. Rev. B. 74, 035112 (2006)]. Additional complexity relating to charge state and orbital occupation arises at the $LaVO_3/SrTiO_3$ interface between these compounds that are d^2 and d^0 respectively in the bulk: the electron-doped ...-TiO_2-LaO-... IF may promote a Ti^{3+} charge state, the hole-doped ...-SrO-VO_2-... IF may encourage a V^{4+} ion, or a metallic IF may result. We will present LDA+U predictions of charge states, orbital and spin order, and conducting behavior at these heterointerfaces, and contrast the results with the $d^1 - d^0$ and $d^0 - d^0$ interfaces mentioned above.

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