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Electronic and magnetic properties of two-dimensional electron gas formed at $LaAlO_3/SrTiO_3$ and $LaTiO_3/SrTiO_3$ interfaces[1] KAROLINA JANICKA, JULIAN VELEV, EVGENY TSYMBAL, Department of Physics and Astronomy, University of Nebraska-Lincoln, Lincoln, Nebraska, USA — We perform first-principles electronic structure calculations to elucidate the electronic and magnetic properties of $LaAlO_3/SrTiO_3$ and $LaTiO_3/SrTiO_3$superlattices. We find that TiO_2-terminated interfaces are n-type conducting which is consistent with experimental observations. In both heterostructures we find that charge resides in Ti conduction band and is localized within a few nanometers from the interface. This charge distribution is consistent with metal induced gap states in the gap of $SrTiO_3$ produced by the interfacial charge. In order to understand the magnetism of these oxide heterostructures, we performed spin-polarized calculations which reveal that this interface in a $(LaAlO_3)_3/(SrTiO_3)_3$ superlattice is magnetic with magnetic moment on the Ti^{3+} atom of $0.2\mu_B$. For thicker $SrTiO_3$ layers the magnetism decreases and eventually disappears because the electron gas spreads over more than one unit cell making the electron delocalized and violating the Stoner criterion for magnetism. The inclusion of electron correlations via the LDA+U approximation with U=5eV on Ti atoms makes the two-dimensional electron gas more localized and half-metallic and strengthens the interface magnetization.

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