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High-carrier-density phase in $LaTiO_3/SrTiO_3$ superlattices[1] SE YOUNG PARK, KARIN RABE, Rutgers University, ANDREW MILLIS, Columbia University — We investigate superlattices composed of alternating layers of Mott insulating $LaTiO_3$ and band insulating $SrTiO_3$ from first principles, using the density functional theory plus U (DFT+U) method. For values of U above a critical threshold, we find that melting of the Mott-insulating phase can extend from the interface into the $LaTiO_3$ layer, resulting in a sheet carrier density exceeding the density of 0.5 electrons per in-plane unit cell found in previous studies. The critical U for the melting transition is larger than the critical Coulomb correlation required for the insulating $LaTiO_3$, suggesting the existence of a high sheet carrier density phase in $LaTiO_3/SrTiO_3$ superlattices. The effects of in-plane strain and varying layer thickness on the melting transition are discussed. For insulating superlattices, we study the strain and thickness dependence of the polarization and its relation to near-interface local atomic distortions.

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