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Confinement induced metal-to-insulator transition in strained $LaNiO_3/LaAlO_3$ superlattices[1] ARIADNA BLANCA ROMERO, Ludwig Maximilians University Munich, Germany, ROSSITZA PENTCHEVA, Ludwig Maximilians University Munich — Using density functional theory calculations including a Hubbard U term we explore the effect of strain and confinement on the electronic ground state of superlattices containing the band insulator $LaAlO_3$ and the correlated metal $LaNiO_3$. Besides a suppression of holes at the apical oxygen, a central feature is the asymmetric response to strain in single unit cell superlattices: For tensile strain a band gap opens due to charge disproportionation at the Ni sites with two distinct magnetic moments of $1.45\mu_B$ and $0.71\mu_B$. Under compressive stain, charge disproportionation is nearly quenched and the band gap collapses due to overlap of $d_{3z^2-r^2}$ bands through a semimetallic state. This asymmetry in the electronic behavior is associated with the difference in octahedral distortions and rotations under tensile and compressive strain. The ligand hole density and the metallic state are quickly restored with increasing thickness of the $(LaAlO_3)_n/(LaNiO_3)_n$ superlattice from $n = 1$ to $n = 3$.

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