

Abstract Submitted
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Designing a Spin-one Mott Insulator: Complete Charge Transfer in Nickelate-Titanate Heterostructures¹ HANGHUI CHEN, Department of Physics, Columbia University, CHRIS MARIANETTI, Department of Applied Physics and Applied Math, ANDREW MILLIS, Department of Physics, Columbia University — *Ab initio* calculations are performed to show that complete charge transfer may occur from the TiO₂ to the NiO₂ layers in (LaTiO₃)₁/(LaNiO₃)₁ superlattices. Although the two component materials are an $S = 1/2$ Mott insulator and a weakly correlated paramagnetic metal, strong correlation effects on Ni d states can render the superlattice an unusual $S = 1$ charge transfer insulator, with the Ti- d band empty, the Ni in the d^8 state and the oxygen bands filled. The charge transfer gap is set by the Ti/Ni d level splitting. Magnetic, photoemission and x-ray scattering experiments are suggested to test the theory. The results show that heterostructuring can lead to very high levels of electron doping of oxides.

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