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Electronic structure, charge modulation, and orbital polarization of LaNiO3/SrTiO3 superlattice[1] MYUNG JOON HAN, MICHEL VAN VEENENDAAL, Argonne National Lab and Northern Illinois University — First-principles density functional theory calculations have been performed to understand the detailed electronic structure for the various (m, n) combinations of (LaNiO3)m/(SrTiO3)n superlattices. Due to the strong covalency of Ni-O bonds, the valence bands are dominated by Ni-d character and the electronic structure is mainly affected by the local environment rather than the ionic potential. Heterostructuring-induced quantum states and the interaction between them leads to the charge redistribution around the Fermi level, which may be responsible for the charge modulation and metal-insulator transition observed in the related systems.

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Myung Joon Han
Argonne National Lab and Northern Illinois University

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