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Lattice instabilities suppress cuprate-like Fermi surfaces in oxide heterostructures JAMES RONDINELLI, NICOLA SPALDIN, UC Santa Barbara — Progress in the layer-by-layer growth of transition metal oxide films motivated the intriguing recent suggestion that oxide heterostructures could be engineered to have band structures close to those of the high- T_c cuprates. Although theoretical candidate materials have been identified, experimental realization has not yet been achieved. In this work, using first-principles density functional theory calculations, we explore the Fermi surface behavior of thin layers of metallic, orbitally degenerate, d^4 SrFeO₃ confined between the d^0 dielectric SrTiO₃ in a superlattice geometry. We show that the conventional heteroepitaxial constraint, which requires the film and substrate to have identical in-plane lattice constants, splits the electronic degeneracy and combines with the two-dimensionality of the superlattice to produce a metallic cuprate-like band structure. We find, however, that the band structure is drastically changed by the existence of lattice instabilities which occur in the superlattice, yet are stable in each bulk component. We show that these enhanced electron-lattice instabilities are strongly sensitive to the superlattice periodicity and compete with the formation of a cuprate-like Fermi surface. We suggest our results provide a plausible explanation for the absence of metallic behavior in ultra-thin orbitally degenerate oxide superlattices that are predicted to be superconducting.

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