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Quantitative measurements and modeling of electronic and atomic surface structure in epitaxial $LaNiO_3$ thin films by ARPES, LEED-I(V), and DFT+DMFT JACOB RUF, ELIZABETH NOWADNICK, Cornell University, HYOWON PARK, Columbia University, PHILIP KING, Cornell University, ANDREW MILLIS, Columbia University, DARRELL SCHLOM, KYLE SHEN, Cornell University — Careful exploration of the phase space available for artificially engineering emergent electronic properties in epitaxial thin films and superlattices of transition-metal oxides requires close feedback between materials synthesis, experimental characterization of both electronic and atomic structures, and modeling based on advanced computational methods. Here we apply this general strategy to the perovskite rare-earth nickelate $LaNiO_3$, using molecular-beam epitaxy to synthesize thin films, performing *in situ* angle-resolved photoemission spectroscopy (ARPES) and low-energy electron diffraction (LEED) measurements, and comparing our results with the predictions of density functional theory plus dynamical mean-field theory (DFT+DMFT). Our study establishes $LaNiO_3$ as a moderately correlated metal in which the quasiparticle mass enhancement can be modeled with quantitative accuracy by DFT+DMFT. Finally, in view of efforts to produce e_g orbital polarization in nickelate heterostructures as a means of mimicking single-band cuprate-like physics, we discuss the extent to which our ARPES and LEED results suggest that such effects are intrinsically present at film surfaces due to the existence of polar distortions, as reported by coherent Bragg rod analysis of surface x-ray diffraction.

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