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Realistic DMFT calculations for nickelate superlattices M.J. HAN, Columbia University, XIN WANG, University of Maryland, CHRIS A. MARIANETTI, ANDREW J. MILLIS, Columbia University — We present phase diagram, photo-emission and RIXS (resonant inelastic X-ray scattering) spectra, orbital polarization, and Fermi surface plots for LaNiO3/LaXO3 superlattice (X=Al, Ga,...) obtained from DMFT (dynamical mean-field theory) calculation based on a realistic multi-band tight-binding model derived from DFT (density functional theory) calculations and in particular including oxygen orbitals. Our results indicate that heterostructuring is unlikely to produce one band model physics and point toward a new view of metal-insulator transition of this system. This work is supported by ARO via grant No. W911NF0910345-56032PH.

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