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Quantifying the

electronic reconstruction in LaTiO₃/LaNiO₃/(LaAlO₃)₃ heterostructures using RIXS¹ GILBERTO FABBRIS, Brookhaven Natl Lab, ANKIT S. DISA, SO-HAB ISMAIL-BEIGI, FREDERICK J. WALKER, CHARLES H. AHN, Yale University, JONATHAN PELLICIARI, YAOBO HUANG, THORSTEN SCHMITT, Swiss Light Source, PSI, LEI XU, LIVIU HOZOI, JEROEN VAN DEN BRINK, IFW Dresden, MARK DEAN, Brookhaven Natl Lab — A novel approach for manipulating the 3d state in transition metal oxide heterostructures has emerged with the growth of trilayer nickelate LaTiO₃/LaNiO₃/(LaAlO₃)₃ (LTNAO) (Disa et al., PRL 114 026801 (2015)). This heterostructure induces a striking reconstruction of the LaNiO₃ electronic structure, which is due to a combination of charge transfer from Ti's 3d state and octahedral elongation along the c axis. We use resonant inelastic x-ray scattering (RIXS) experiments at Ni L_{2.3} and O K edges to spectroscopically resolve the LTNAO electronic structure. Surprisingly, our results show that the octahedral elongation generates minor changes in crystal fields at Ni's 3d state compared to bulk LaNiO₃. Instead, heterostructuring creates an anisotropic reconstruction of the Ni 3d - O 2p hybridization. The x^2 - y^2 orbital is significantly more hybridized with O p, leading to a $3z^2-r^2/x^2-y^2$ hole ratio of ~ 0.55 and large orbital polarization as measured by x-ray absorption spectroscopy. This work establishes RIXS as an ultra-sensitive probe of complex oxide heterostructures.

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