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Orbital Reflectometry and the Electronic Structure of Oxide Interfaces

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The occupation of d -orbitals has a key influence on the physical properties of transition-metal (TM) oxides.¹ Due to the strong hybridization with neighboring oxygen ions, the electronic structure is very sensitive to changes in the TM-oxygen bond distances induced by strain and/or by the chemical bonding to other ions with different electronic configuration. Both effects might be important in oxide heterostructures,² but thus far it has been difficult to probe atomic-scale modulations of the orbital occupation in a quantitative manner.³ We present results from polarized soft x-ray resonant reflectivity, which demonstrate that it is possible to derive quantitative, spatially resolved orbital polarization profiles. We show that this method is sensitive enough to resolve differences of $\sim 3\%$ in the occupation of Ni e_g orbitals in adjacent atomic layers of a LaNiO₃-LaAlO₃ superlattice, and the experimental findings are in good agreement with electronic-structure calculations. The possibility to quantitatively correlate theory and experiment on the atomic scale opens up new perspectives for orbital physics in oxide heterostructures.

¹Tokura, Y. & Nagaosa, N. *Science* **288**, 462-468 (2000).

²Han, M. J., Marianetti, C. A. & Millis, A. J. *Phys. Rev. B* **82**, 134408 (2010).

³Chakhalian, J. *et al.* *Science* **318**, 1114-1117 (2007).