

Using Resonant X-ray Reflectometry to Study Orbital Degrees of Freedom in Oxide Heterostructures

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Orbital degrees of freedom make transition-metal oxides (TMOs) particularly prone to dimensionality effects since the occupation of the five d-orbitals delicately depends on the electronic surroundings of individual TM atoms. This occupation can be tuned away from its balance in the bulk by breaking certain symmetries: For instance, the deposition on lattice-mismatched substrates breaks both local discrete rotational symmetries and translational symmetry by creating an interface and a surface, while in a TMO heterostructure different interfaces can be combined. Hitherto available spectroscopic tools can hardly provide information about the interfacial electronic properties, in particular the orbital occupation. X-ray linear dichroism can provide some insight into the orbital reconstruction at a single buried interface, relying on the shallow electron escape depth in the TEY mode – however, without any depth-resolved information.

In this presentation I will show that it is possible to derive quantitative, spatially resolved orbital polarization profiles from soft-x-ray reflectivity data, without resorting to model calculations [1]. The method is sensitive enough to resolve differences of ~3% in the occupation of Ni eg orbitals in adjacent atomic layers of a LaNiO_3 – LaAlO_3 superlattice, in good agreement with theoretical calculations. The possibility to quantitatively correlate theory and experiment on the atomic scale opens up many new perspectives for orbital physics in transition-metal oxides.

[1] E. Benckiser, V. Hinkov, B. Keimer et al., “Orbital reflectometry of oxide heterostructures,” *Nature Materials* 10, 189 (2011).