

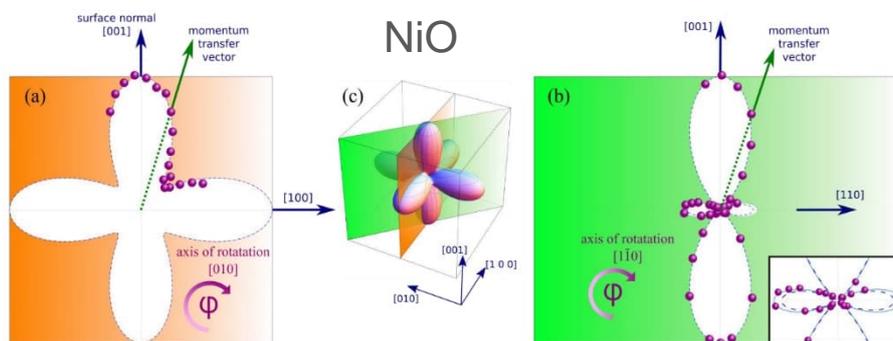
"Direct imaging of the local charge density in quantum materials"

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The search for new quantum materials with novel properties is often focused on materials containing transition-metal, rare-earth and/or actinide elements. The presence of the atomic-like d or f orbitals provides a fruitful playground to generate novel phenomena. The intricate interplay of band formation with the local electron correlation and atomic multiplet effects leads to phases that are nearly iso-energetic, making materials' properties highly tunable by doping, temperature, pressure or magnetic field. Understanding the behavior of the d and f electrons is essential for designing and controlling novel quantum materials. Therefore, identifying the d or f orbitals that actively participate in the formation of the ground state is crucial. So far, these orbitals have mostly been deduced from optical, X-ray and neutron spectroscopies in which spectra must be analyzed using theory or modelling. This, however, is also a challenge in and of itself, since *ab-initio* calculations hit their limits due to the many-body nature of the problem.

Here we developed a new experimental method that circumvents the need for involved analysis and instead provides the information as measured. With this technique, we can make a direct image of the active orbital and determine what the atomic-like object looks like in a real solid. The method, X-Ray Raman spectroscopy or non-resonant inelastic X-ray scattering using an s-core level (s-NIXS), relies on high momentum transfer in the inelastic scattering process, which is necessary for dipole-forbidden terms to gain spectral weight. To demonstrate the strength of the technique, we imaged the text-book example, ground-state $x^2-y^2/3x^2-r^2$ hole orbital of the Ni^{2+} ion in NiO single crystal (see Figure). We will present the basic principles of s-NIXS and details of its experimental implementation. We will show how we can apply this technique to unveil the active orbitals in a wide range of single crystalline materials. We will also lay out what instrumental improvements are needed to advance this method further.



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