

XAS and RXES study of the O 2*p* and Ru 4*d* orbital occupation in Ruddlesden-Popper strontium ruthenates Sr_{*n*+1}Ru_{*n*}O_{3*n*+1} (*n* = 1, 2, 3): the influence of the lattice distortions on the electronic structure.

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We report the polarization-dependent XAS and RXES study results of the electronic and local atomic structures of the Ruddlesden-Popper (RP) layered strontium ruthenate series, Sr_{*n*+1}Ru_{*n*}O_{3*n*+1}.¹⁻⁴

Ruthenium oxides are a particularly interesting class of materials exhibiting fascinating physical properties like unconventional superconductivity, ferromagnetism and metamagnetism, antiferromagnetic insulating behavior, and orbital ordering, resulting from the intimate interplay between charge, spin, orbital, and lattice degrees of freedom. In particular, the Sr_{*n*+1}Ru_{*n*}O_{3*n*+1} layered system have become a prototype for exploring intriguing physical phenomena due to a subtle interplay between structural anisotropy and distortions, multi-band effects and magnetic fluctuations. Infact, despite the fact that the Sr_{*n*+1}Ru_{*n*}O_{3*n*+1} compounds are all based on Ru⁴⁺ ions, octahedrally coordinated by oxygen atoms, with electronically inactive Sr-site counterions, they show a rich variety of magnetic and electronic states with experimental signatures of strong coupling to the lattice distortions driven by the number *n* of perovskite RuO₆ layers in the unit cell.

Oxygen K-edge XAS and RXES spectroscopy has a proven ability to shed light on the site symmetry and the occupation of empty states hybridized with O 2*p* orbitals, and have been successfully employed in 3*d* correlated transition metal oxides such as cuprates⁵, manganites⁶ and cobaltates⁷.

By comparing the temperature and angle resolved polarization-dependent O K-edge XAS and RXES data measured on Sr₂RuO₄, Sr₃Ru₂O₇ and Sr₄Ru₃O₁₀ with the complementary structural information provided by the x-ray diffraction study, we show how the occupied and unoccupied density of states resulting from the hybridization of O 2*p*-Ru 3*d* and O 2*p*-Sr 3*d* are affected by the rotations and tilting of the RuO₆ octahedra. We also present results on the O K edge XAS and XES spectra and partial density of states simulated by means of DFT-LDA and directly compared with the experimental data.

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