

Magnetic Correlations in the Spectroscopy of NiO Across the Néel Transition

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Abstract. The nature of strong electronic correlations in NiO has been under debate for decades. The traditional assumption that this system behaves as a Mott or charge-transfer insulator [1,2] has been recently challenged by works highlighting the crucial role played by structural and magnetic motifs, which break lattice and spin symmetries [3,4]. An important element in this discussion is how the electronic properties evolve when temperature is increased and fluctuations are strong enough to disrupt long-range and short-range order. Previous works have provided contradictory evidence, ranging from negligible changes [5] to marked differences [6] in the measured spectra. To address this question, we employ hard X-ray photoelectron spectroscopy to investigate the core-level and valence spectra of NiO across the Néel transition. Multi-scale methods based on first-principles electronic structure calculations are then used to model the evolution of the magnetic and electronic structure over this temperature range, providing a microscopic basis for interpreting the experimental data. Our results demonstrate that short-range magnetic correlations dominate the behavior of the electronic structure, which opens important questions concerning the temporal and spatial scales of the experimental probe in this type of analysis.

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