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EINLADUNG zum IFP-SEMINAR

LDA+DMFT approach to core-level spectroscopy : application to 3d transition metal compounds

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Host:	Jan Kunes
Termin:	Mittwoch, 10. Mai 2017, 16:00 Uhr
Ort:	Institut für Festkörperphysik, TU Wien
	Wiedner Hauptstraße 8-10, 1040 Wien
	Seminarraum DC rot 07 (roter Bereich, 7. OG)

Abstract:

We present a computational study of 2p core-level X-ray photoemission spectra (XPS) of transition metal monoxides MO (M=Ni, Co, Mn) and sesquioxides M_2O_3 (M=V, Cr, Fe) using a theoretical framework based on the local-density approximation (LDA) + dynamical mean-field theory (DMFT). We find a very good description of the fine spectral features, which improves considerably over the cluster model conventionally employed in spectral analysis. We analyze the role of the non-local screening in 2p XPS and its relationship to the long-range magnetic order and the lattice geometry. We also present selected applications of the framework to L-edge X-ray absorption spectroscopy and L-edge resonant inelastic X-ray scattering. Our results reveal the potential of the present method for the analysis and interpretation of the modern high-energy-resolution experiments.