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EINLADUNG zum IFP-SEMINAR

Core-Level Spectra in the Dynamical Mean-Field Theory

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Host:	Jan Kuneš
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The combination of the density-functional theory with the dynamical mean-field theory is a powerful tool for theoretical modeling of compounds with strongly correlated electrons. I illustrate how this framework can be used to analyze core-level spectra on the same footing as the valence-band electronic structure. The valence-band selfenergy as well as the core-level spectra are calculated in an impurity model, in which the hybridization of the (localized) correlated electrons with the surrounding electronic states, the crystal field, and the strength of the spin-orbital coupling are all determined from first principles. I apply this method to (a) photoemission from core levels in actinide and rare-earth oxides and discuss how the satellite features observed in these spectra do (or do not) reflect the chemical bonding, (b) and to the pressure-induced intermediate valency in elemental praseodymium, in particular to its signatures in the resonant x-ray emission spectra (RXES).