

**Thursday, 25<sup>th</sup> June 2015**

**09:30**

**AER 19 Seminar Room 4.14**

**Core-Level Spectra  
in the Dynamical Mean-Field Theory**

by

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The combination of the local-density approximation with the dynamical mean-field theory (LDA+DMFT) is a powerful tool for a theoretical investigation of compounds with correlated electrons. We illustrate how the core-level spectra can be analyzed on the same footing as the valence-band electronic structure.

The valence-band self-energy as well as the core-level spectra are calculated in the Anderson impurity model, in which the hybridization of the (localized) correlated electrons with the surrounding electronic states, the crystal field, as well as the spin-orbital coupling are all determined from first principles. We apply this method to

a) the actinide and rare-earth dioxides and discuss why their core-level x-ray photoelectron spectra (XPS) differ despite their valence-band electronic structure being very similar.

b) the pressure-induced intermediate valence in the elemental praseodymium, in particular to its signatures in the resonant x-ray emission spectra (RXES).