DFT+DMFT studies of metal-insulator transitions in complex 3d transition metal oxides

A talk by Claude Ederer

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DATE / TIME: Monday, Nov 20th 2017, 4:00 p.m.

LOCATION: TU Wien, Seminarraum 138C (Freihaus, Turm B/yellow, 9. OG)

In this talk, I will discuss two examples of how we use density functional theory plus dynamical mean-field theory (DFT+DMFT) to explore the properties of complex transition metal oxides close to metal-insulator transitions.

The first part of the talk is focused on early transition metal oxides such as vanadates and titanates, which are close to a Mott metal-insulator transition. Here, we explore ways to tune the metal-insulator transition via strain engineering and hetero-structuring. Specifically, I will discuss the case of CaVO3, where a thickness-dependent MIT has been recently observed [Gu et al., J. Appl. Phys. 113, 133704 (2013)]. Our calculations allow us to separate finite-size effects in ultra-thin films from the effects of epitaxial strain and from interfacial effects, and thus to clearly identify the main source for the observed behavior.

In the second half of the talk, I will discuss the case of rare-earth nickelates, RNiO3, where a metal-insulator transition is coupled to a structural distortion that splits the Ni sites into two inequivalent subsets. This poses additional challenges to the DFT+DMFT method, and we explore how accurately the energetics of this structural distortion can be described within DFT+DMFT.