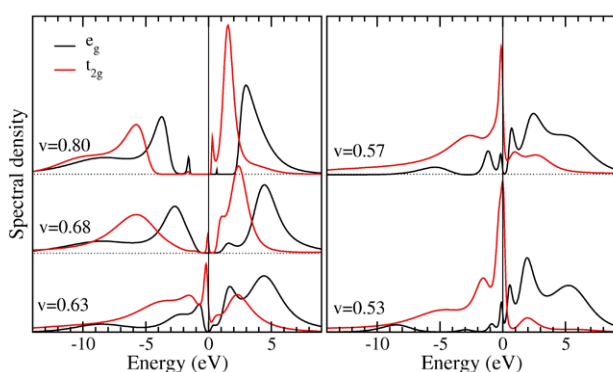


## Dynamical correlations in transition metal compounds

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The standard methods of density functional theory describe the electronic structure of materials in terms of Slater determinants. While such description proved useful in many cases, in transition metal compounds it is often not sufficient. We use the dynamical mean-field theory (DMFT) [1] to study such systems and phenomena related to electronic correlations. The examples include the spin state transitions in MnO [2] and Fe<sub>2</sub>O<sub>3</sub> [3], driven by pressure, and in LaCoO<sub>3</sub> [4], driven by temperature. We discuss the relationship of the spin transition to the metal-insulator transition and tendencies towards long-range ordering.



**Figure 1:** The orbital resolved Mn-*d* spectral density in MnO for various specific volumes. The results correspond to the temperature of 1160 K.

We will show how the local electronic correlation leads to emergence of non-fermionic degrees of freedom, such as the local magnetic moments, and how their fluctuations influence the material properties. The talk will focus on the qualitative differences between the DMFT description and static mean-field theories such as LDA or LDA+U.

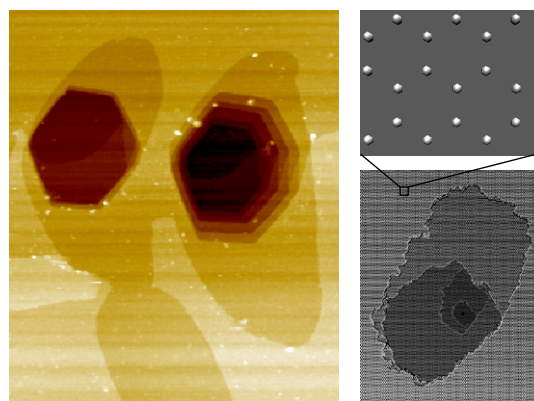
- [1] Georges *et al.* (1996) *Rev. Mod. Phys.* **68**, 13–125.  
 [2] Kunes *et al.* (2008) *Nature Mater.* **7**, 198–202. [3] Kunes *et al.* (2009) *Phys. Rev. Lett.* **102**, 146402. [4] Kunes & Krapek (2011) arXiv, 1103.2249.

## Phyllosilicate dissolution kinetics: experimental observations and Kinetic Monte Carlo modeling

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We present our recent results in the study of phyllosilicate dissolution kinetics. The major problem in this field is the influence of the layered structure on dissolution mechanism and the difference in reactivity between edge and basal faces. We use an integrated approach including experiments and modelling to understand real crystallographic control of dissolution kinetics. Vertical Scanning Interferometry allows us to observe mineral surface topography during the dissolution process, measure dissolution rates and access their spatial and temporal variability. Detailed information about surface structure has also been obtained from AFM work. We simulate the dissolution of phyllosilicates using Kinetic Monte Carlo (KMC) approach. This stochastic method links elementary reactions taking place on the mineral surface with the topographic outcome of these processes. The KMC model has been parameterised using activation energies of elementary bond-hydrolysis reactions obtained from quantum mechanical calculations. As a result, we have reproduced experimentally-observed dissolution patterns in our KMC simulations (Fig.1). The combination of these techniques will help us to understand complex behaviour of crystalline systems in the dissolution process.



**Figure 1:** Left: AFM image of etch pit on muscovite {001} face 3x3 μm; Right: Etch pit (50 x 70 nm) obtained from KMC simulations with the enlarged area above showing arrangement of cations (Si/Al)