# Correlation induced Peierls transition in $VO_2$

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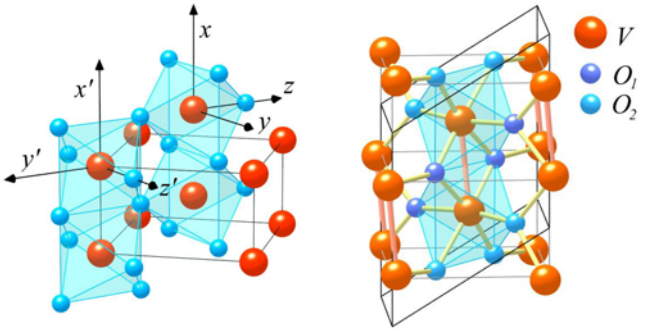
## Metal-Insulator Transition at 340 K

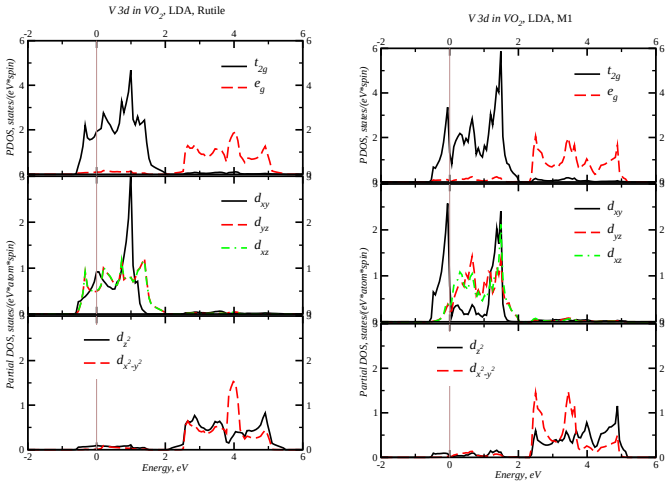
High temperature : rutile phase (metallic)  Low temperature : monoclinic phase (insulating)

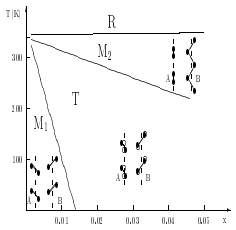



The metal-insulator transition is accompanied by a structural transition with dimerization of the V atoms and tilting of the pairs out of the z axis.
(From V. Eyert, Ann. Phys. (Leipzig) 11, 650-702 (2002))

## Peierls or Mott ? - the nature of the transition

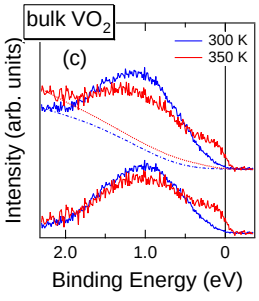
Density functional theory (DFT) within the local density approximation (LDA) does not describe the *insulating* phase :




- DFT-LDA describes structural properties rather well (Wentzcovitch et al.) → Peierls?
- DFT-LDA opens a gap if distortions are exaggerated (Eyert) → Peierls?
- Existence of mixed phases (Pouget et al.) → Mott?
- Magnetic properties → Mott?

## Spectral properties




- qualitative disagreement with LDA in the monoclinic phase (T < 340 K)
- quantitative disagreement with LDA in the rutile phase (T > 340 K)

Photoemission (Okazaki et al., see also Koethe et al., Shin et al. and Sawatzky et al.)

## Dynamical mean field theory ...

... maps a lattice problem onto a single-site (Anderson impurity) problem

with a self-consistency condition

## Cluster Dynamical Mean Field Theory ...

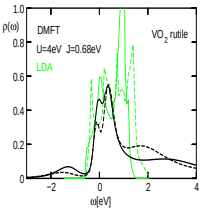
... maps a lattice problem onto a cluster impurity problem

Here, we combine DFT-LDA with Cluster-DMFT for a 2-site $V_2O_4$ cluster using

- Nth order muffin tin orbitals (NMTO) (Andersen et al., 2001)
- an effective Hamiltonian for V-$t_{2g}$ states
- QMC sampling (Hirsch-Fye) for the solution of the cluster impurity problem

## The Rutile Phase

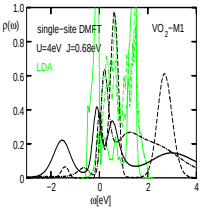
within single-site DMFT (U=4 eV) (or cluster-DMFT (not shown))




- agreement with photoemission spectra : coexistence of quasiparticle peak with Hubbard bands
- ∼ 30 % bandwidth renormalization

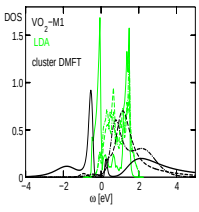
## The Monoclinic Phase ...

... within single-site DMFT at U=4 eV



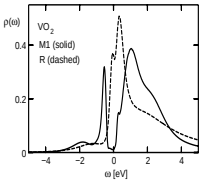

- insulating character not captured by single-site DMFT at U=4 eV
- to open a Mott gap direct Coulomb interactions as strong as U=5eV are required

... within cluster DMFT (U=4 eV)




- agreement with spectra
- self-energy is of Fermi liquid type (→ Peierls !) not Mott type
- strong intra-pair fluctuations, large intra-pair self-energy between $a_{1g}$ bands
- Peierls gap coexists with Hubbard bands
- strong charge transfer to $a_{1g}$ bands

## Comparison : total $t_{2g}$ spectral function




- coherent peak at -0.7 eV in M1 phase
- Hubbard band at -1.3 eV in R phase

## Conclusions

- Single-site LDA+DMFT describes rutile phase, but not monoclinic phase of $VO_2$
- Cluster extension of LDA+DMFT describes both, rutile and monoclinic phase
- Mixed Peierls-Mott character of the insulating phase of $VO_2$
- For more details and refs see: Phys. Rev. Lett. 94 026404 (2005)