Materials Design using Correlated Materials? – A Dynamical Mean Field View

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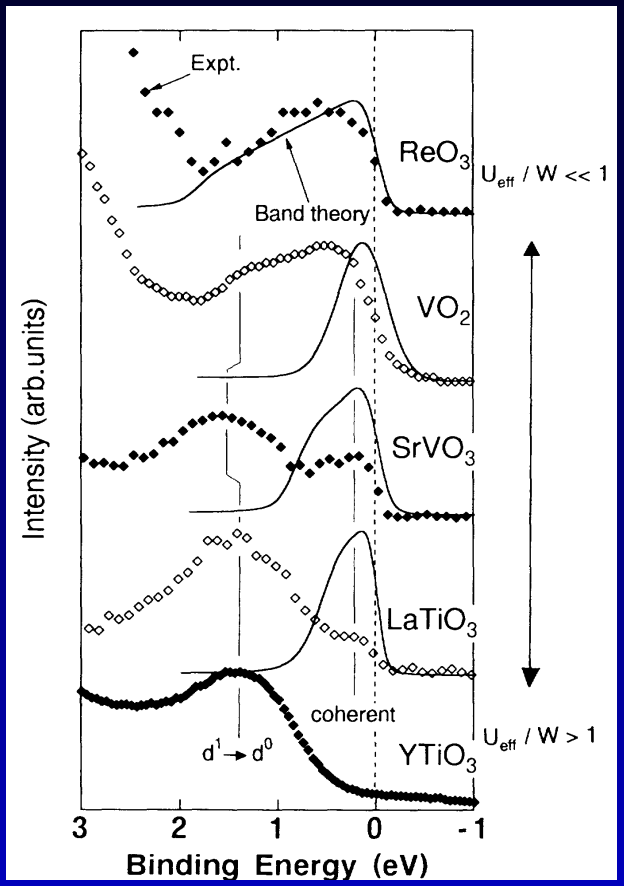
Why Dynamical Mean Field Theory?



Mott insulating phases: not accessible in one-particle picture

Correlated metals: Coex-istence of quasi-particle bands with Hubbard bands
NB: several energy scales!

(Photoemission data from Fujimori et al., 1992)

What's a mean field theory?

Example of the Ising Model:

$$H = -J \sum_{ij} S_i^z S_j^z \tag{1}$$

Mean field theory: map onto single-spin problem in an effective field

$$H = -\mu_B B_{eff} S_o^z \tag{2}$$

with a self-consistency condition restoring translational invariance

What's a mean field theory?

Two ingredients:

1. Reference system: single site (or cluster of sites) in an effective mean field

2. Self-consistency condition relating the effective problem to the original one

... a *dynamical* mean field theory?

Two ingredients:

1. Reference system: single site (or cluster of sites) in an effective mean field
   - Mean field can be **energy-dependent ($\longrightarrow$ dynamical)**
   - Reference system can be **interacting**
2. Self-consistency condition relating the effective problem to the original one

From basic concepts ...

- DMFT – basic ideas (example: Hubbard model)
- “LDA+DMFT”
- Different implementations
- What can we calculate?

... to real materials ...

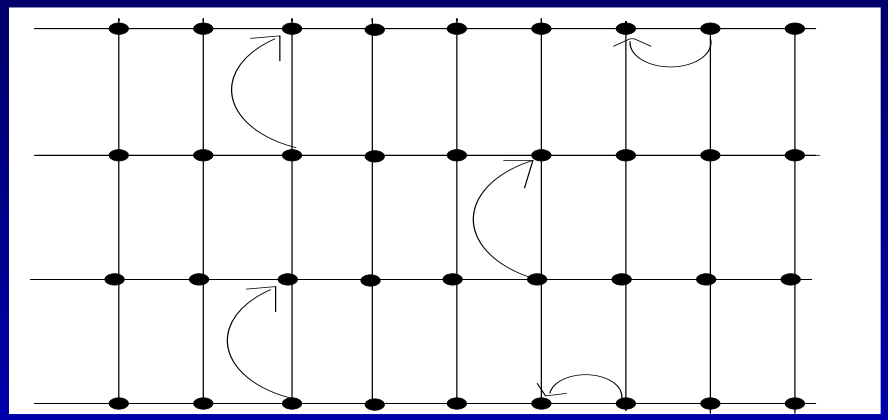
- transition metals and their oxides
- f-electron materials
- iron oxypnictides

... and back (?)

- Current challenges and perspectives

The Hubbard model

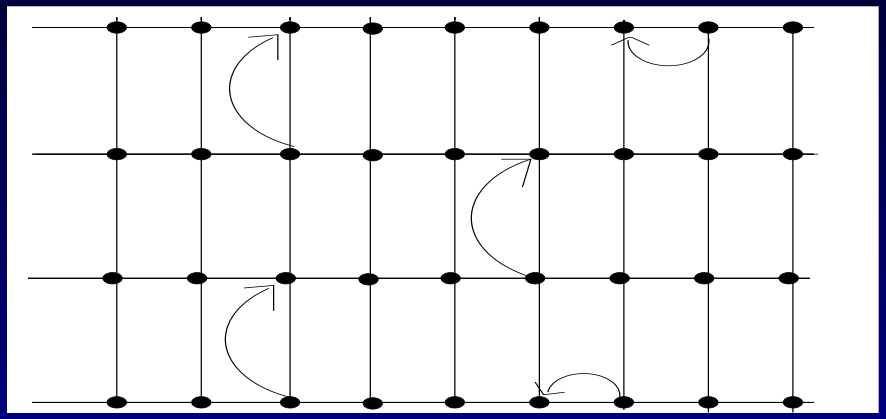
$$H = -\frac{D}{2} \sum_{<ij>\sigma} \left(c^{\dagger}_{i\sigma} c_{j\sigma} + c^{\dagger}_{j\sigma} c_{i\sigma} \right) + U \sum_{i} n_{i\uparrow} n_{i\downarrow}$$



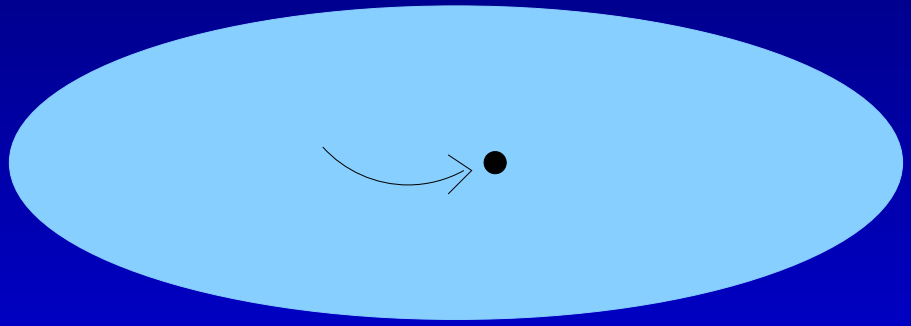
(Hubbard, 1963)

Dynamical mean field theory ...

... maps the lattice problem



onto a single-site (Anderson impurity) problem



with a self-consistency condition

(for a review see Georges et al., Rev. Mod. Phys. 1996)

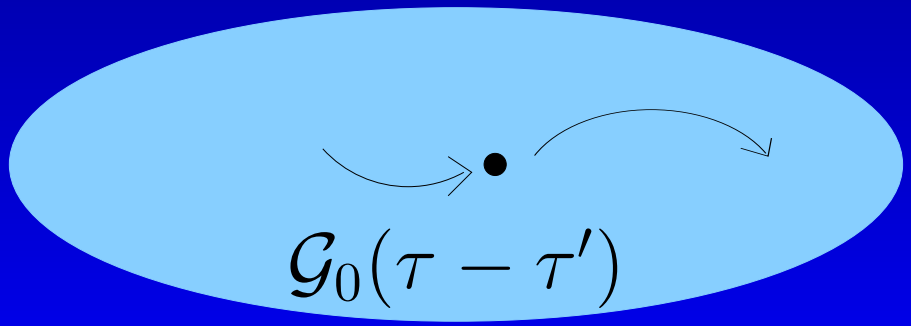
Effective dynamics ...

... for *single-site* problem

$$S_{eff} = -\int_0^\beta d\tau \int_0^\beta d\tau' \sum_\sigma c_\sigma^\dagger(\tau)\mathcal{G}_0^{-1}(\tau-\tau')c_\sigma(\tau')$$

$$+ U\int_0^\beta d\tau n_\uparrow n_\downarrow$$

with the dynamical mean field $\mathcal{G}_0^{-1}(\tau-\tau')$



DMFT (contd.)

Green's function:

$$G_{impurity}(\tau) = -\langle \hat{T} c(\tau) c^{\dagger}(0) \rangle$$

Self-energy (k-independent):

$$\Sigma_{impurity}(\omega) = \mathcal{G}_0^{-1}(\omega) - G_{impurity}^{-1}(\omega)$$

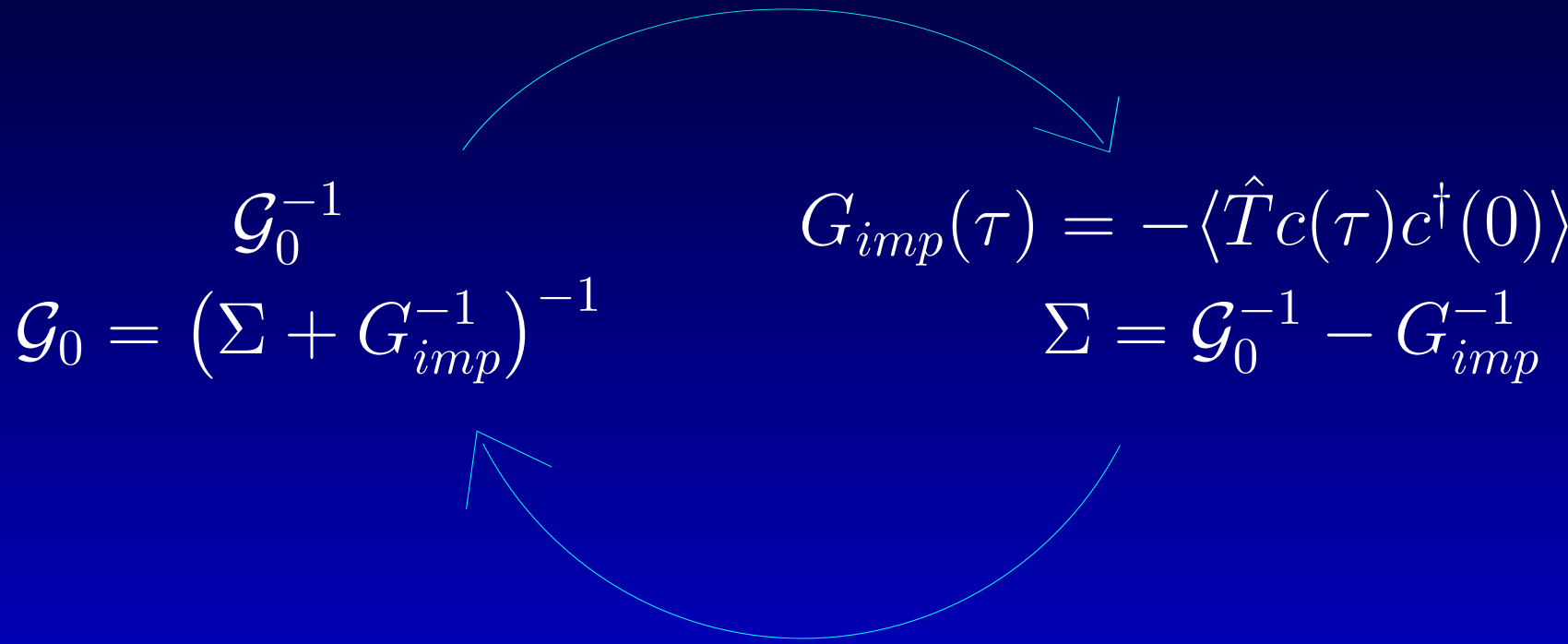
DMFT assumption :

$$\begin{aligned} \Sigma_{impurity} &= \Sigma^{lattice} \\ G_{impurity} &= G_{local}^{lattice} \end{aligned}$$

$\longrightarrow$ Self-consistency condition for $\mathcal{G}_0^{-1}$

The DMFT self-consistency cycle

Anderson impurity model solver



Self-consistency condition:

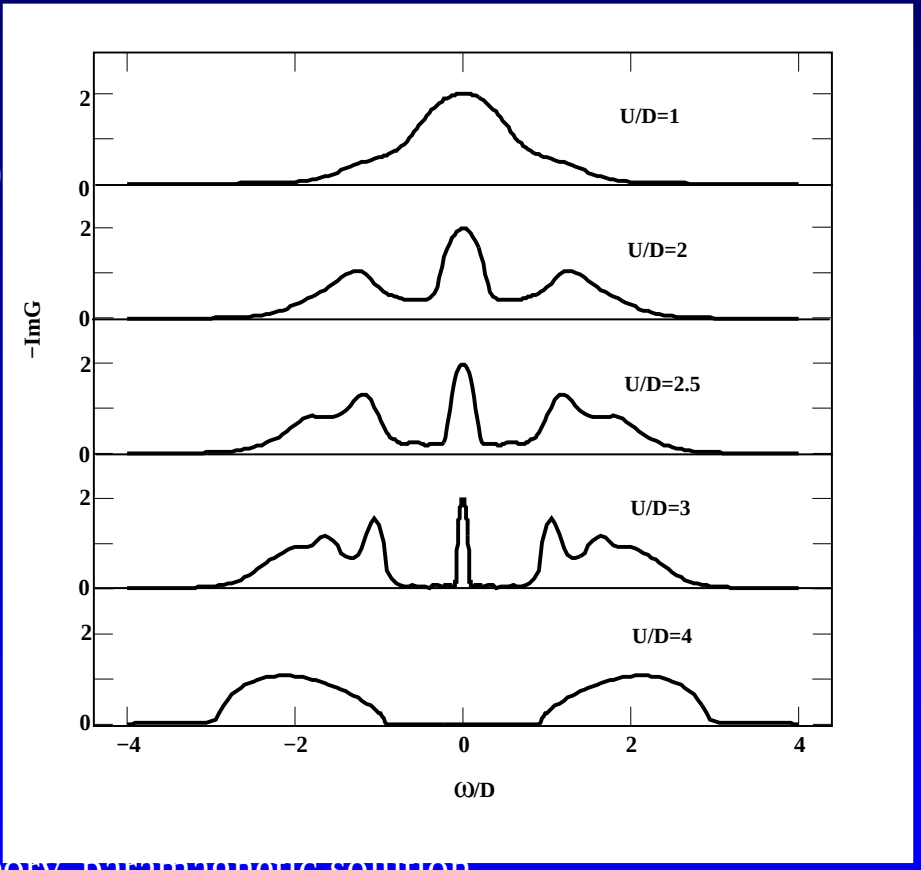
$$G(\omega) = \sum_k \frac{1}{\omega + \mu - \epsilon_k - \Sigma(\omega)}$$

Hubbard model within DMFT

$$H = -\frac{D}{2} \sum_{<ij>\sigma} \left(c^{\dagger}_{i\sigma} c_{j\sigma} + c^{\dagger}_{j\sigma} c_{i\sigma} \right) + U \sum_{i} n_{i\uparrow} n_{i\downarrow}$$

(Hubbard, 1963)

$\rho(\omega)$

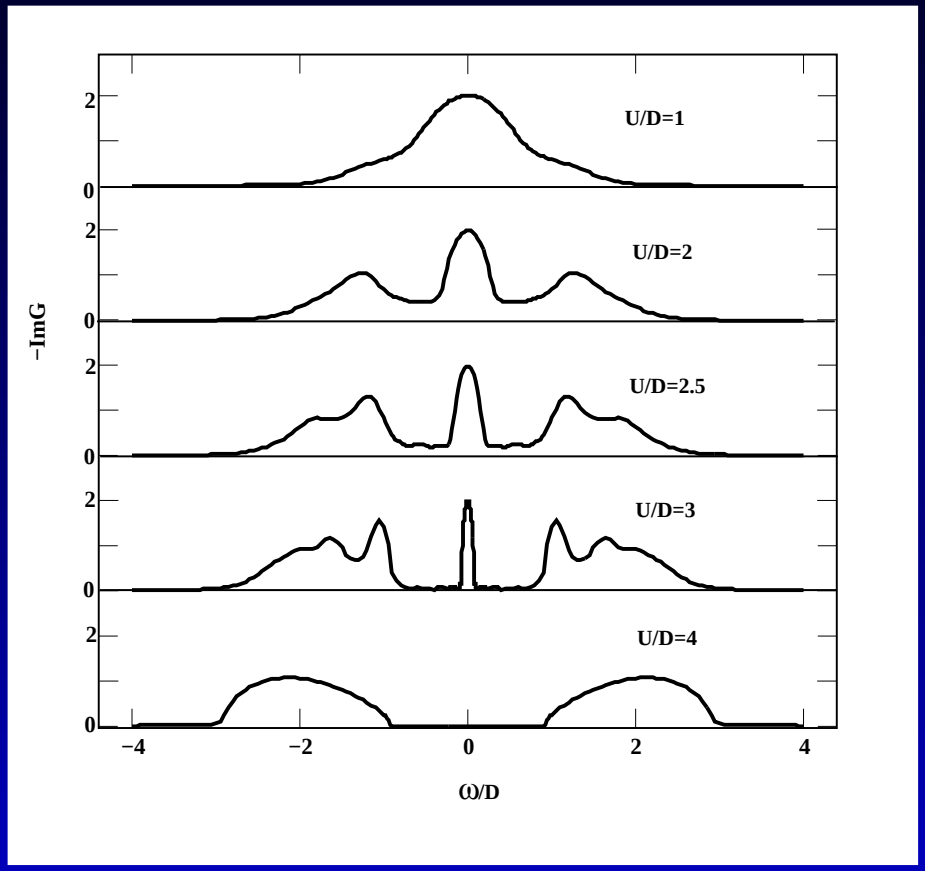


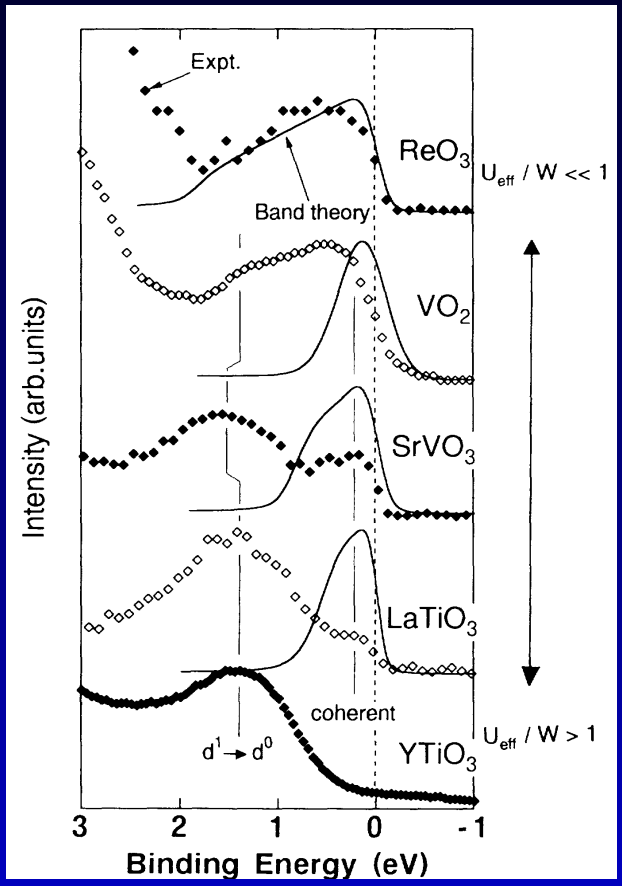
Quasi-particle peak
Hubbard bands

Georges & Kotliar 1992

(∗) DMFT = Dynamical Mean Field Theory, paramagnetic solution

Photoemission vs. Hubbard model spectral function





(from Fujimori et al., 1992)

From basic concepts to real materials ...?

Wanted: techniques for materials-specific calculations of electronic properties beyond band theory

Strategy:

- materials-specific $\longrightarrow$ "first principles" (i.e. without adjustable parameters)
- beyond band theory $\longrightarrow$ many-body techniques based on dynamical mean field theory (DMFT)

$\longrightarrow$ combine both ...

“LDA+DMFT” – basic strategy

$\longrightarrow$ effective one-particle Hamiltonian within LDA

$\longrightarrow$ represent in localized basis

$\longrightarrow$ add Hubbard interaction terms

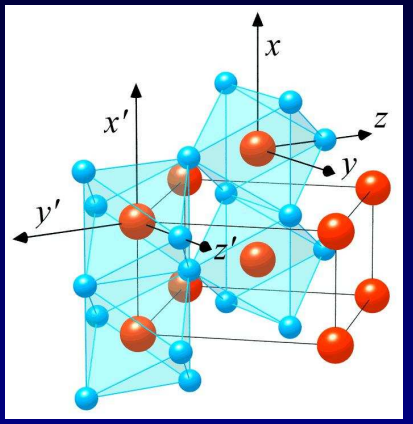
$$
\begin{aligned}
H &= \sum_{\{im\sigma\}} (H^{LDA}_{im,i'm'} - H^{double\ counting}_{im,i'm'}) a^{+}_{im\sigma} a_{i'm'\sigma} \\
&+ \frac{1}{2} \sum_{imm'\sigma\ \text{(correl. orb.)}} U_{mm'} n_{im\sigma} n_{im'-\sigma} \\
&+ \frac{1}{2} \sum_{im\neq m'\sigma\ \text{(correl. orb.)}} (U_{mm'} - J_{mm'}) n_{im\sigma} n_{im'\sigma}
\end{aligned}
$$

$\longrightarrow$ solve within Dynamical Mean Field Theory

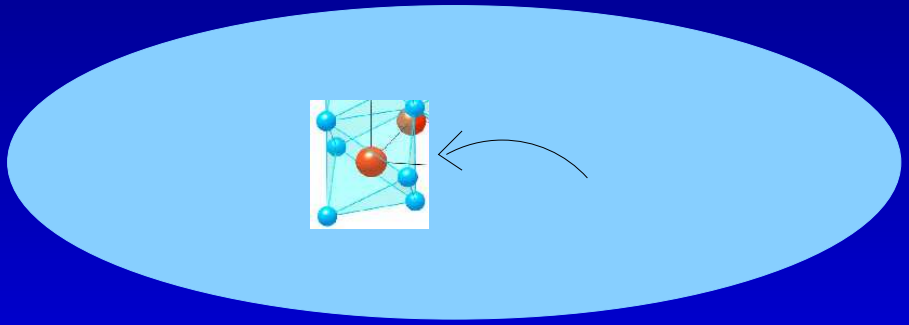
(Anisimov et al. 1997, Lichtenstein et al. 1998)

Dynamical mean field theory ...

... maps a lattice problem [a solid]



onto a single-site problem [an effective atom]



with a self-consistency condition

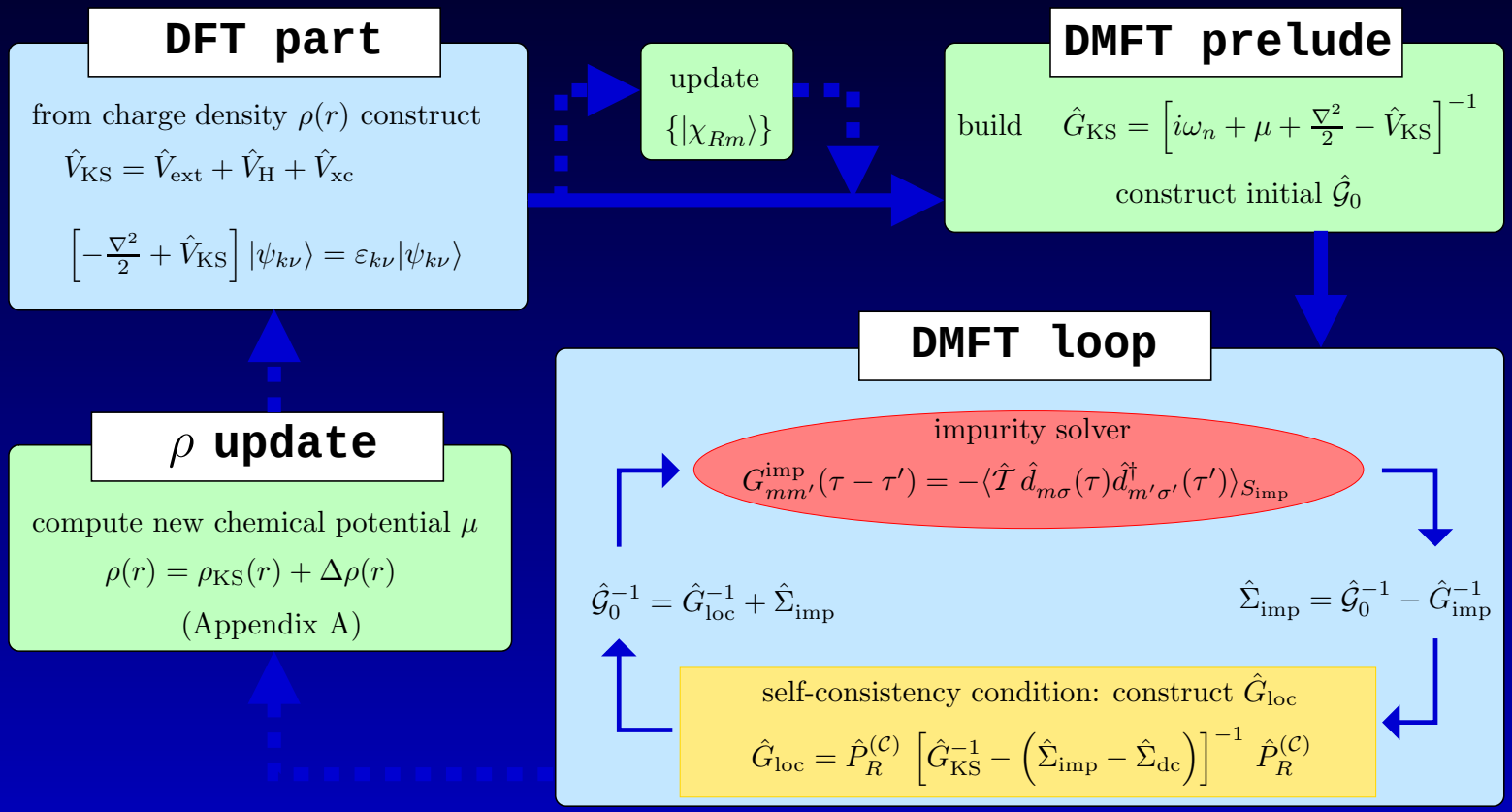
Spectral density functional theory

Update of “non-interacting” (LDA) Hamiltonian!

- Functional of density and spectral function of correlated orbitals
- DMFT a way to (approximately) evaluate that functional

(Kotliar and Savrasov, 2004)

LDA+DMFT – full scheme



see e.g. F. Lechermann, A. Georges, A. Poteryaev, S. B., M. Posternak, A. Yamasaki, O. K. Andersen, Phys. Rev. B **74** 125120 (2006)

Different implementations

- muffin-based (LMTO, NMTO ...)
- maximally localised Wannier functions
  $\longrightarrow$ use your favorite LDA implementation ...!
- Wannier-like functions generated from projected atomic orbitals
  $\longrightarrow$ use your favorite LDA implementation ...!
- ...

(see, e.g., Aichhorn et al., PRB 2009)

cf X. Gonze's talk

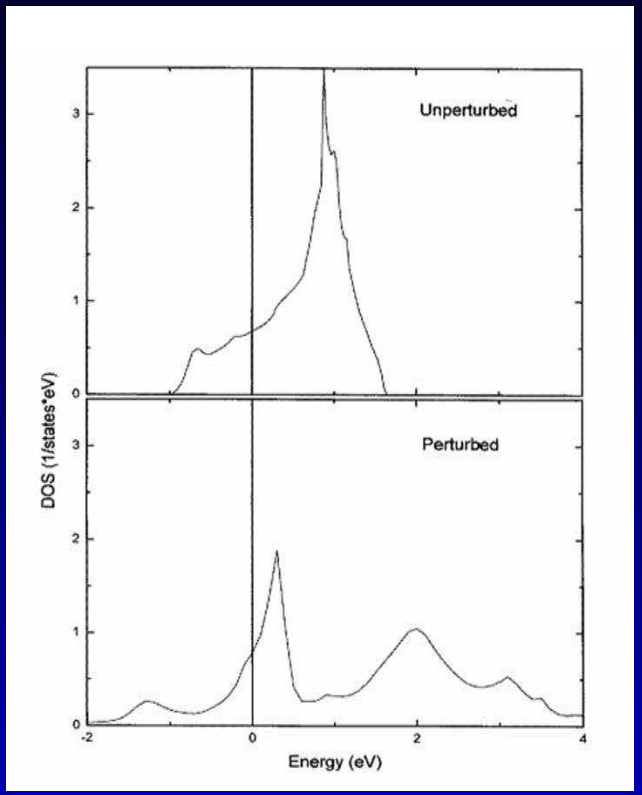
Solvers?

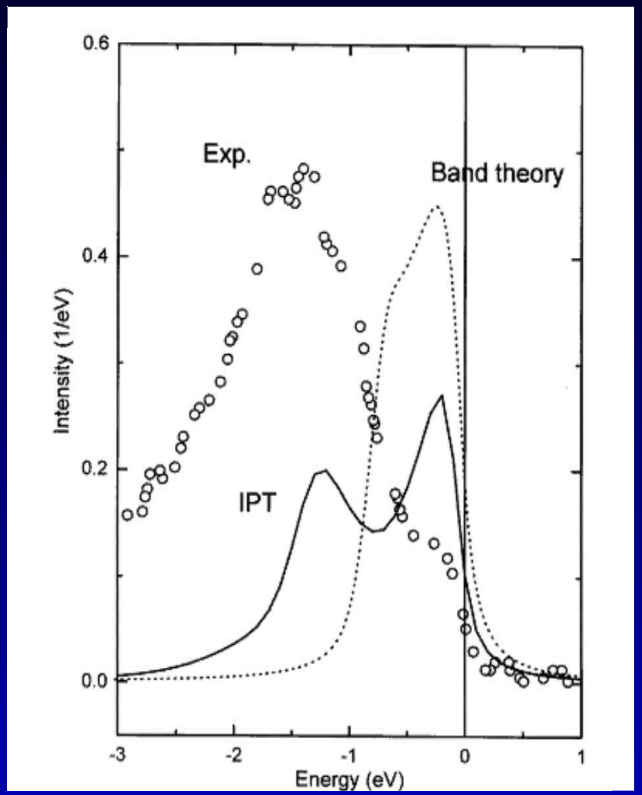
How to solve the (multi-orbital) Anderson impurity model?

- “numerically exact” schemes (QMC)
- approximate techniques, e.g. based on diagrammatic (NCA and extensions, FLEX, ...) or physical (Hubbard I, slave bosons ...) considerations

NB. Can build in knowledge about the solution (and save hours of Monte Carlo time ...).

doped $LaTiO_3$



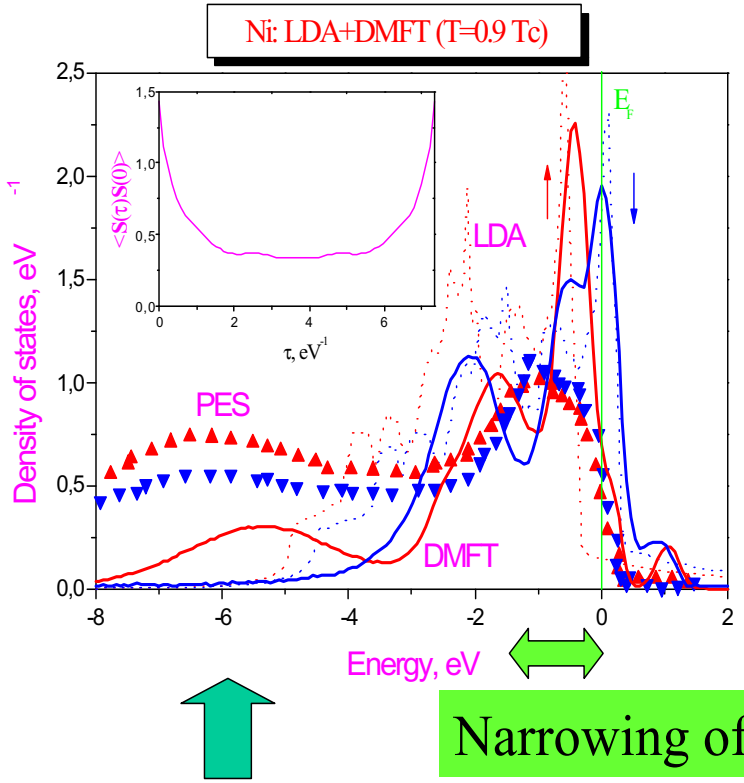


Anisimov et al., 1997

Nickel within LDA+DMFT

(from: Lichtenstein et al. 2001)

Local spectral function: Nickel



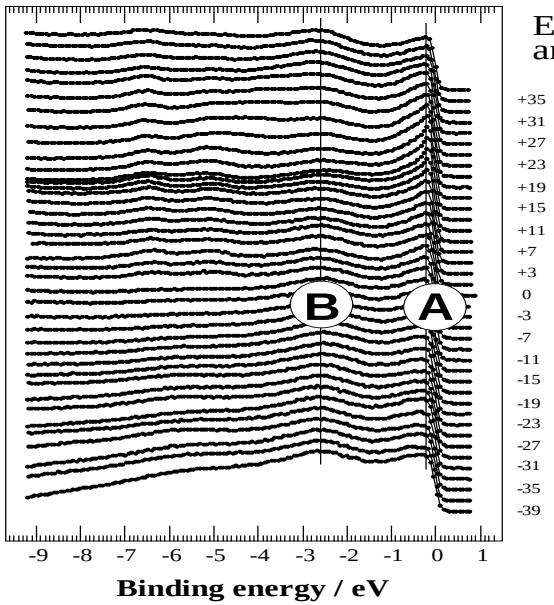
Three correlation effects:

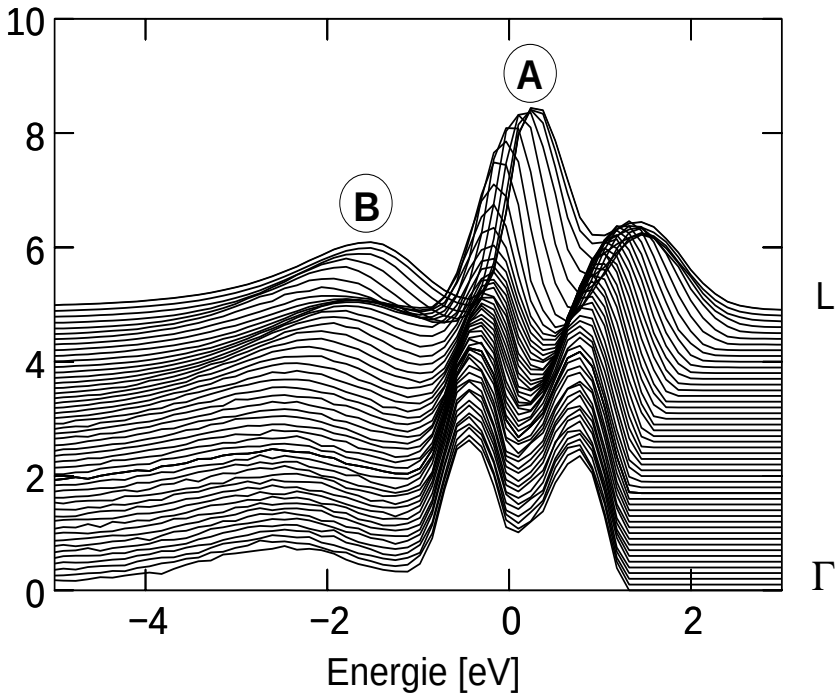
50% decrease of exchange splitting

Narrowing of occupied d-band (30%)

6 eV satellite, spin polarized

γ-Manganese



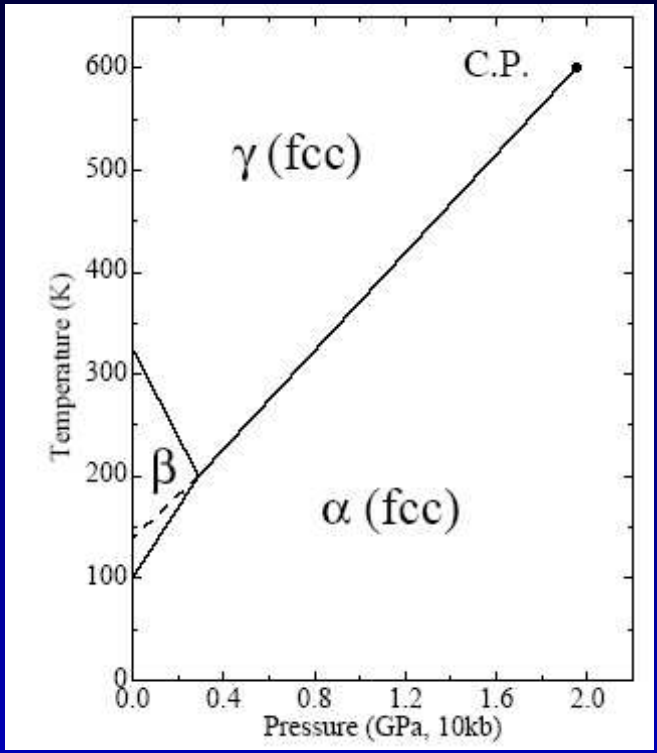


Quasi-particle bands (A) coexisting with Hubbard bands (B)

Experiment: Dallmeyer et al.

LDA+DMFT: SB, Lichtenstein, Katsnelson (2000)

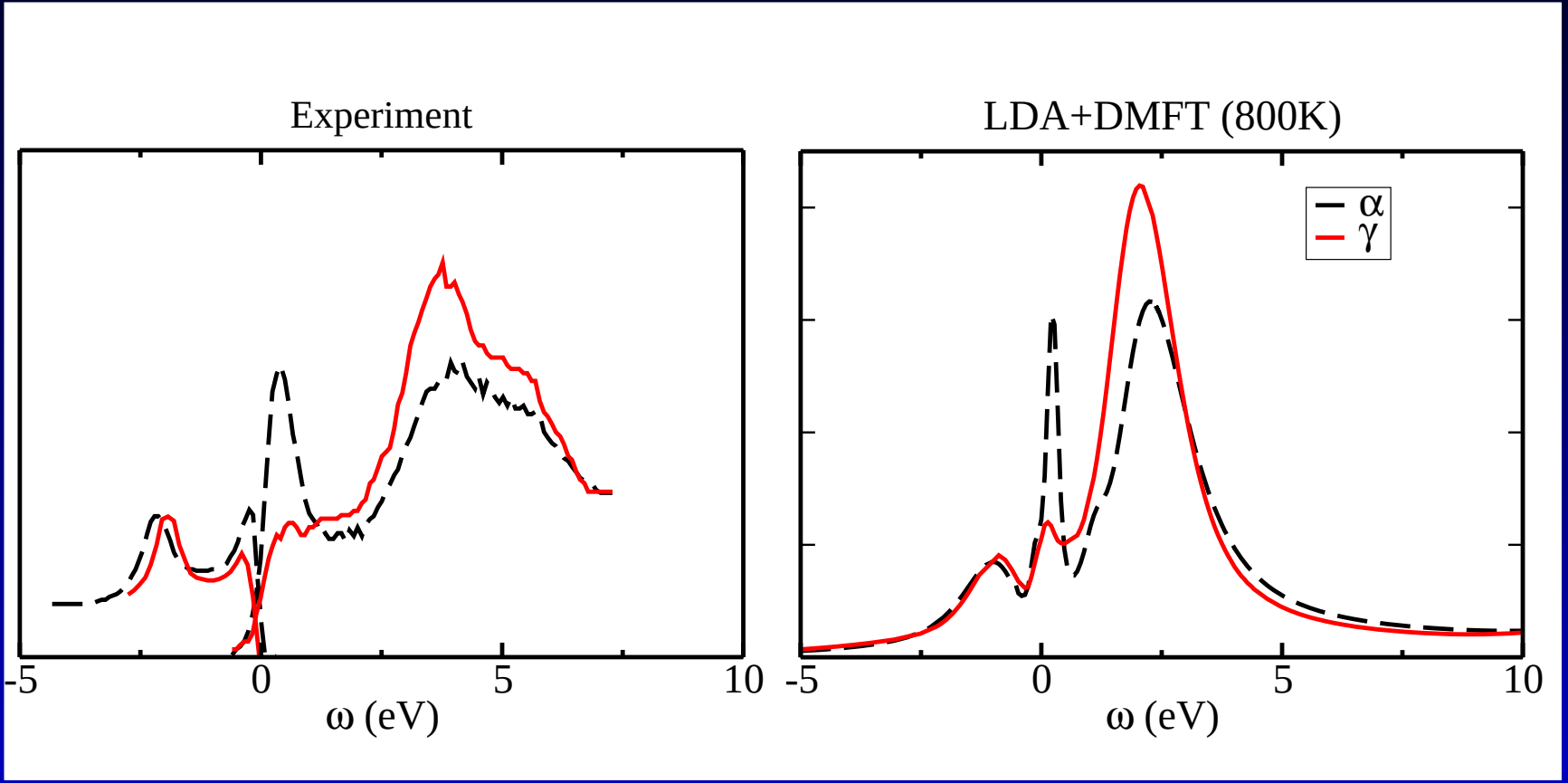
Cerium



α-phase:
small volume, delocalized f-electrons
γ-phase:
large volume, localized f-electrons

Several studies using LDA+DMFT:
Held et al., Zölfl et al., Haule et al., Sakai et al., MacMahan et al., Amadon et al.

Spectral properties

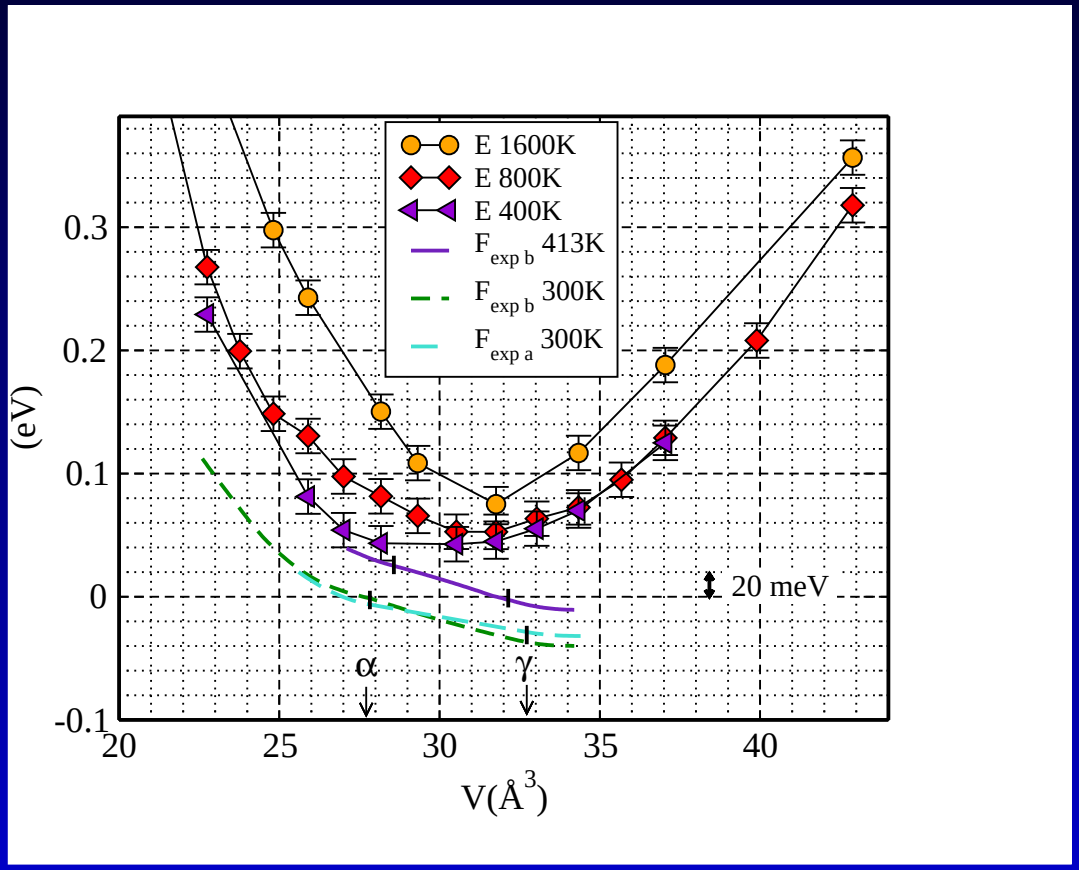


Experimental data: Wuilloud et al, Wieliczka et al.

LDA+DMFT: Amadon, SB., Georges, Aryasetiawan, PRL 2005

Total energy

LDA+DMFT calculations

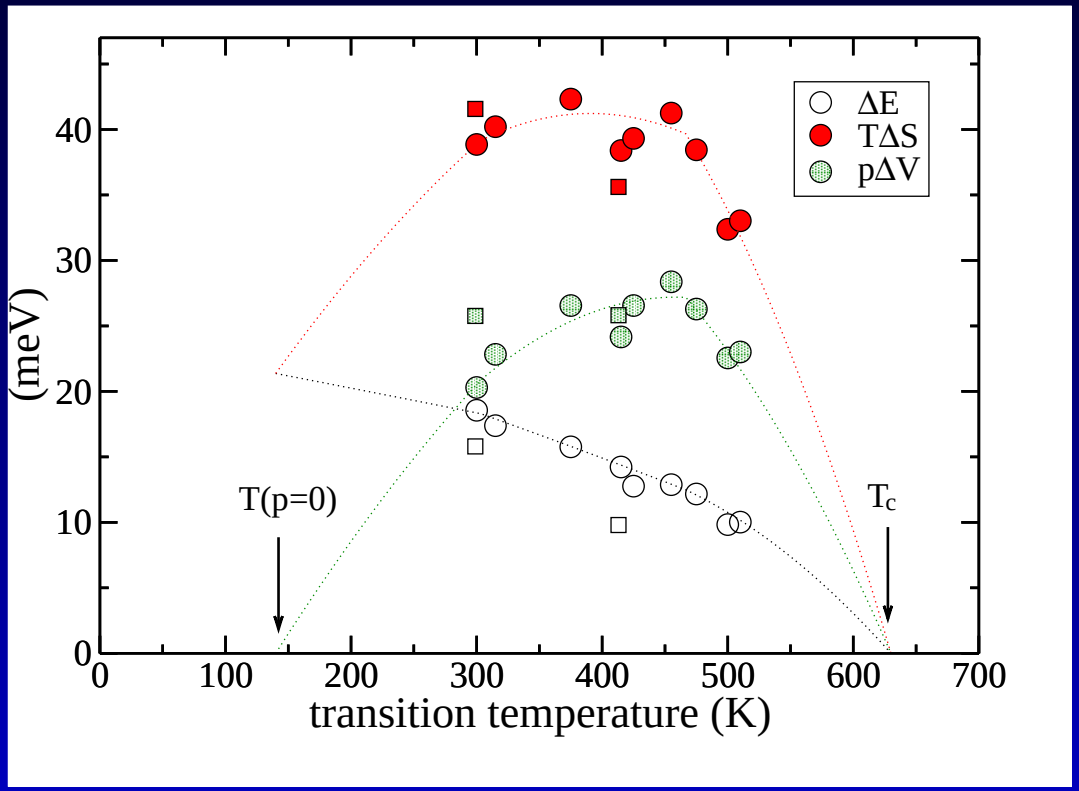


No double minimum

(B. Amadon et al., PRL 2005)

Energetic contributions

Exploit available experimental data!

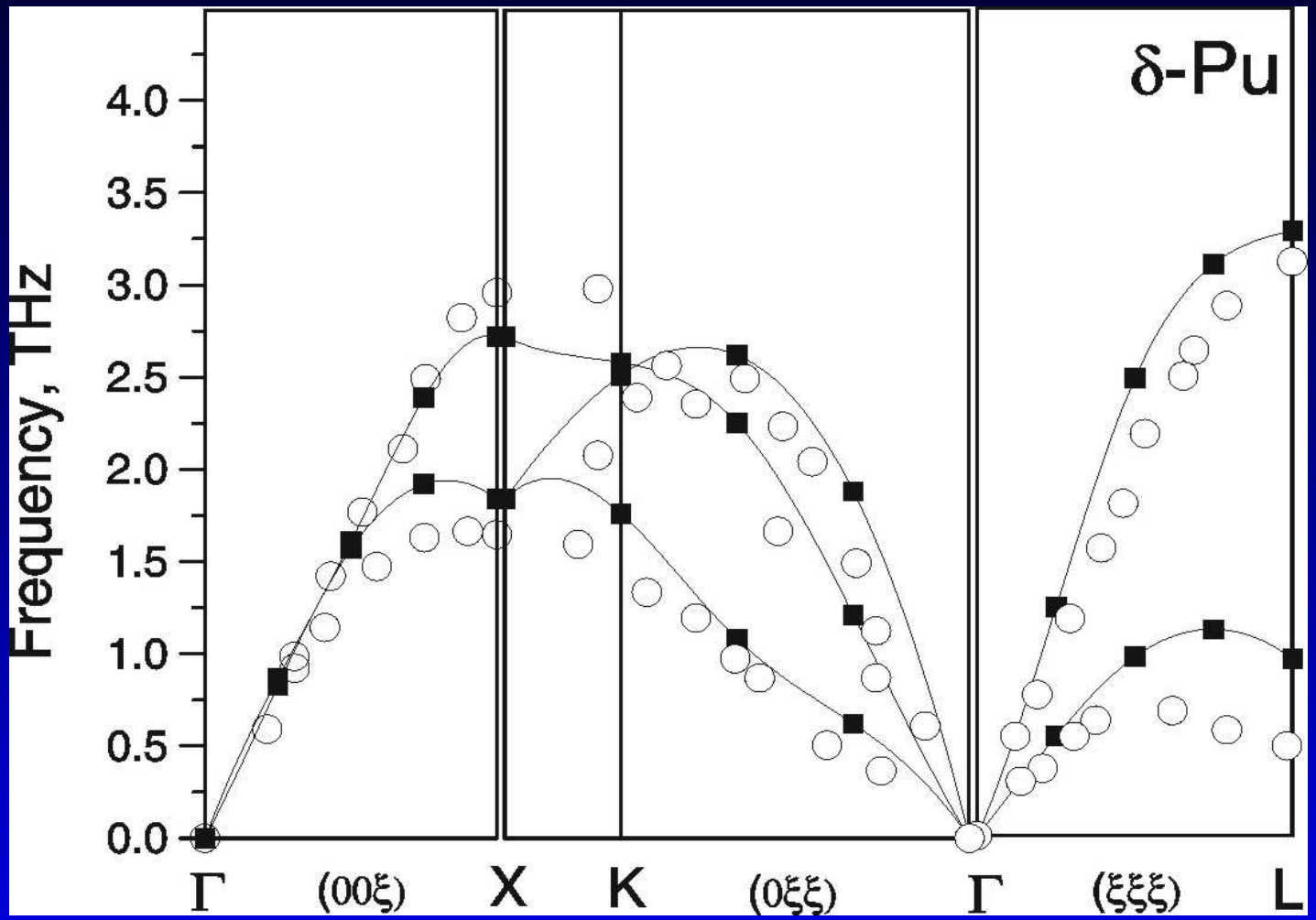


$$\Delta E = E_\gamma - E_\alpha > 0$$
$$\Delta F = F_\gamma - F_\alpha = \Delta E - T\Delta S = -p\Delta V < 0$$

Transition is entropy-driven!

Phonons in Pu

LDA+DMFT vs. experiment (Dai et al., 2004)

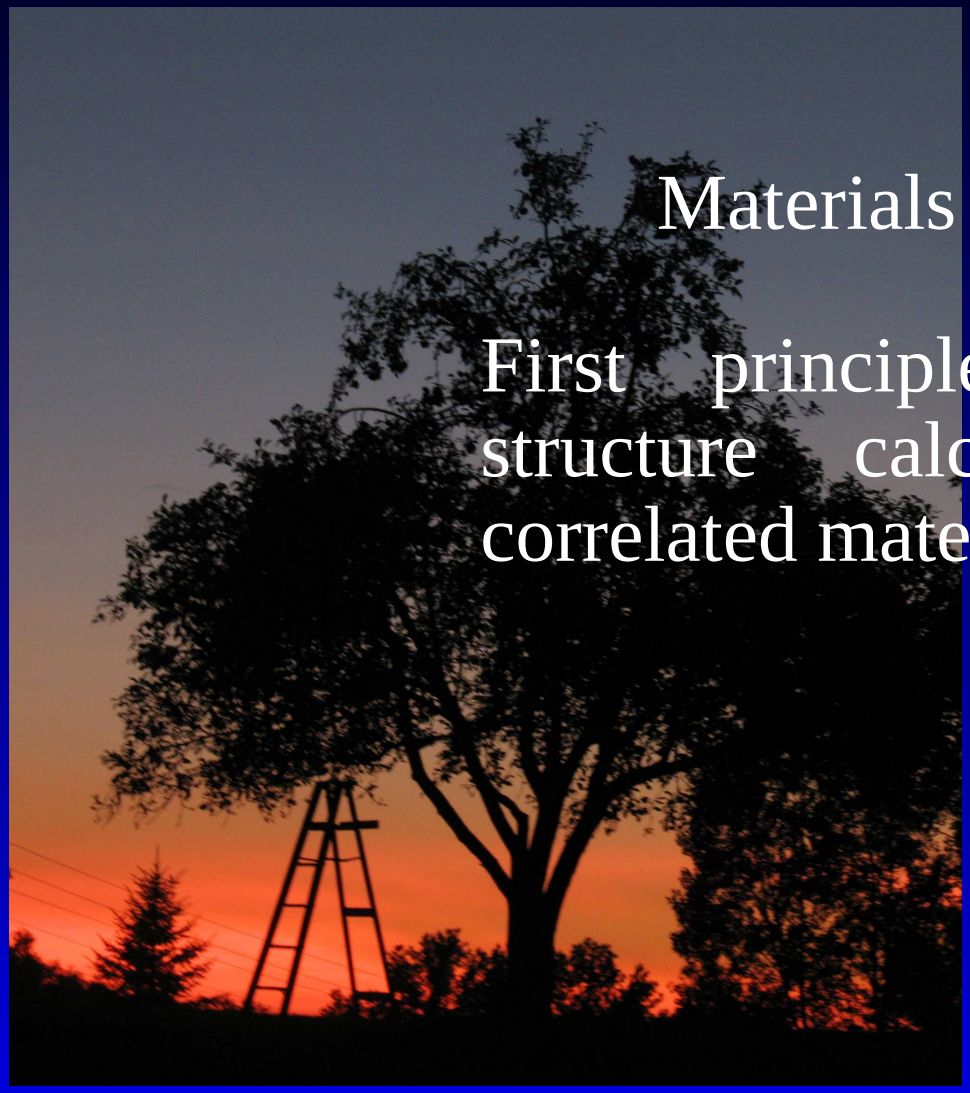


What can we calculate?

- spectral functions
- k-resolved spectral functions
- optical conductivities
- total energies
- phonons
- magnetic properties (but: local self-energy)

Jacob’s ladder ?

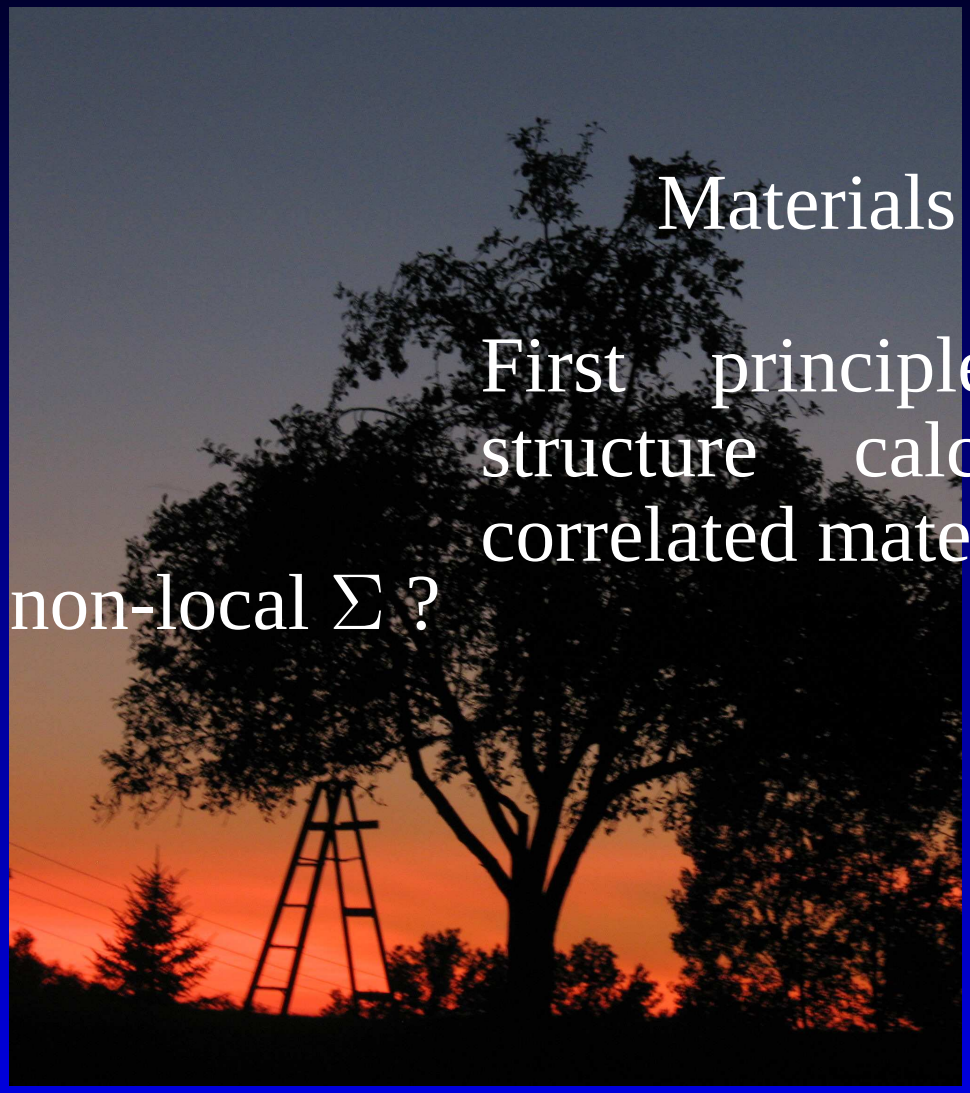
Jacob's ladder ?



Materials Design

First principles electronic structure calculations for correlated materials

Jacob's ladder ?



Materials Design

First principles electronic structure calculations for correlated materials

non-local Σ ?

Intelligent Windows ?

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Last Updated: Wednesday, 25 August, 2004, 09:56 GMT 10:56 UK

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'Heat-proof' glass could save on air-con

A new coating for glass that can keep the heat from the sun out, saving on air-conditioning costs, has been developed by scientists in London.

The benefits will be most felt in the buildings of the world's hottest cities

The glass has a microscopic coating that allows glazing to keep heat out of buildings while allowing light to pass through.

The key is a thin coating of vanadium dioxide, around the thickness of a human hair, that is placed on normal window glass.

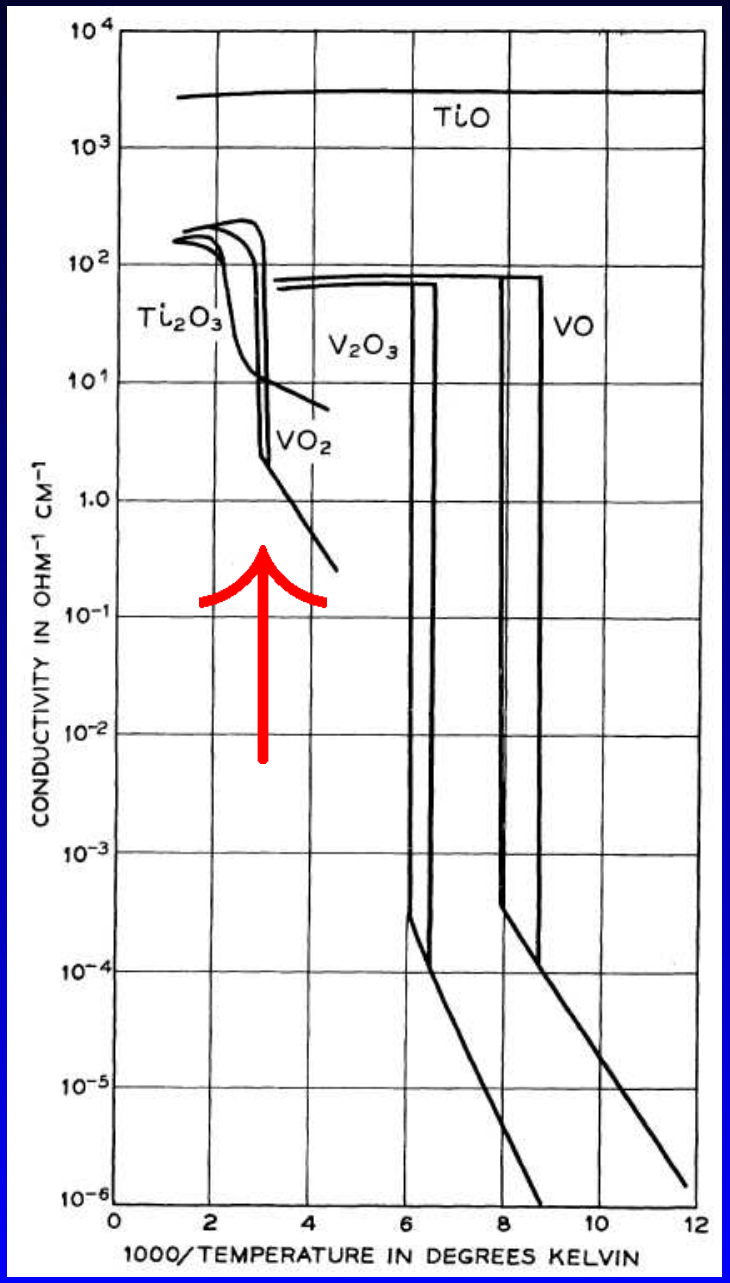
"This coating can actually be used for modifying the properties of the glass," said Ivan Parkin, of the team at University College London that has developed the coating.

"When put onto a window, it will let in only a certain fraction of the sunlight," he told the BBC World Service programme, Science In Action.

"When the window gets hot, it becomes more reflective. But it only becomes more reflective of the heat portion of the sunlight, not in the visible portion."

Vanadium dioxide VO_2 proposed as a coating material

Metal-Insulator Transitions

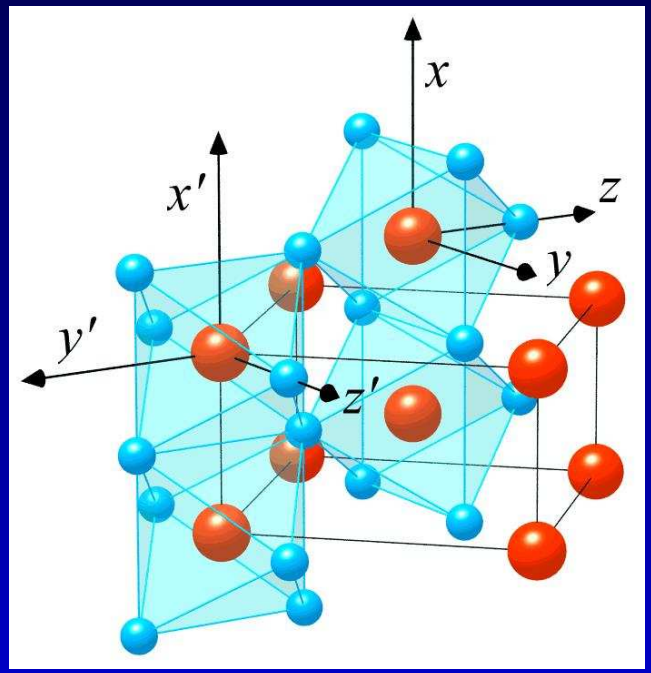


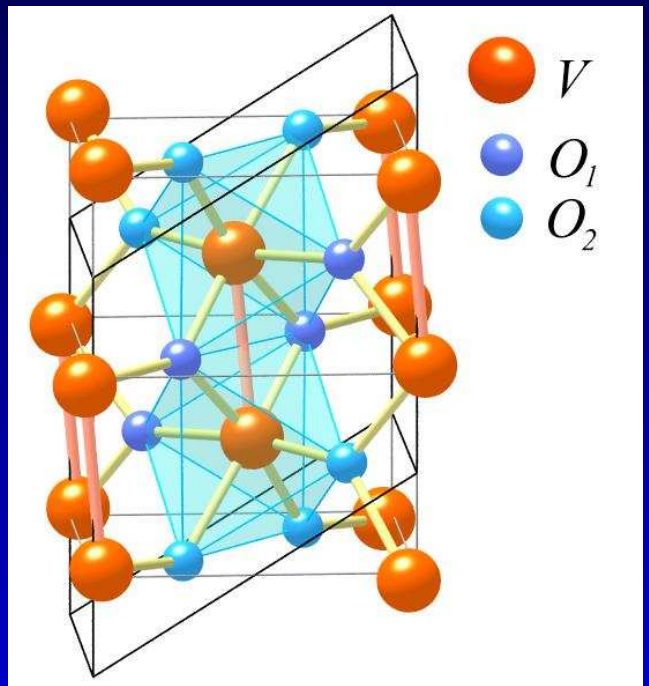
Metal-insulator transition in VO_2 at T_c=340 K

Morin et al., 1959

Structures of VO_2

Metal-insulator transition accompanied by dimerization of V atoms:
High-T: Rutile Low-T: Monoclinic





(pictures from V. Eyert)

VO_2: Peierls or Mott ?

PHYSICAL REVIEW B VOLUME 11, NUMBER 11 1 JUNE 1975

Metal-insulator transition in vanadium dioxide*

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Laboratoire Central de Recherches, Thomson-C.S.F., 91401 Orsay, France

N. F. Mott
Cavendish Laboratory, University of Cambridge, Cambridge, England
(Received 27 November 1974)

VOLUME 35, NUMBER 13 PHYSICAL REVIEW LETTERS 29 SEPTEMBER 1975

Electron Localization Induced by Uniaxial Stress in Pure VO_2

J. P. Pouget and H. Launois
Laboratoire de Physique des Solides, Université Paris XI, 91405 Orsay, France

and

J. P. D'Haenens and P. Merenda
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and

T. M. Rice
Bell Laboratories, Murray Hill, New Jersey 07974
(Received 7 August 1975)

VOLUME 72, NUMBER 21 PHYSICAL REVIEW LETTERS 23 MAY 1994

VO_2: Peierls or Mott-Hubbard? A View from Band Theory

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Department of Physics, State University of New York at Stony Brook, Stony Brook, New York 11794-3800
(Received 24 November 1993)

The electronic and structural properties of VO_2 across its metal-insulator transition are studied using the local-density approximation. Band theory finds a monoclinic distorted ground state in good agreement with experiment, and an almost open gap to charge excitations. Although rigid criteria for distinguishing correlated from band insulators are not available, these findings suggest that VO_2 may be more bandlike than correlated.

PRL 97, 266401 (2006) PHYSICAL REVIEW LETTERS week ending 31 DECEMBER 2006

Monoclinic and Correlated Metal Phase in VO_2 as Evidence of the Mott Transition: Coherent Phonon Analysis

Hyun-Tak Kim,[1,*] Yong Wook Lee,[1] Bong-Jun Kim,[1] Byung-Gyu Chae,[1] Sun Jin Yun,[1] Kwang-Yong Kang,[1] Kang-Jeon Han,[2] Ki-Ju Yee,[2] and Yong-Sik Lim[3]

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(Received 23 July 2006; published 26 December 2006)

In femtosecond pump-probe measurements, the appearance of coherent phonon oscillations at 4.5 and 6.0 THz indicating the rutile metal phase of VO_2 does not occur simultaneously with the first-order metal-insulator transition (MIT) near 68 °C. The monoclinic and correlated metal (MCM) phase between the MIT and the structural phase transition (SPT) is generated by a photoassisted hole excitation, which is evidence of the Mott transition. The SPT between the MCM phase and the rutile metal phase occurs due to subsequent Joule heating. The MCM phase can be regarded as an intermediate nonequilibrium state.

Evidence for a Mott-Hubbard metal-insulator transition in VO_2

R. Eguchi,[1,*] M. Taguchi,[1] M. Matsunami,[1] K. Horiba,[1] K. Yamamoto,[1] Y. Ishida,[1] A. Chainani,[1] Y. Takata,[1] M. Yabashi,[2,3] D. Miwa,[2] Y. Nishino,[2] K. Tamasaku,[2] T. Ishikawa,[2,3] Y. Senba,[3] H. Ohashi,[3] Y. Muraoka,[4] Z. Hiroi,[4] and S. Shin[1,4]

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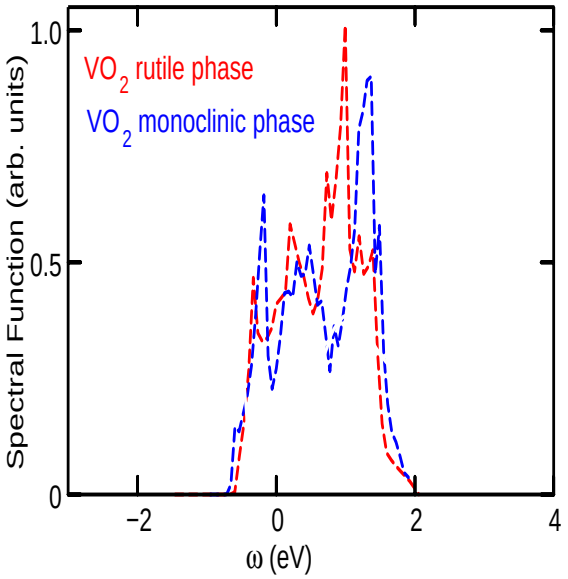
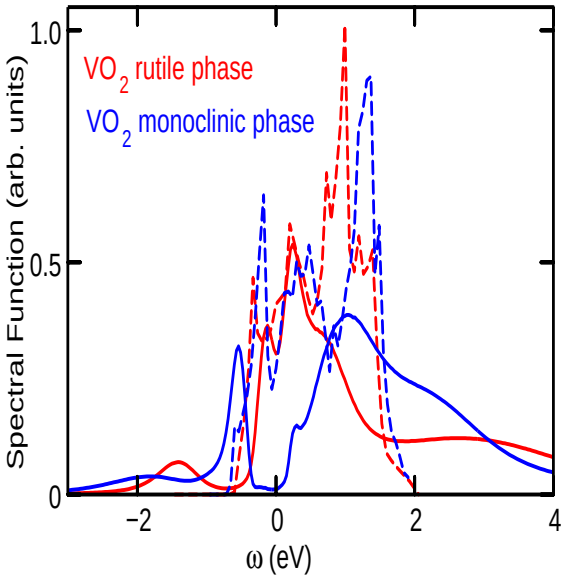
[3]*JASRI/SPring-8, Sayo-cho, Sayo-gun, Hyogo 679-5198, Japan*
[4]*Institute for Solid State Physics, University of Tokyo, Kashiwanoha, Kashiwa, Chiba 277-8581, Japan*
(Dated: July 28, 2006)

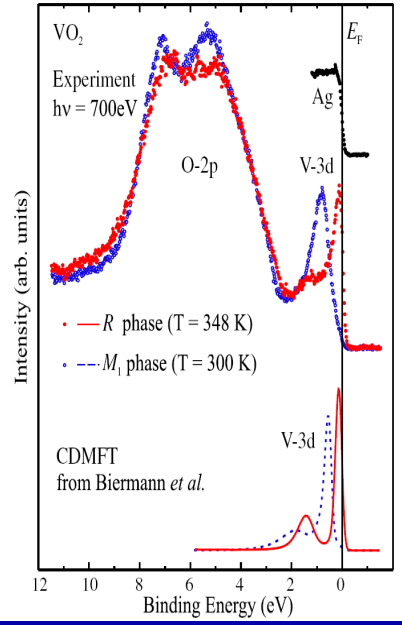
see also: Liebsch et al., Tanaka, Laad et al., Qazilbash et al., ...

VO_2 : Spectra

LDA-DOS LDA+DMFT PES vs. LDA+DMFT







PES: Koethe et al., PRL 2006

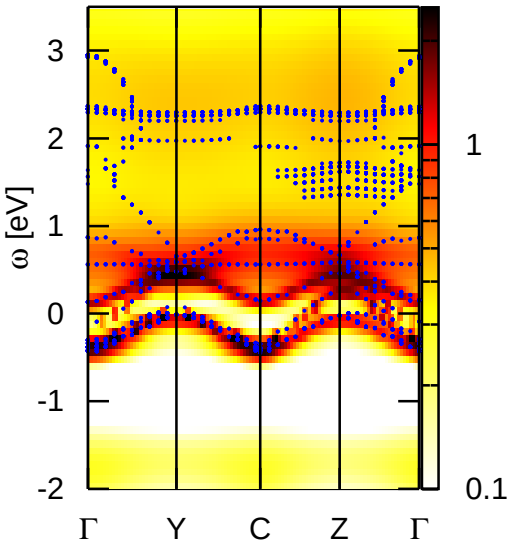
LDA+(cluster-)DMFT: S. Biermann, A. Poteryaev, A. I. Lichtenstein, A. Georges, PRL 2005

see also work by Liebsch et al., Laad et al.

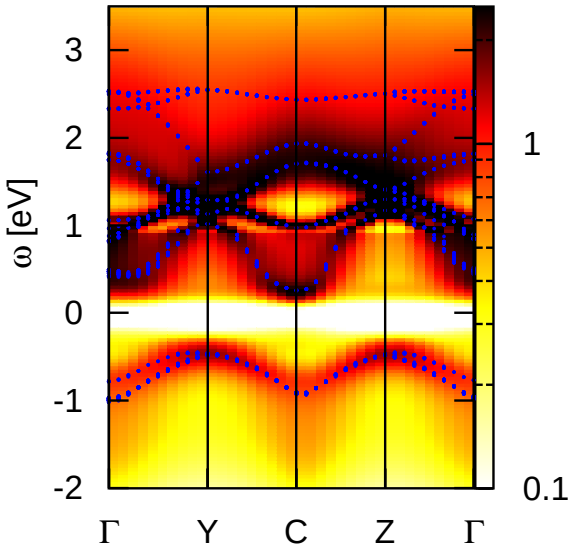
VO_2 : the physical picture

Charge transfer $e_g^\pi \rightarrow a_{1g}$ and bonding-antibonding splitting

metallic phase:



insulating phase:



Spectral functions and "band structure"

$$\det\left(\omega_{\mathbf{k}} + \mu - H^{\mathrm{LDA}}(\mathbf{k}) - \Re\Sigma(\omega_{\mathbf{k}})\right) = 0$$

J.M. Tomczak, S.B., J.Phys.:Cond.Mat. 2007; J.M. Tomczak, F. Aryasetiawan, S.B., PRB 2008

Susceptibility

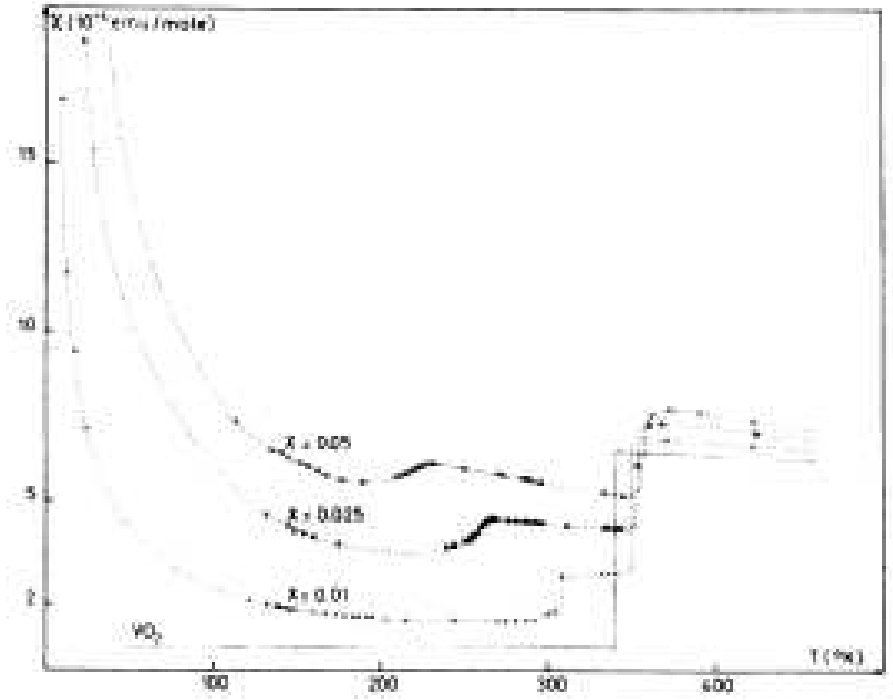
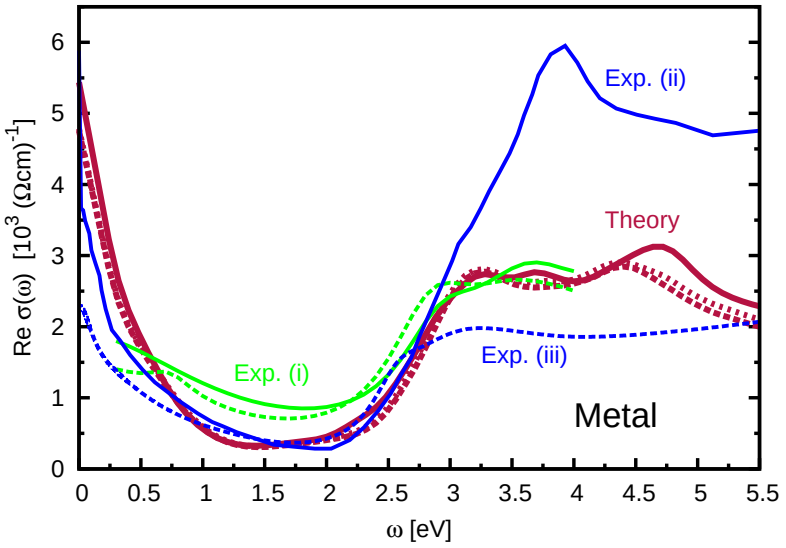


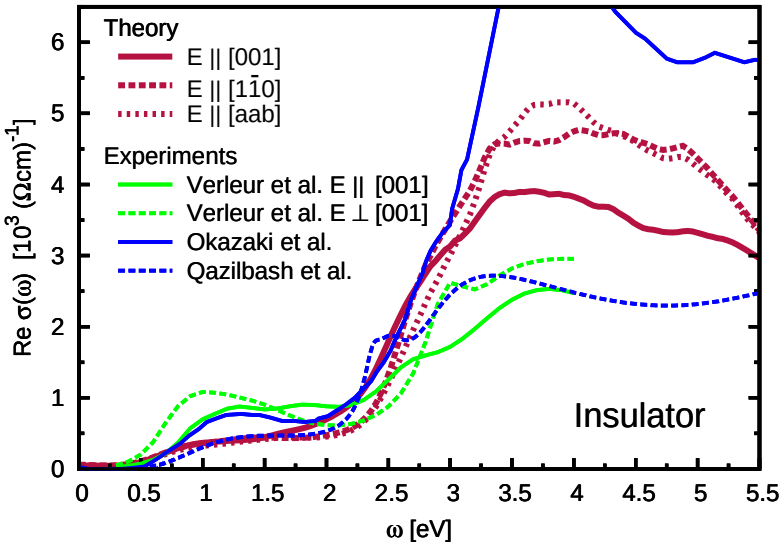
FIG. 6. Magnetic susceptibility of $V_{1-x}Cr_xO_2$ vs temperature.

From Pouget et al.

flat susceptibility in monoclinic phase, corresponding to singlet state

Optical Conductivity of VO_2





[Verleur *et al.*] : single crystals

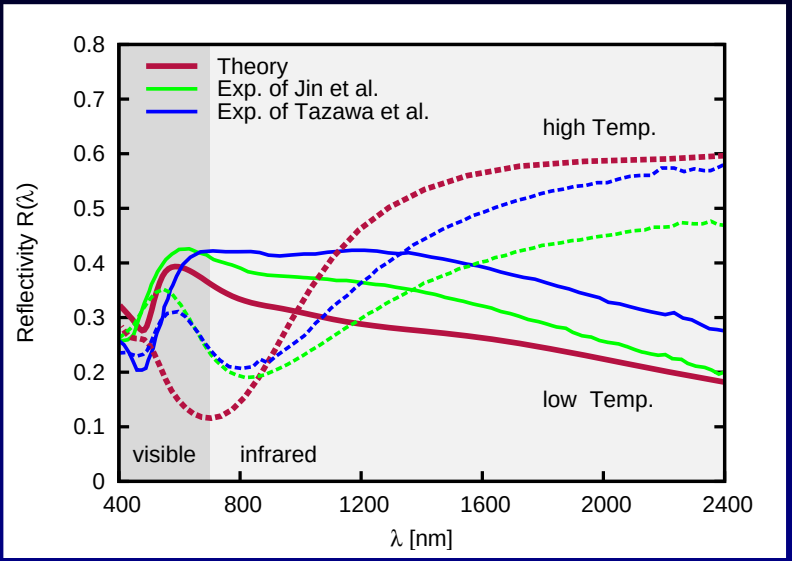
[Okazaki *et al.*] : thin films $E \perp [001]$, T_c=290 K

[Qazilbash *et al.*] : polycrystalline films, preferential $E \perp [010]$, T_c=340 K

J.M. Tomczak, PhD thesis 2007.

J.M. Tomczak, S.B., Europhys. Lett. 2009.

Setup of an Intelligent Window?

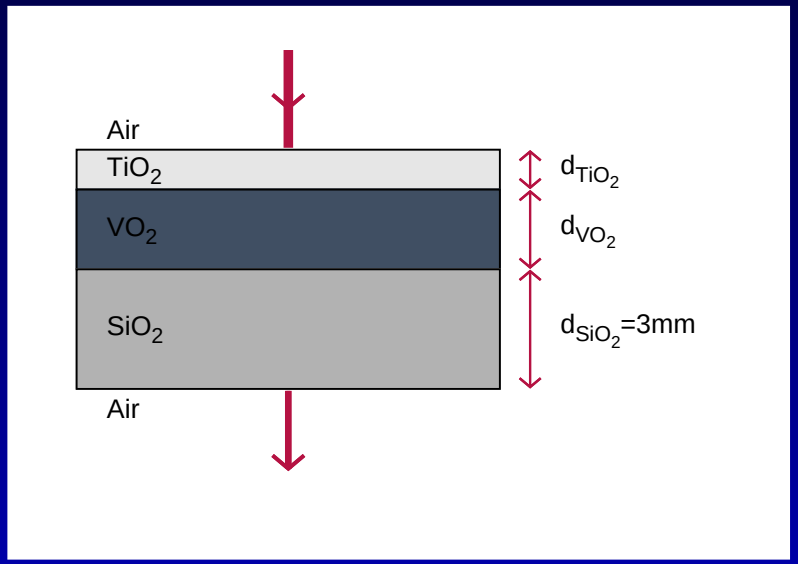


50nm VO_2 on SiO_2

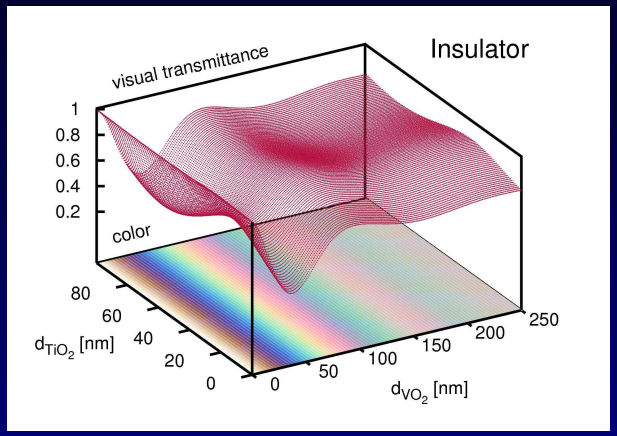
- infrared switching
- non uniform reflectivity for visible light
- reflectivity for visible light not low

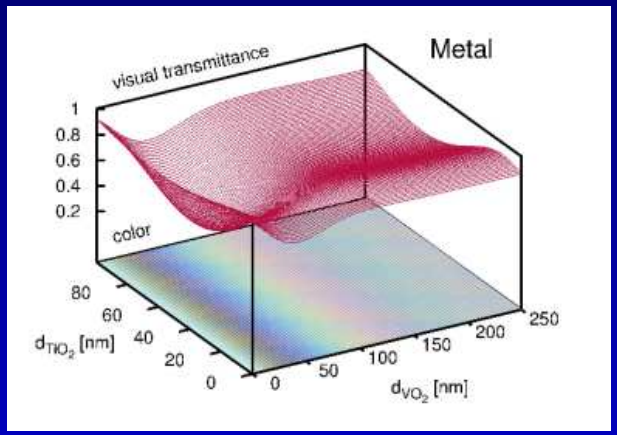
Intelligent Window?

TiO_2 on VO_2 on SiO_2



Visual transmittance





visual transmittance (S : spectrum of the light source) :

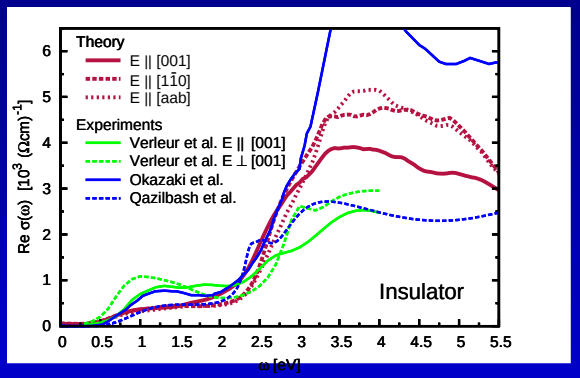
$\int_{400nm}^{700nm} d\lambda S(\lambda)T(\lambda) / \int_{400nm}^{700nm} d\lambda S(\lambda)$

J.M. Tomczak, S.B., Europhys. Lett. 2009.

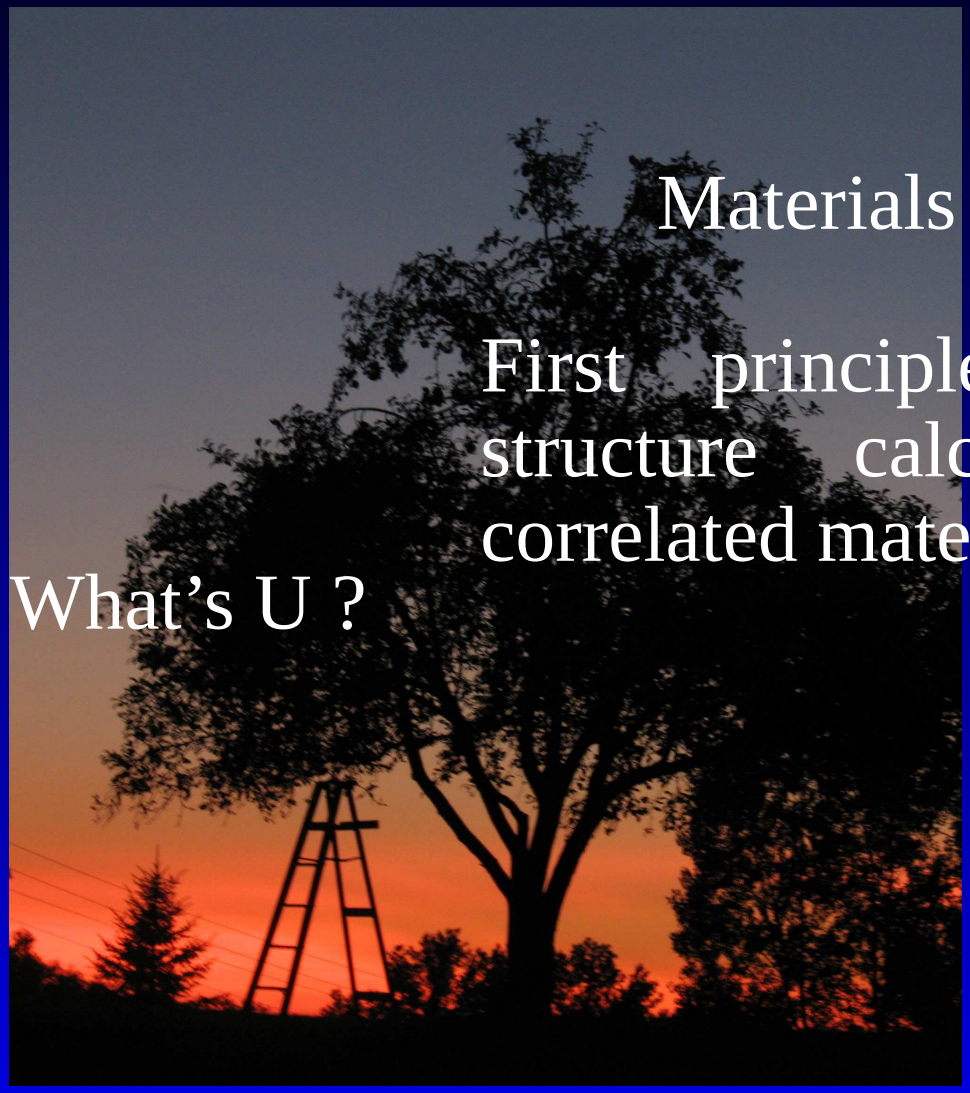
- Optics calculations in *semi-quantitative* agreement with experiments
- predictions become possible, even for correlated materials

$\longrightarrow$ theoretically guided design of materials?

Example: VO_2



Jacob's ladder ?

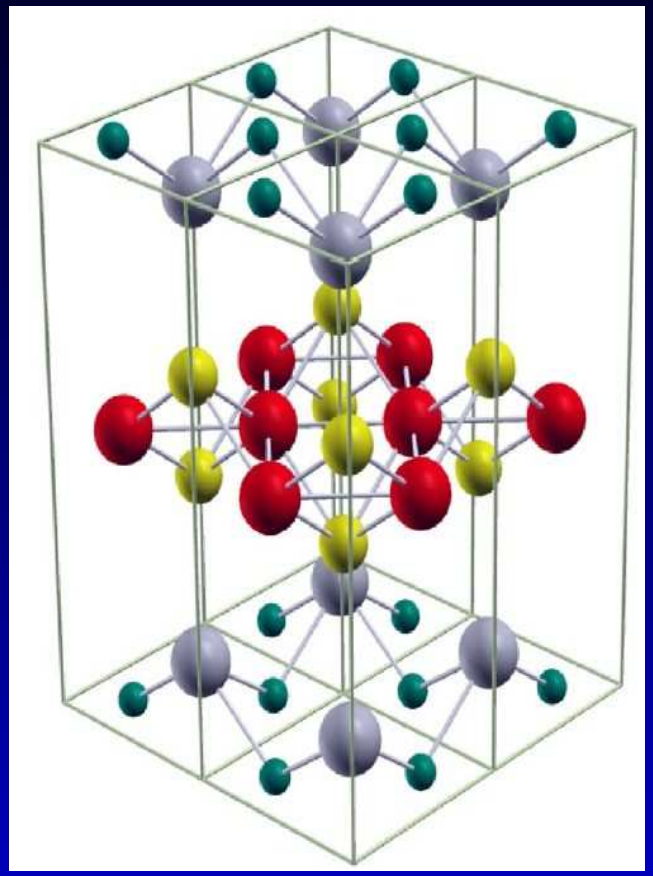


Materials Design

First principles electronic structure calculations for correlated materials

What's U ?

LaFeAsO



Fe

As

RE=La, Ce,
Pr, Sm,...

O

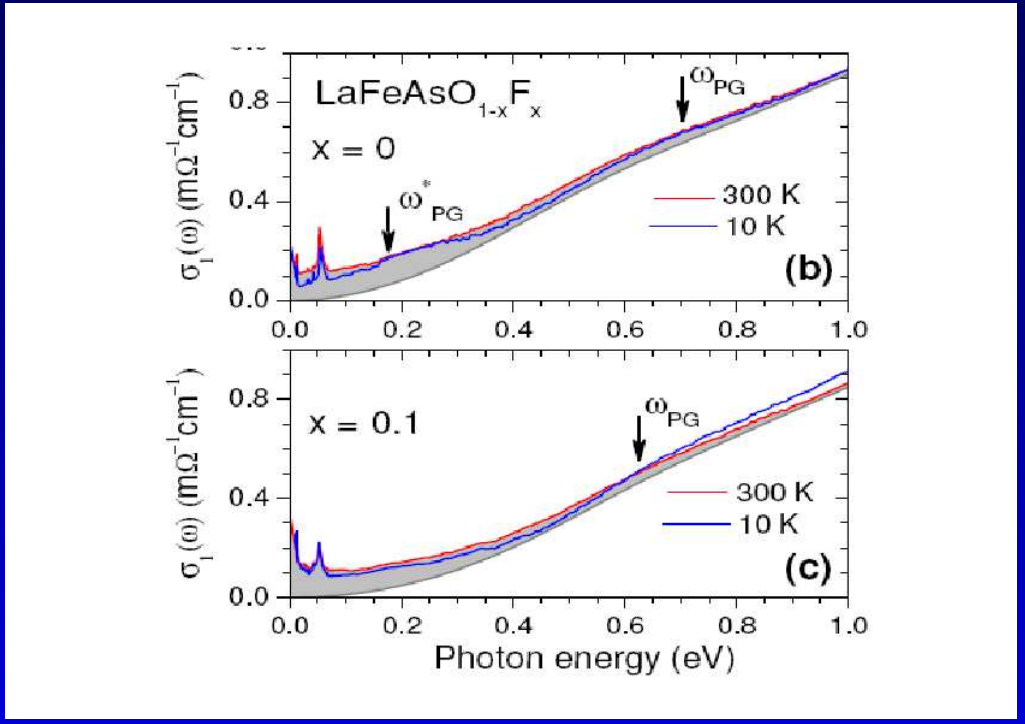
Parent compound of new iron oxypnictide superconductors
Fe-d states, hybridising with As-p and O-p bands

Correlations in LaFeAsO?

Experimental (ARPES, XAS, optics ...) indications of weak or moderate correlations

Mass enhancement from ARPES $\sim$ 1.8 - 2.2

Optics (Boris et al.):



DMFT work: Shim et al., Anisimov et al., Craco et al. (also related compounds: Skornyakov et al.)

What's U in LaFeAsO?

"d-model" within cRPA (cf. Ferdi Aryasetiawan's talk)

$$U^{\sigma\bar{\sigma}}_{mm'}| = \begin{pmatrix} 3.17 & 2.02 & 1.72 & 2.22 & 2.22 \\ 2.02 & 3.36 & 2.16 & 2.04 & 2.04 \\ 1.72 & 2.16 & 2.17 & 1.73 & 1.73 \\ 2.22 & 2.04 & 1.73 & 2.73 & 1.84 \\ 2.22 & 2.04 & 1.73 & 1.84 & 2.73 \end{pmatrix}$$

Very anisotropic!

Very extended orbitals! cf Vildosola et al., PRB 2008

U=2.14 eV, J=0.6 eV

(Aichhorn, ... , **Miyake**, ... PRB 2009), see also Nakamura et al., JPSJ 2009.

CRPA: Aryasetiawan et al., PRB 2004.

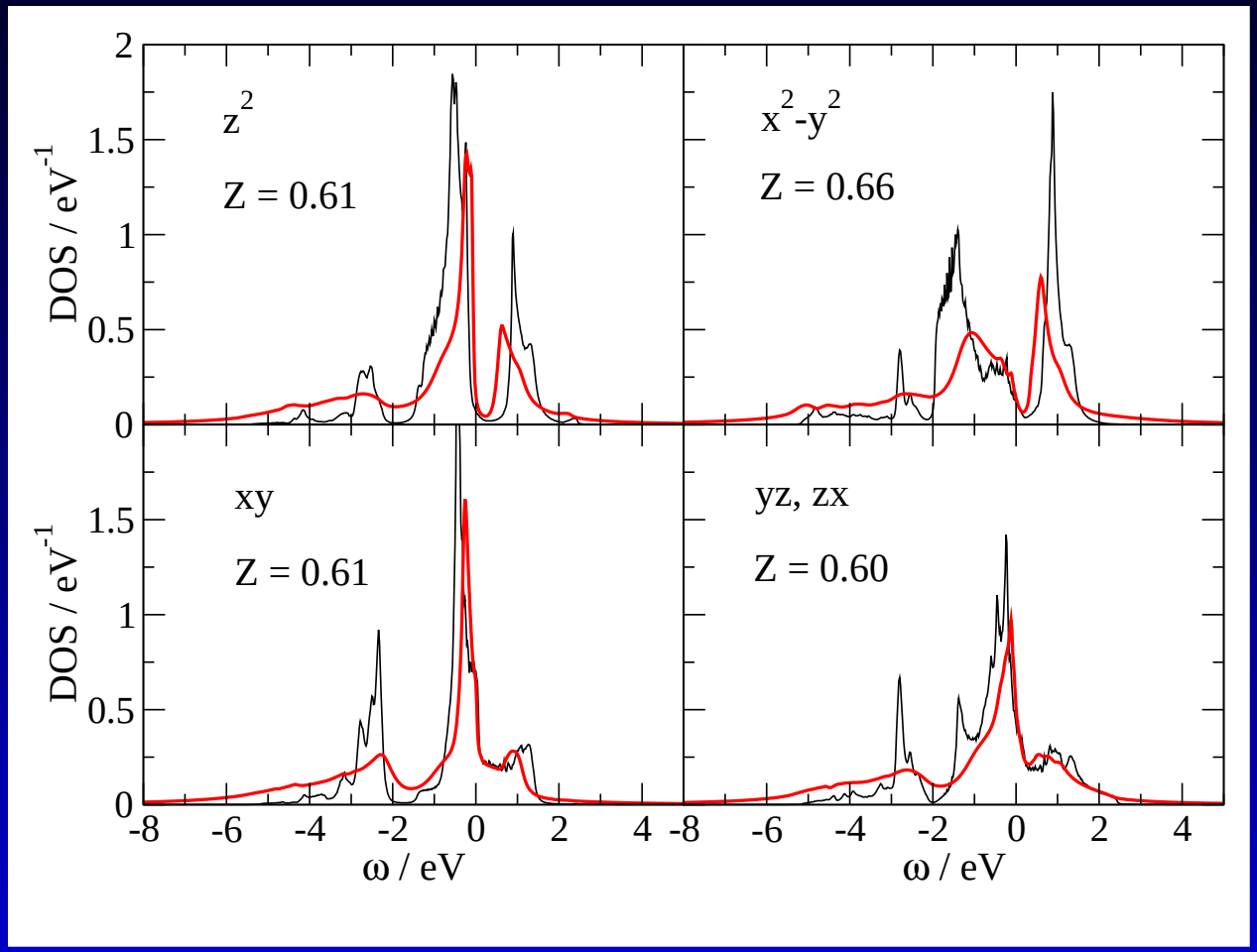
What's U in LaFeAsO?

"dpp-model" comprising Fe-d, As-p, O-p

$$U^{\sigma\bar{\sigma}}_{mm'} = \begin{pmatrix} 3.77 & 2.35 & 2.21 & 2.71 & 2.71 \\ 2.35 & 3.94 & 2.87 & 2.44 & 2.44 \\ 2.21 & 2.87 & 3.31 & 2.29 & 2.29 \\ 2.71 & 2.44 & 2.29 & 3.48 & 2.29 \\ 2.71 & 2.44 & 2.29 & 2.29 & 3.48 \end{pmatrix}$$

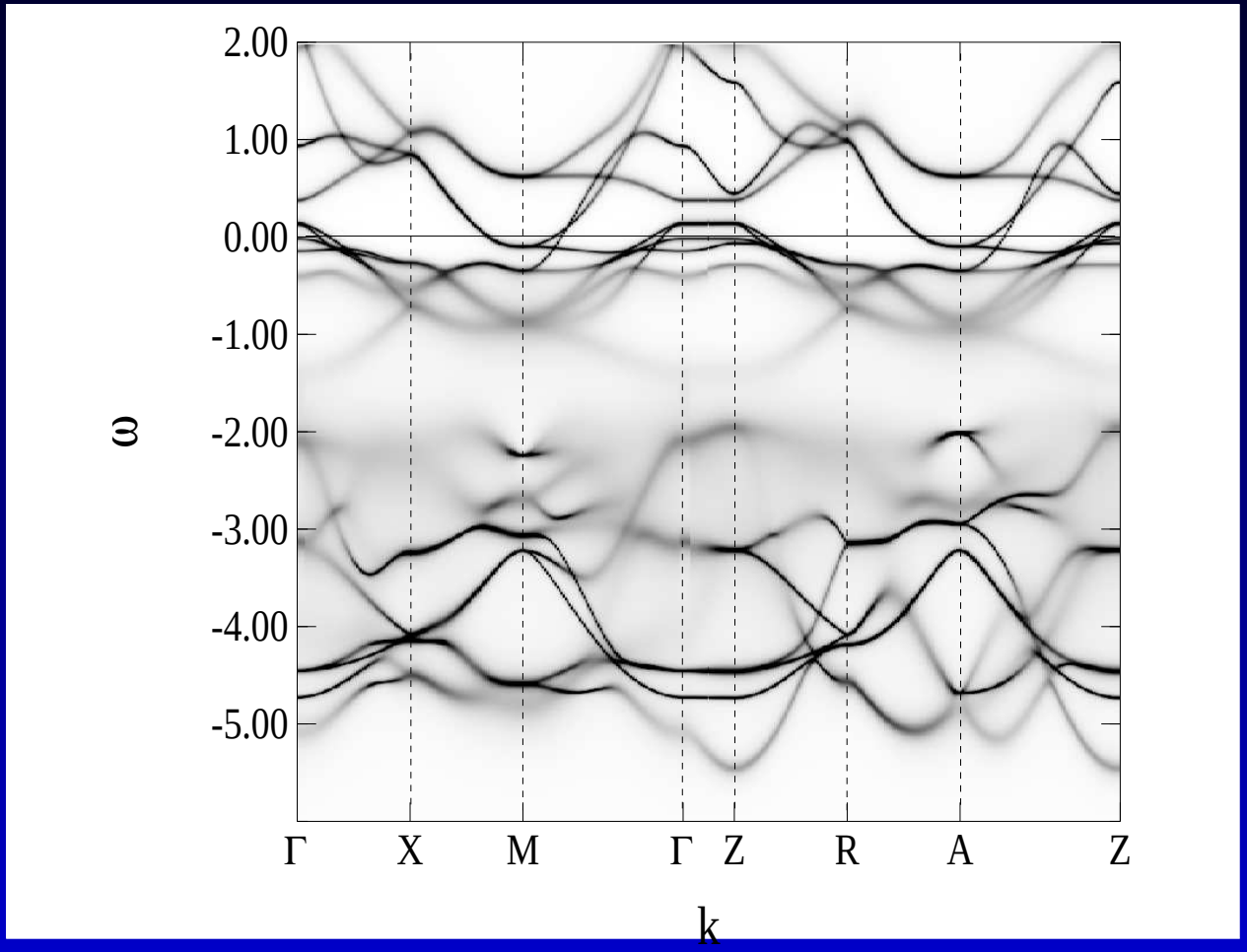
U=2.7eV, J=0.8eV

LaFeAsO in DMFT



Aichhorn, Pourovskii, Vildosola, Ferrero, Parcollet, Miyake, Georges, SB, PRB 2009

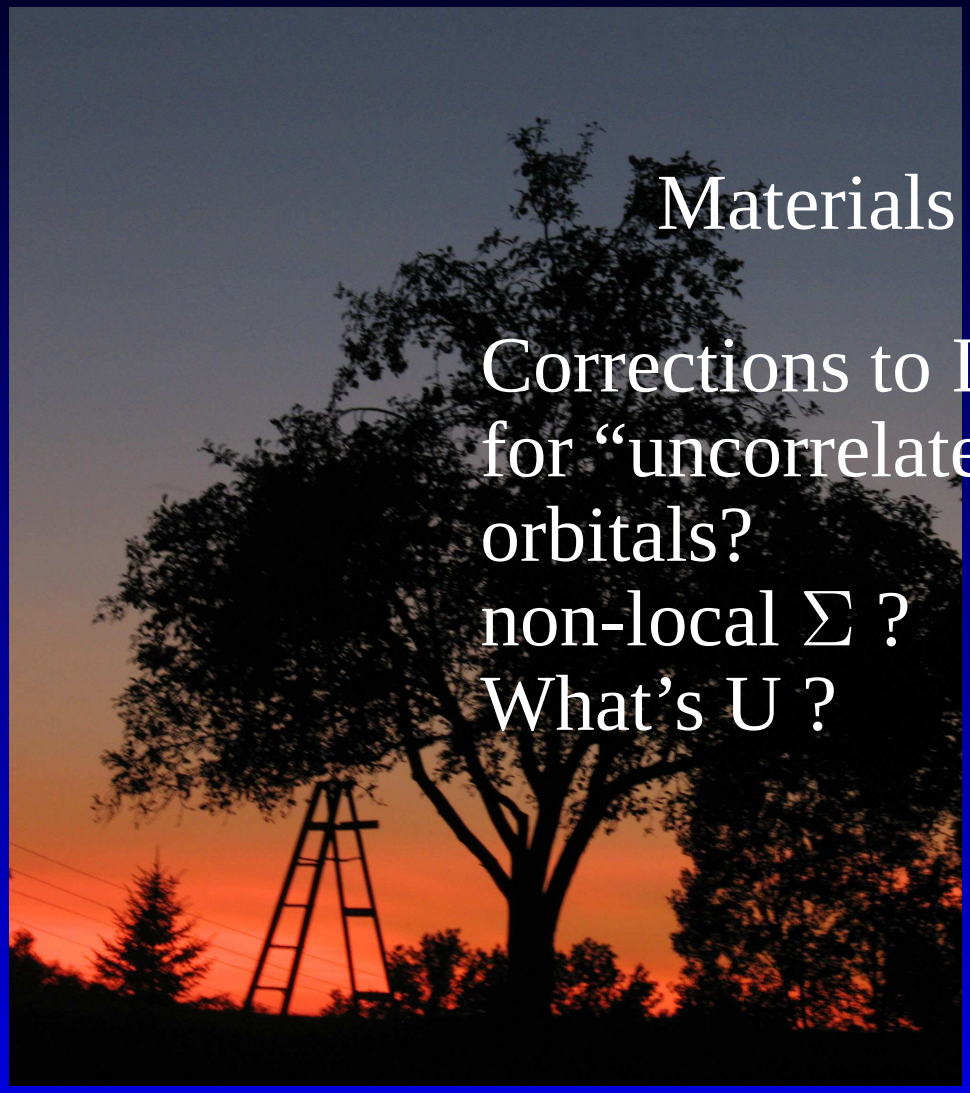
LaFeAsO in DMFT



Well-defined quasi-particles close to E_F, damping effects beyond ~ 0.5 eV.

Aichhorn, Pourovskii, Vildosola, Ferrero, Parcollet, Miyake, Georges, SB, PRB 2009

Jacob's ladder ?



Materials Design

Corrections to LDA
for "uncorrelated"
orbitals?
non-local Σ ?
What's U ?

LDA+DMFT without LDA?

LDA+DMFT without LDA?

$\longrightarrow$ GW+DMFT

(somewhere high up on the Jacob's ladder ...)

A functional point of view

[Chitra & Kotliar, 2001, Almbladh et al. 1999]

$$\Gamma[G,W] = \mathrm{Tr}\ln G - \mathrm{Tr}[(G_H{}^{-1} - G^{-1})G]$$
$$-\frac{1}{2}\mathrm{Tr}\ln W + \frac{1}{2}\mathrm{Tr}[(V^{-1} - W^{-1})W] + \Psi[G,W]$$

Free energy Γ is a functional of

- one-electron Green's function
  $G(\mathbf{r},\mathbf{r}';\tau-\tau') \equiv -\langle T_\tau\, \psi(\mathbf{r},\tau)\psi^\dagger(\mathbf{r}',\tau')\rangle$
- the screened Coulomb interaction
  $W = V - V\chi V$

G_H = bare (Hartree) Green's function

Approximations to Psi ?

GW: $\Psi_{GW}[G,W] = -\frac{1}{2} TrGWG$

Extended DMFT ("E-DMFT"):
$\Psi_{DMFT}[G,W] = \Psi_{impurity}[G_{impurity}, W_{impurity}]$

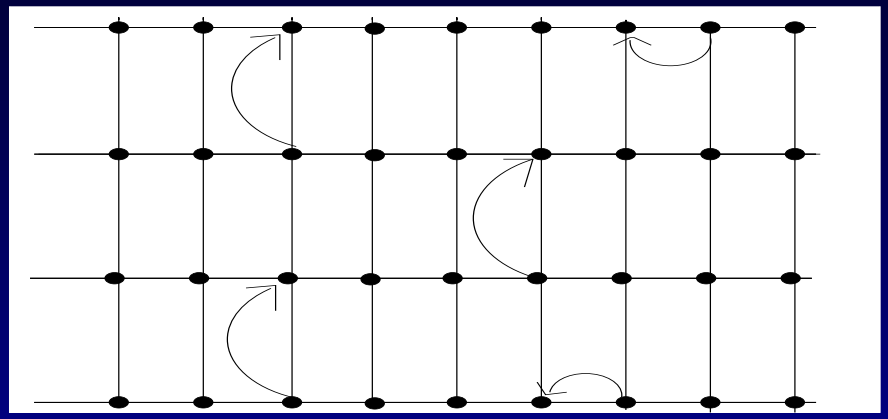
E-DMFT for local part of correlated orbitals + GW for nonlocal part and *uncorrelated* orbitals:
$\Psi_{GW+DMFT}[G,W] = \Psi_{DMFT} + \Psi_{GW}^{nonlocal}$

S.B., F. Aryasetiawan, A. Georges PRL **90** *086402 (2003) + cond-mat/0401653*

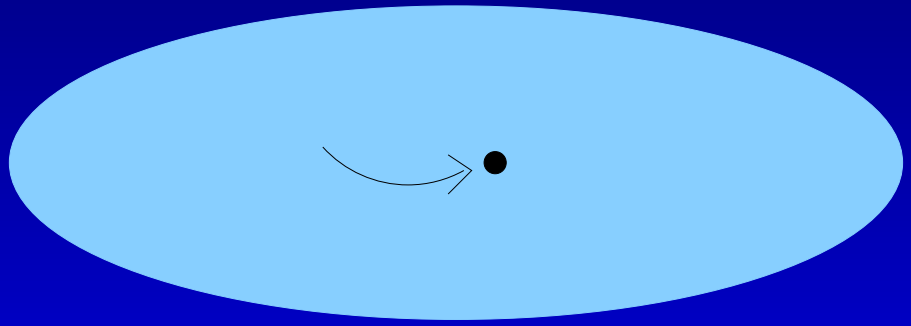
NB: "local" = "onsite" is a basis-set dependent notion!

Extended DMFT ...

... maps a lattice problem



onto a single-site (Anderson impurity) problem



with a *dynamical* interaction $\mathcal{U}(\tau - \tau')$

GW+DMFT: local part

$\Psi_{imp}[G_{imp}, W_{imp}]$ calculated from local impurity model:

$$S_{imp} = \int d\tau d\tau' \Big[-\sum c^\dagger_L(\tau) \mathcal{G}^{-1}_{LL'}(\tau - \tau') c_{L'}(\tau') + \sum : c^\dagger_{L_1}(\tau) c_{L_2}(\tau) : \mathcal{U}_{L_1 \ldots L_4}(\tau - \tau') : c^\dagger_{L_3}(\tau') c_{L_4}(\tau') : \Big]$$

$$\begin{aligned} G^{LL'}_{imp} &= -\langle T_\tau c_L(\tau) c^+_{L'}(\tau') \rangle_S \\ \chi_{L_1 L_2 L_3 L_4} &= \langle : c^\dagger_{L_1}(\tau) c_{L_2}(\tau) :: c^\dagger_{L_3}(\tau') c_{L_4}(\tau') : \rangle_S \\ W_{imp} &= \mathcal{U} - \mathcal{U} \chi \mathcal{U} \end{aligned}$$

Self-consistency loop

$$\text{Impurity model :}$$

$$\mathcal{G}(\tau), \mathcal{U}(\tau)$$

$$G_{imp} \equiv -\langle T_\tau \, c c^\dagger \rangle_S \;\rightarrow\; \Sigma^{xc}_{imp} = \mathcal{G}^{-1} - G^{-1}_{imp}$$

$$W_{imp} = \mathcal{U} - \mathcal{U}\chi\mathcal{U} \qquad P_{imp} = \mathcal{U}^{-1} - W^{-1}_{imp}$$

$$\uparrow \qquad\qquad \downarrow$$

$$\text{Update} \qquad\qquad \text{Combine :}$$

$$\mathcal{G}^{-1} = G^{-1}_{loc} + \Sigma_{imp} \qquad \Sigma = \Sigma_{imp} + \Sigma^{nonlocal}_{GW}$$

$$\mathcal{U}^{-1} = W^{-1}_{loc} + P_{imp} \qquad P = P_{imp} + P^{nonlocal}_{GW}$$

$$\uparrow \qquad\qquad \downarrow$$

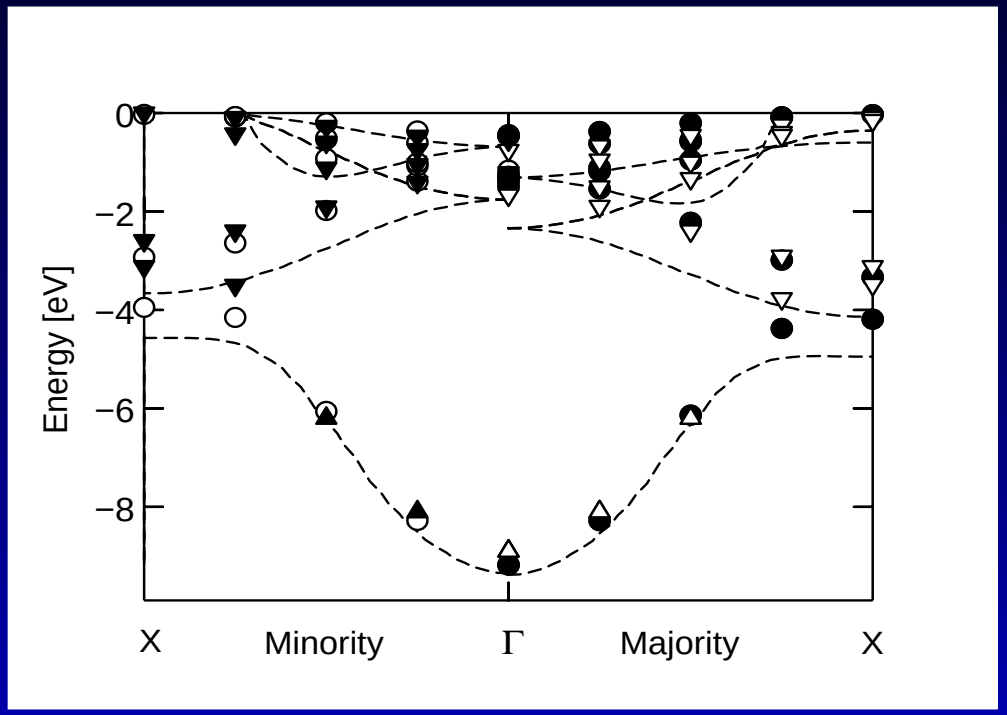
$$\text{Self} - \text{consistency}$$

$$G_{loc} = \sum_{\mathbf{k}} [{G_H}^{-1} - \Sigma^{xc}]^{-1}$$

$$W_{loc} = \sum_{\mathbf{q}} [V^{-1}_{\mathbf{q}} - P]^{-1}$$

Simplified GW+DMFT

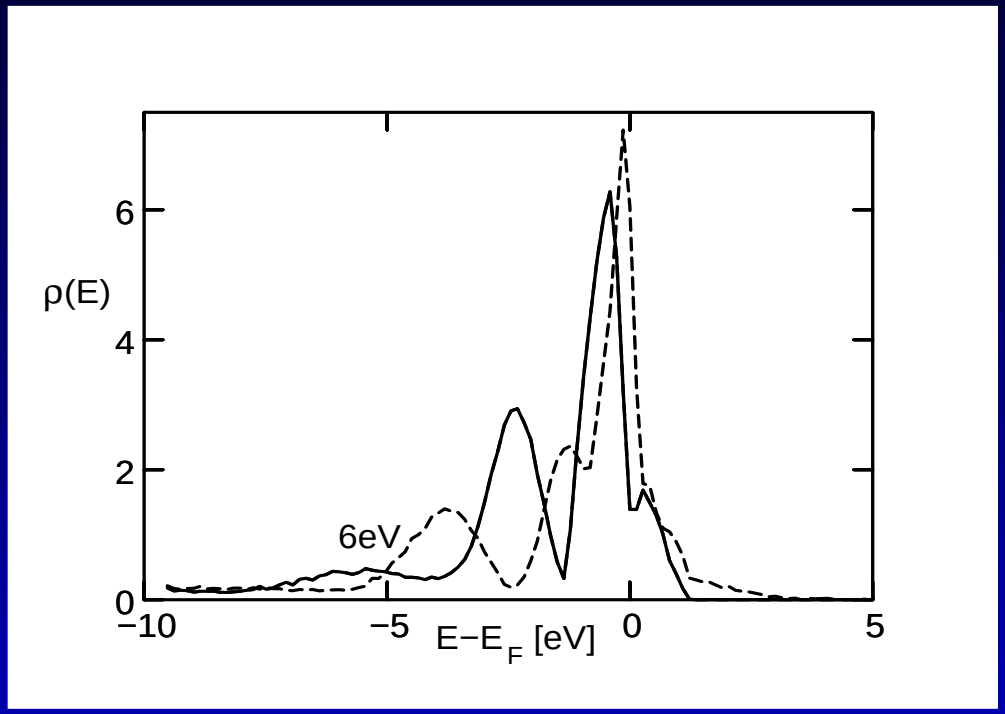
Ni band structure



Circles: GW+DMFT
Dashed: LDA
Triangles: photoemission data
(Bünemann et al. 2002, Mårtensson et al., 1984)
Simplified GW+DMFT = non-sc GW and local self-energy from impurity model

Simplified GW+DMFT:

Spectral function of Ni



Majority and minority spins

Satellite at 6eV correct!

Conclusions

- LDA+DMFT useful tool for a wide range of properties of correlated materials
- More and more versatile implementations
- Consistency between different choices of orbitals
- Challenge: first principles U! $\rightarrow$ CRPA ?
- Get rid of LDA ...? $\rightarrow$ GW+DMFT

Collaborations and references

- Different LDA+DMFT implementations:
  Aichhorn, Pourovskii, Vildosola, Ferrero, Parcollet, Miyake, Georges, SB, PRB 2009
  F. Lechermann, A. Georges, A. Poteryaev, SB, M. Posternak, A. Yamasaki,O. K. Andersen, PRB 2006
- Constrained RPA:
  F. Aryasetiawan, M. Imada, A. Georges, G. Kotliar, S. B., A. I. Lichtenstein, Phys. Rev. B 70, 195104 (2004)
- Manganese: S. Biermann, PhD thesis 2000
  S. Biermann, A. Dallmeyer, C. Carbone, W. Eberhardt, C. Pampuch, O. Rader, M. I. Katsnelson, A. I. Lichtenstein, JETP Letters (2004) and arXiv 2001.
- Cerium: B. Amadon, S. B., A. Georges, F. Aryasetiawan, PRL 2006

Collaborations and references

- Pnictides:

  Aichhorn, Pourovskii, Vildosola, Ferrero, Parcollet, Miyake, Georges, SB, PRB 2009

  Miyake, Pourovskii, Vildosola, SB, Georges, JPSJ 2009.

  Pourovskii, Vildosola, Biermann, Georges, EPL 2009.

  Vildosola, Pourovskii, Arita, Biermann, Georges, PRB 2008.

- VO_2: Metal-insulator transition, effective potential, optics scheme, and dirty windows:

  J. Tomczak and SB, EPL, 2009.

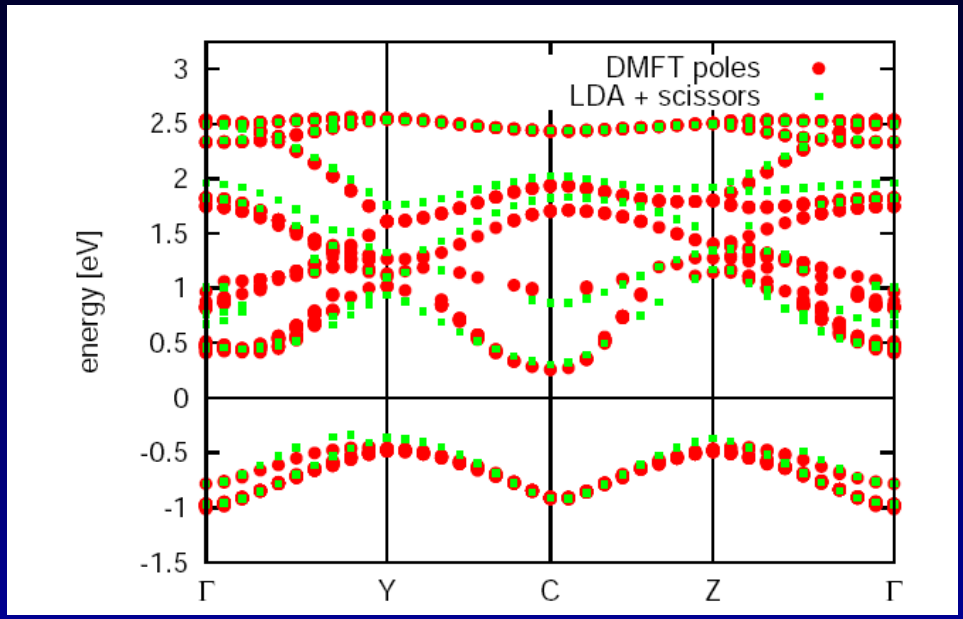
  J. Tomczak and SB, PRB 2009, Phys. Stat. Solidi, 2009.

  J. Tomczak, F. Aryasetiawan, S.B., PRB 2007;

  J. Tomczak and S.B., J. Phys. Cond. Mat. 2007;

  S.B., A. Poteryaev, A. Georges, A. Lichtenstein, PRL 2005

VO_2 monoclinic phase



quasi-particle poles (solutions of det[$\omega + \mu - H(k) - \Sigma(\omega)$]=0) and band structure from effective (orbital-dependent) potential

$\longrightarrow$ gap opening obtained from static (beyond-LDA-) potential

$\longrightarrow$ Result of DMFT: DMFT not really necessary ... !

(Tomczak and S.B., J. Phys. Cond. Mat, 2007)

NB. Confirmed by the fact that the band structure obtained from QP-self-consistent GW indeed also displays a gap! (Gatti et al, PRL 2007, Sakuma et al., PRB)