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Electronic structure of strongly correlated materials with dynamical mean-field theory: Challenges and Perspectives

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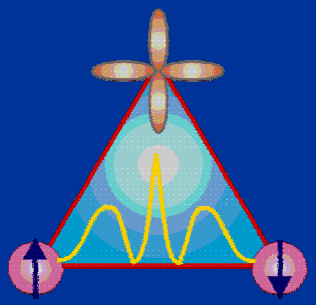
Electronic structure of strongly correlated materials with Dynamical Mean-Field Theory: Challenges and Perspectives



Antoine GEORGES

Ecole Polytechnique

Trieste, January 2007

http://www.cpht.polytechnique.fr/cpht/correl/mainpage.htm

Status report on recent achievements

- Flexible implementations within basically any electronic structure method (in progress)
- Calculation of quasiparticle band-structure (momentum-resolved spectral density) and of Fermi surfaces
- Optical spectra, Phonons
- Total energy
- Significant recent progress in computational efficiency of DMFT from alternative forms of QMC algorithms

Aim of this lecture…

- DMFT will be only briefly introduced and motivated
- In this talk I want to point out a few issues, both conceptual and practical, regarding implementation within electronic structure methods, e.g:

- Conceptual difference between correlated orbitals and basis set
- Choice of basis set and implementation in any electronic structure method, Wannier functions.

Illustrated by some recently studied physical examples

- Frontier of the field: challenges ahead.

I. MOTIVATIONS: DMFT aims at overcoming some of the limitations of DFT-LDA for correlated materials, which are twofold:

- **A) Ground-state issues**

When some of the electrons are rather well localized in certain orbitals (typically, d- and f-orbitals), LDA has a tendency to **OVERBIND**

i.e the participation of those electrons in the electronic cohesive energy of the solid is overestimated, resulting in a too small (sometimes MUCH too small) value of the unit-cell volume at equilibrium

Example (a dramatic one): delta-Plutonium

GGA underestimates unit-cell volume by ~ 30 % !

(cf. work of several groups)

Bulk modulus one order of magnitude too large

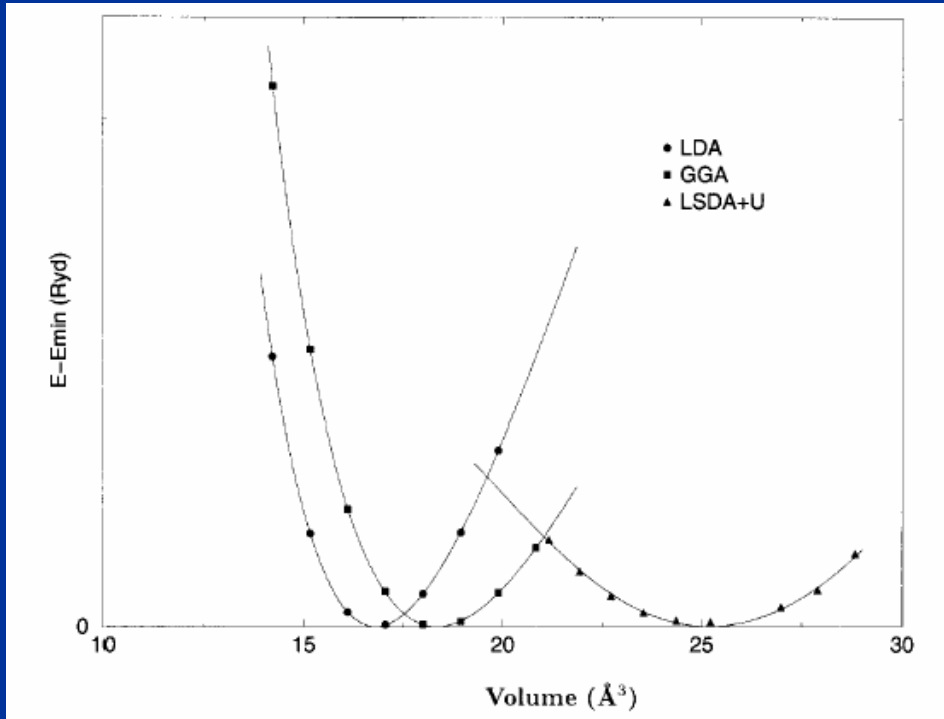


Figure 1. The total energy of δ-Pu versus the volume calculated using the LDA, the GGA and the LSDA + U method.

Bouchet et al. J.Phys.C 2000
Savrasov&Kotliar, PRL 2000

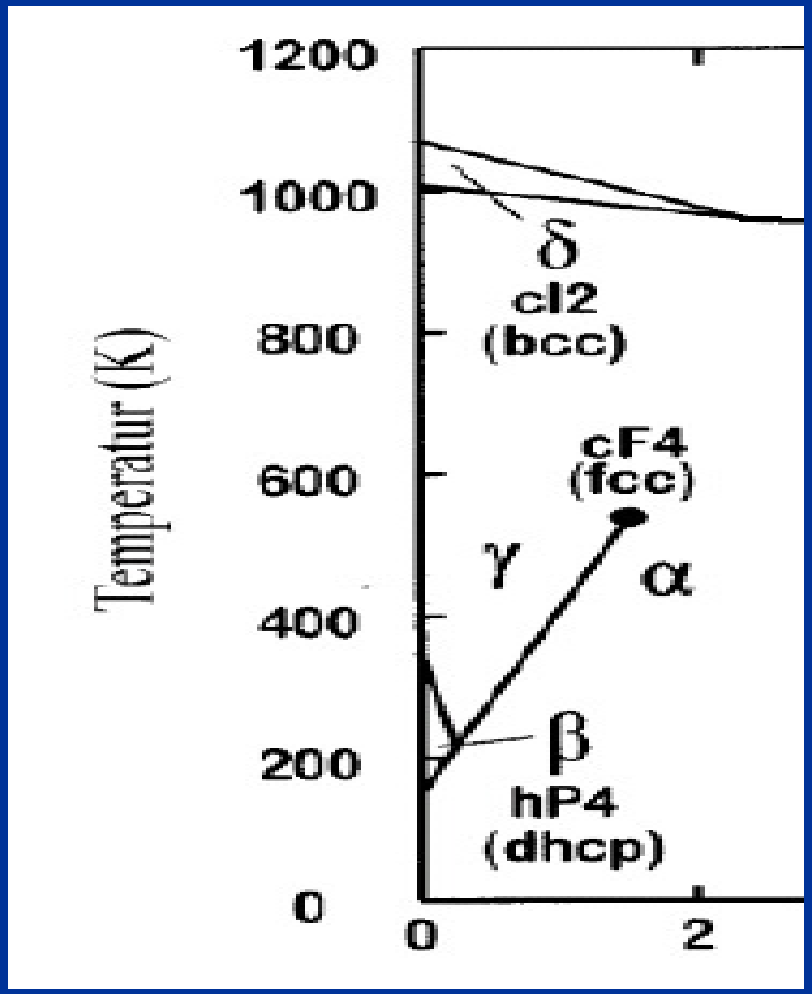
L(S)DA+U corrects the volume but leads to long-range magnetic order, in contradiction to experiments

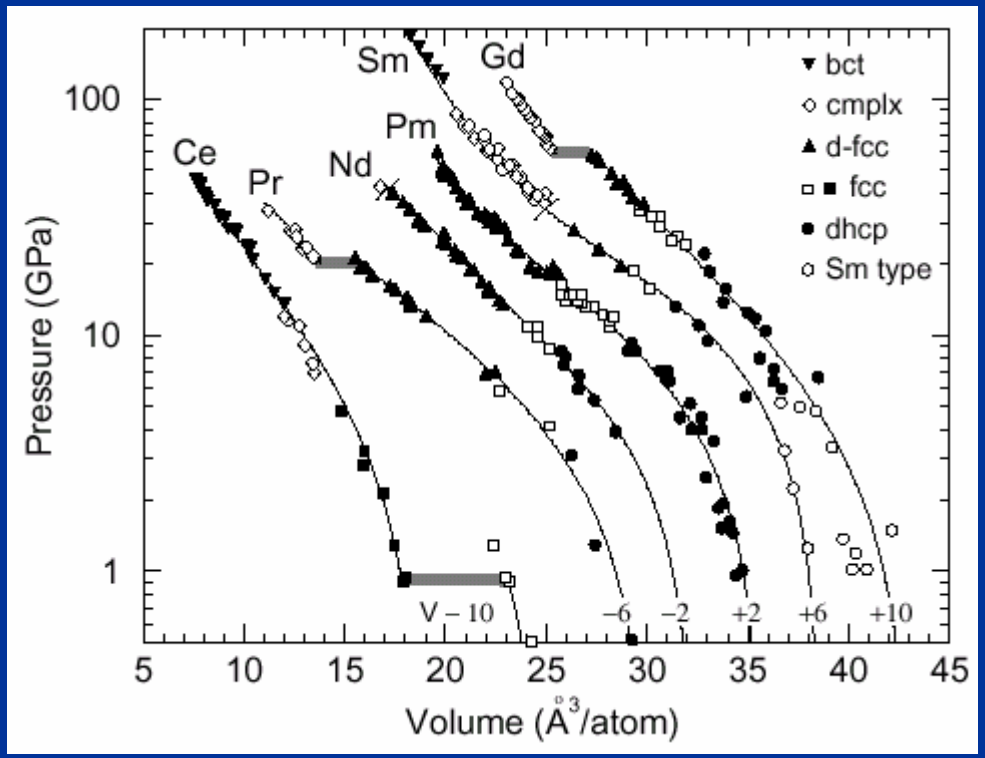
When the electrons are well localized, the problem can be fixed (to some extent) by **treating these orbitals as core**.
However:
-Generally leads to underestimate of cohesive energy
-Hence, too large volumes (cf. rare-earths)

The problem becomes crucial when electrons are in ***an intermediate regime between being localized and being itinerant***, and especially when a phase transition takes place from one behaviour to the other (as a function of e.g pressure)

Well-known examples:
f-states: alpha-gamma transition of Cerium, Americium under pressure, etc…
d-states: metal- Mott insulator transition

Delocalization/localization transition in rare-earths (e.g cerium α-γ)

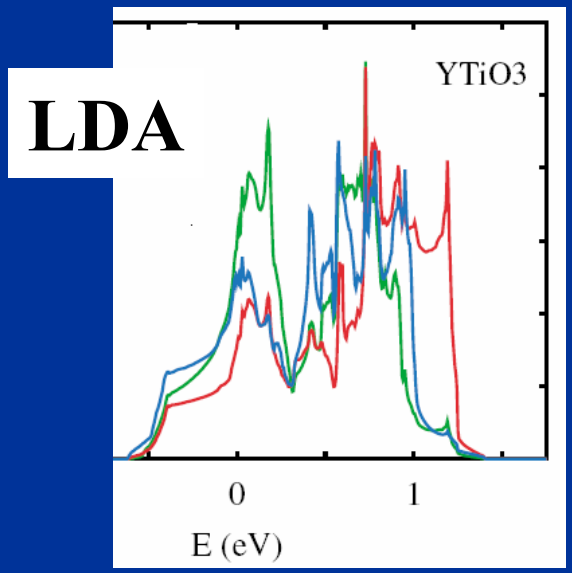


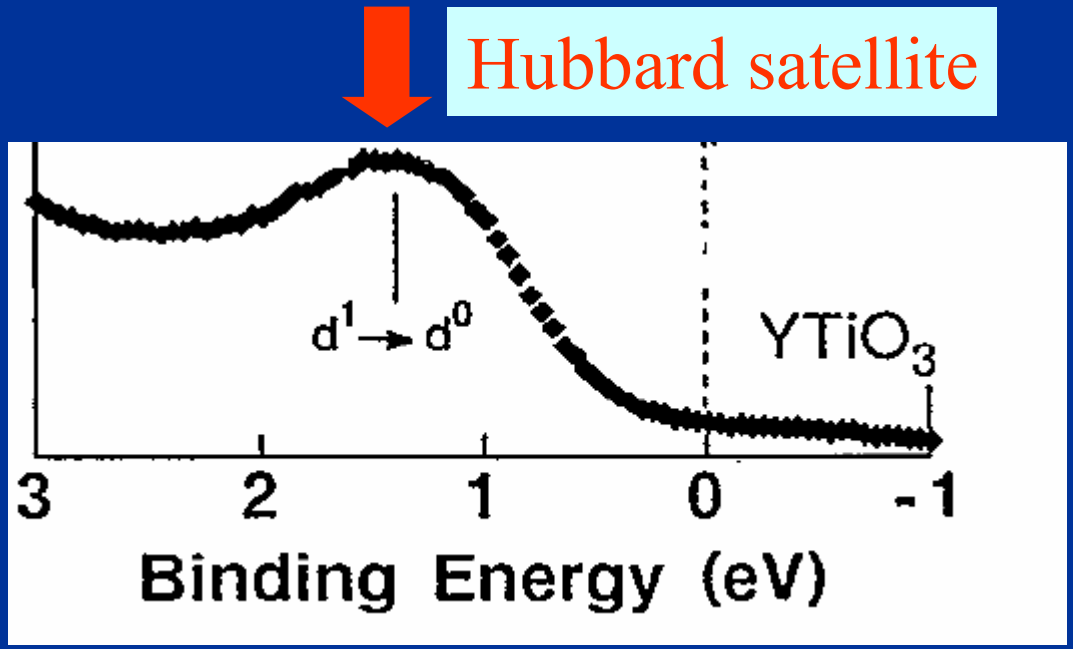


B) Difficulties with excited states

The interpretation of Kohn-Sham spectra as excitations is in serious trouble in the case of correlated materials

- The most dramatic examples are Mott insulators:



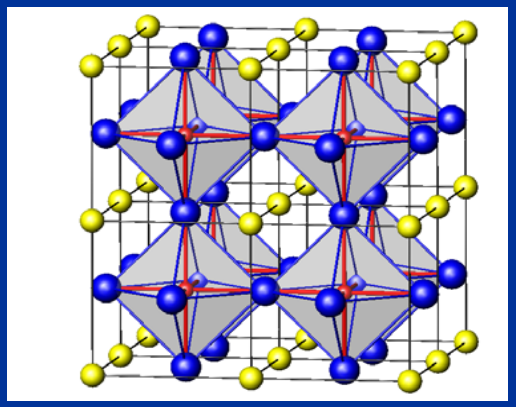


Photoemission: Fujimori et al., PRL 1992

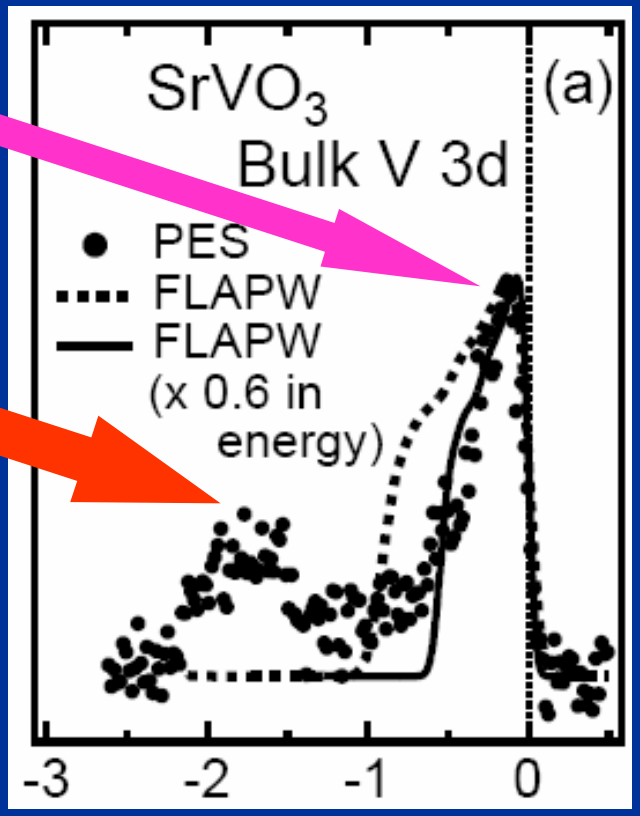
Correlated metals:

Even when ground-state is indeed metallic,
KS spectra from LDA fail to reproduce:

- **Narrowing of quasiparticle bands** due to correlations (the Brinkman-Rice phenomenon)
- **Hubbard satellites** (i.e extension to the solid of atomic-like transitions)



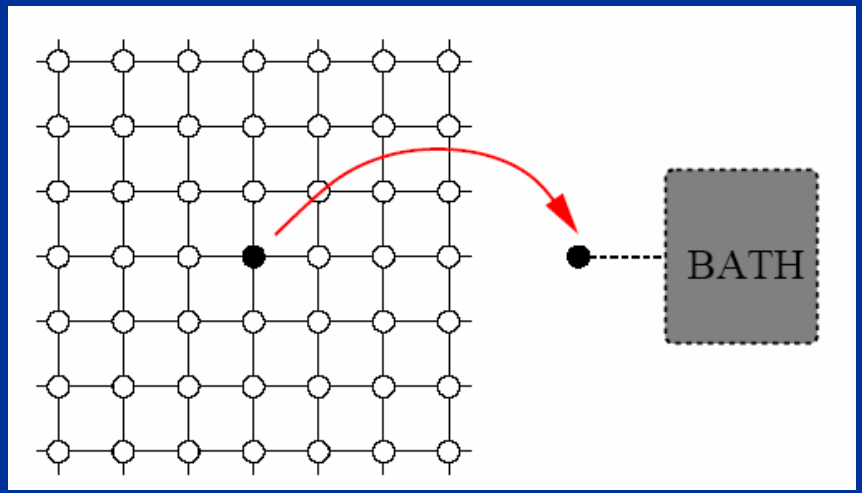
$SrVO_3$



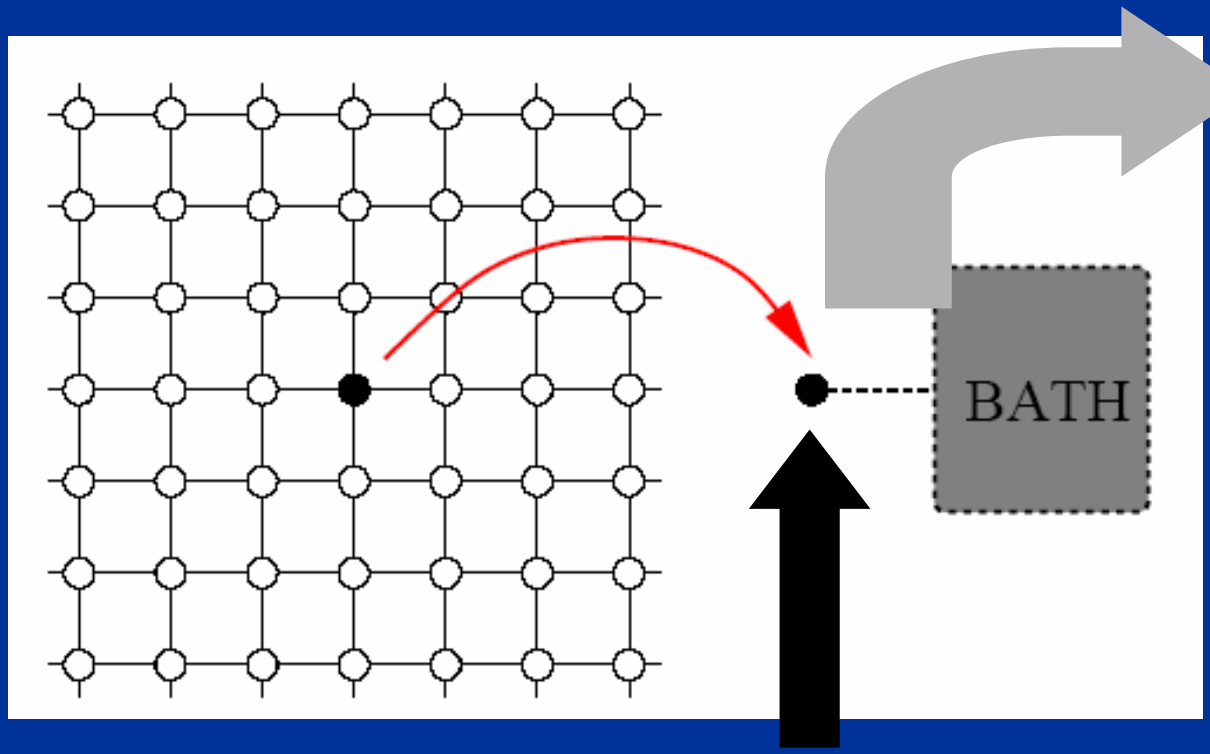
Sekiyama et al., PRL 2004

II. Main concept behind DMFT:

Replace the full solid
*by an **effective atom***
*hybridized, in a **self-consistent manner**,*
*to an **energy-dependent environment***
(effective medium)



Think of the local spectral function as that of of an **effective atom** hybridised to a well-chosen bath of free electrons



$$\Delta(\omega)$$

Effective hybridisation function, chosen such as to reproduce local Green's function

$$H_{atom} = U\, n^c_\uparrow n^c_\downarrow + (\varepsilon_0 - \mu)\,(n^c_\uparrow + n^c_\downarrow)$$

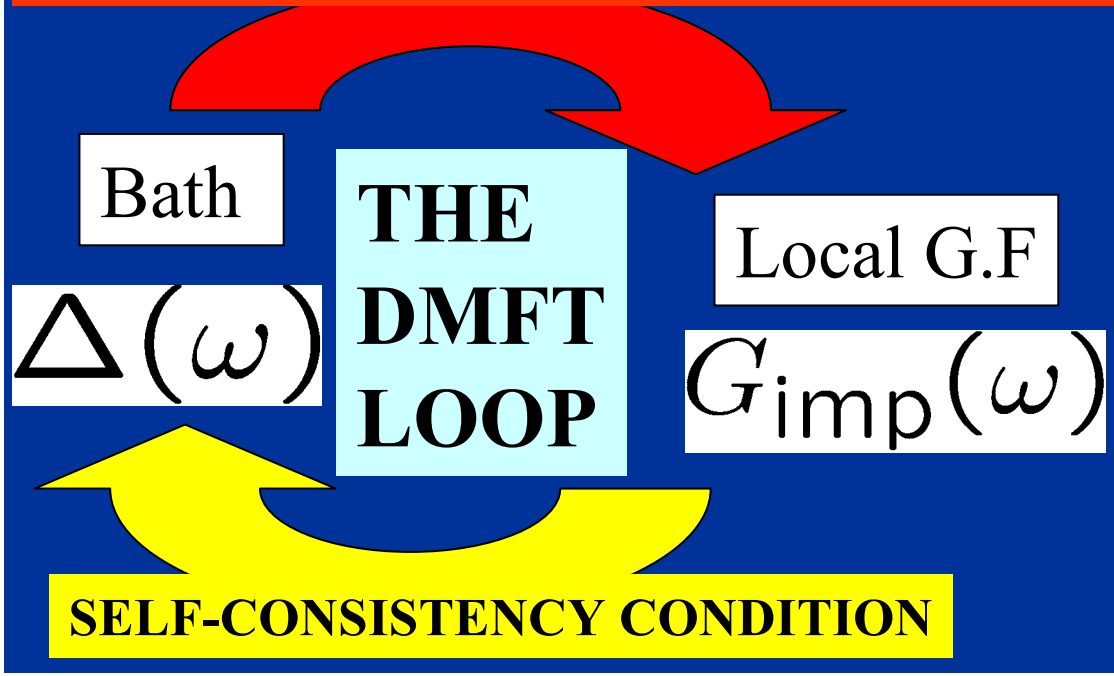
$$H = -\sum_{ij,\sigma} t_{ij}\, c^\dagger_{i\sigma} c_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow} + \varepsilon_0 \sum_{i\sigma} n_{i\sigma}$$

Illustrated here for a simple Hubbard model

Self-consistency condition which fully determines both the local G and Δ:

$$G_{\mathrm{imp}}[\Delta(\omega)] = \sum_{\mathbf{k}} \frac{1}{\omega + \mu - \Sigma_{\mathrm{imp}}[\Delta(\omega)] - \varepsilon_{\mathbf{k}}}$$

EFFECTIVE LOCAL IMPURITY PROBLEM



(Kotliar&A.G, PRB 1992)

In the large-d limit pioneered by **Metzner&Vollhardt (PRL 1989)** this construction becomes exact

``Impurity solvers''
(Key to DMFT computational efficiency)

- Many established algorithms (eg Hirsch-Fye QMC, NRG, etc…)

- **Recent breakthrough: continuous-time QMC method** starting from strong-coupling side

(P.Werner, M.Troyer, A.Millis)

III. The (happy) marriage of DFT-LDA and DMFT. Extending the DMFT construction to a real solid:

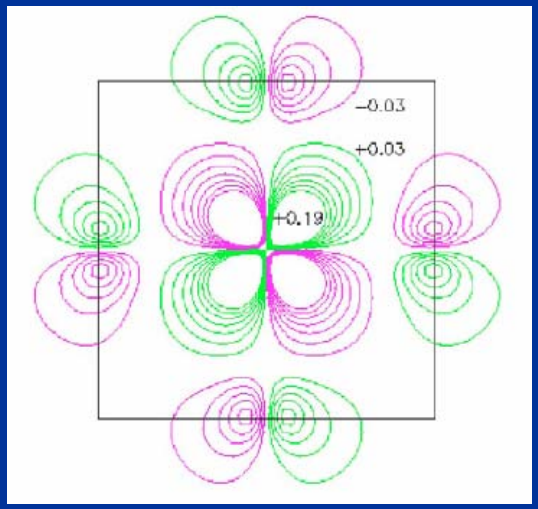
- ***Basis-set independent*** **formulation**
- **Flexible implementation within any kind of electronic structure code (eg plane wave) using e.g Wannier functions with a high degree of localization**

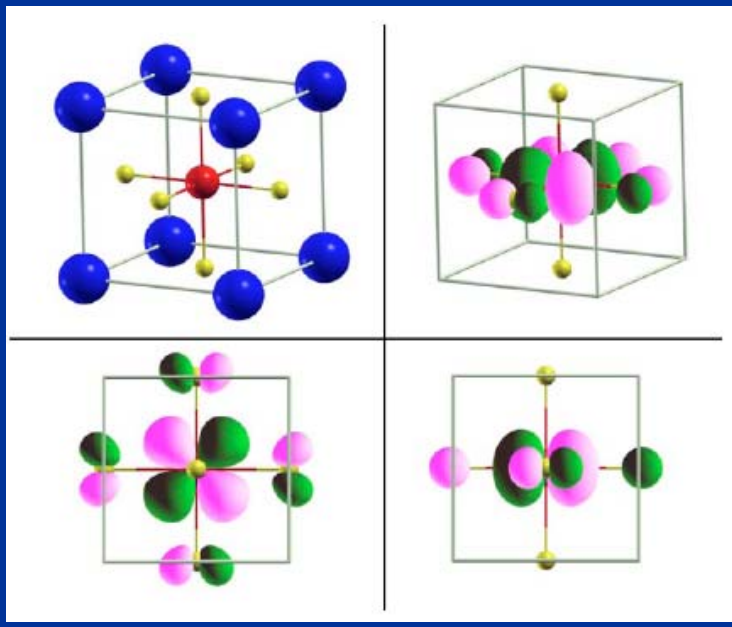
(we used: LMTO/NMTO, FLAPW, mixed-basis pseudo MBPP)

cf: F.Lechermann, AG, S.Biermann, A.Poteryaev, M.Posternak, O.K. Andersen, A. Yamazaki PRB 74, 125120 (2006)

Identify **set of ``correlated'' orbitals** for which many-body effects will be treated w/DMFT, beyond LDA:

e.g d- or f- subset denoted $\{|\chi_{\mathbf{R}m}\rangle\}$





e.g t_{2g} Wannier functions for SrVO3

In practice:

-e.g LMTOs, or LMTO heads only (not necessarily basis functions !)

-Or Wannier functions e.g NMTOs, or maximally localized, etc..

cf. Pavarini et al, Anisimov et al

*** Focus on two key quantities:**

- Total charge density in the solid (all orbitals) $\rho(\mathbf{r})$

- Components of on-site Green's function (and self-energy) ***projected on the correlated subset:***

$$G^{\mathrm{loc}}_{mm'}(i\omega_n) = \int\int d\mathbf{r}d\mathbf{r}'\chi^*_m(\mathbf{r}-\mathbf{R})\chi_{m'}(\mathbf{r}'-\mathbf{R})G(\mathbf{r},\mathbf{r}';i\omega_n).$$

$$= \hat{P}^{(C)}_{\mathbf{R}}\hat{G}\hat{P}^{(C)}_{\mathbf{R}}$$ projection on correlated space

* Add to the exchange-correlation functional $E^{xc}_{LDA}[\rho]$ on-site many-body terms of the form:

$$\sum_{\mathbf{R}} \left(\Phi_{\mathrm{imp}}[G^{\mathbf{RR}}_{ab}] - \Phi_{\mathrm{dc}}[G^{\mathbf{RR}}_{ab}] \right)$$

Calculated from an effective embedded atom, defined by **on-site interaction parameters $\mathbf{U_{abcd}}$.**
(The 2nd term is a double-counting correction, cf. LDA+U)

* The `impurity' self-energy is upfolded to the whole solid:

$$\Delta\Sigma(\mathbf{r},\mathbf{r}';i\omega_n) \equiv \sum_{\mathbf{T}mm'} \chi^*_m(\mathbf{r}-\mathbf{R}-\mathbf{T})\chi_{m'}(\mathbf{r}'-\mathbf{R}-\mathbf{T})\Delta\Sigma_{mm'}(i\omega_n)$$

Incidentally: what is really the (in)famous Hubbard U in a solid ?

~ something like :

$$U \sim \int d\mathbf{r} d\mathbf{r}' |\chi_m(\mathbf{r})|^2 W^{\text{int}}_{\text{screened}}(\mathbf{r}-\mathbf{r}') |\chi_m(\mathbf{r}')|^2$$

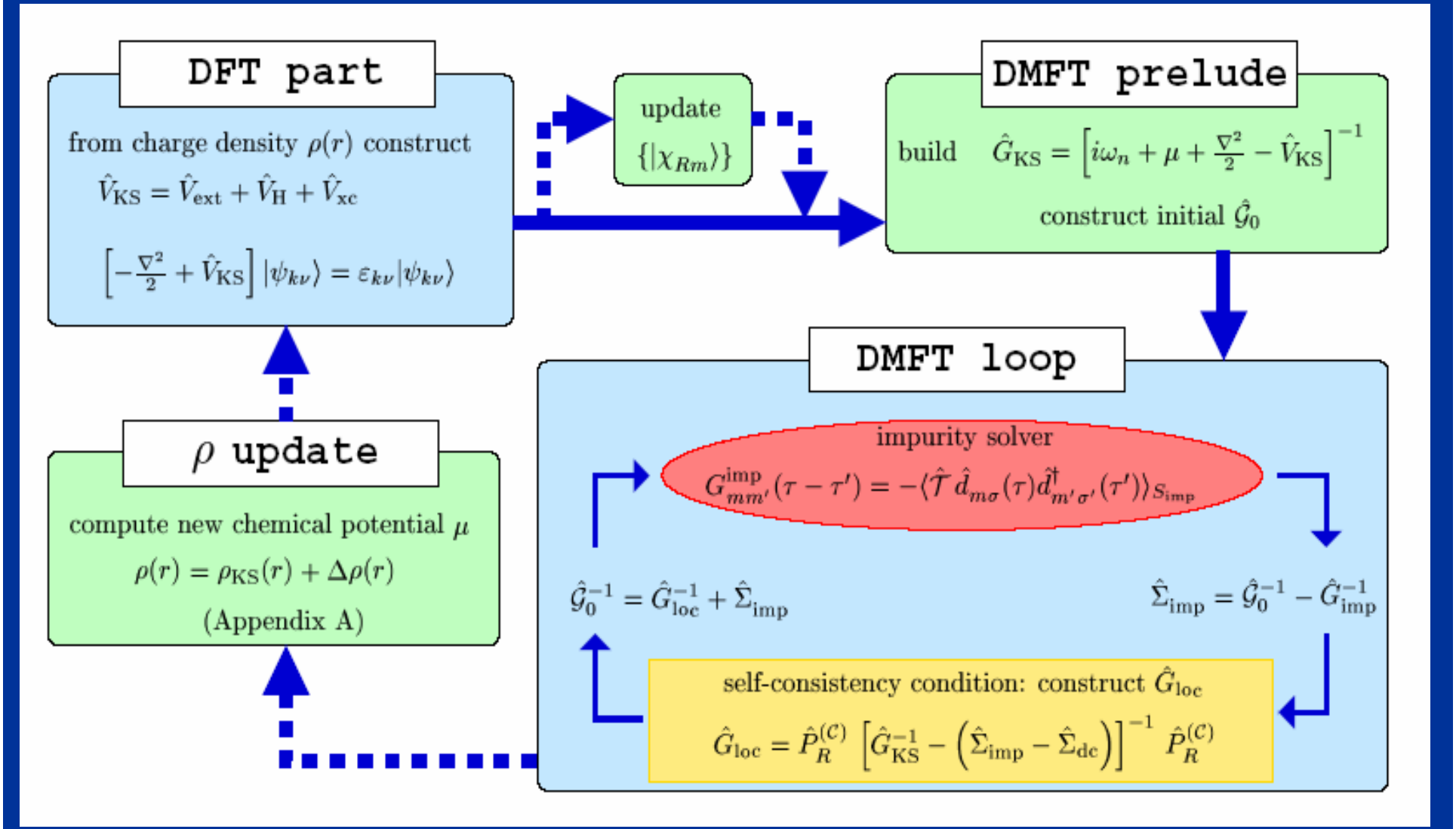
SCREENING plays a key role

Naive –unscreened- value is **HUGE** (10-20 eV !)
and applies at high-energy
while in fact low-energy U is a few eV's

Hence U is in fact an energy scale-dependent notion: U(ω)

This is an important question: see recent work by F.Aryasetiawan et al. I.Solovyev and M.Imada, ***and full GW+DMFT formalism***

Realistic DMFT, in a nutshell…



NOTE: No basis set has been specified

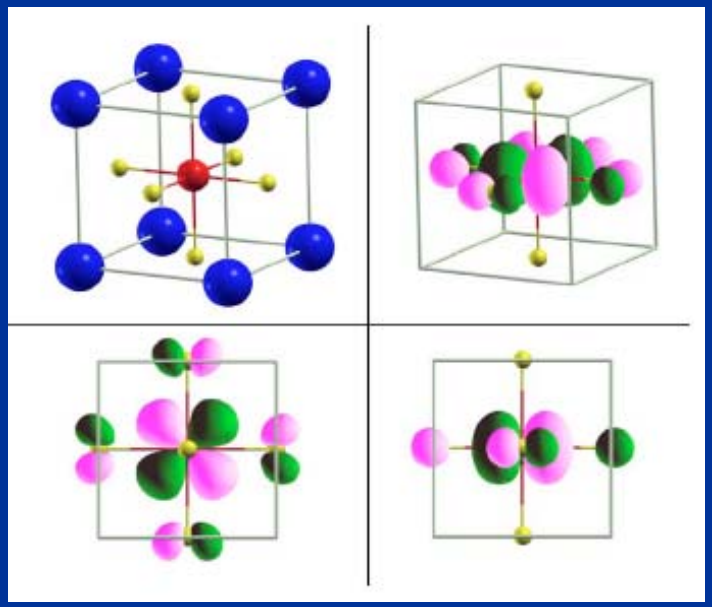
Question:

How sensitive are the results to the choice of the correlated orbitals ?

(e.g for a simple case like SrVO3, LMTO in full spd formulation, or LMTO head, or more extended t_{2g} Wannier function -NMTO or `maximally localized'-

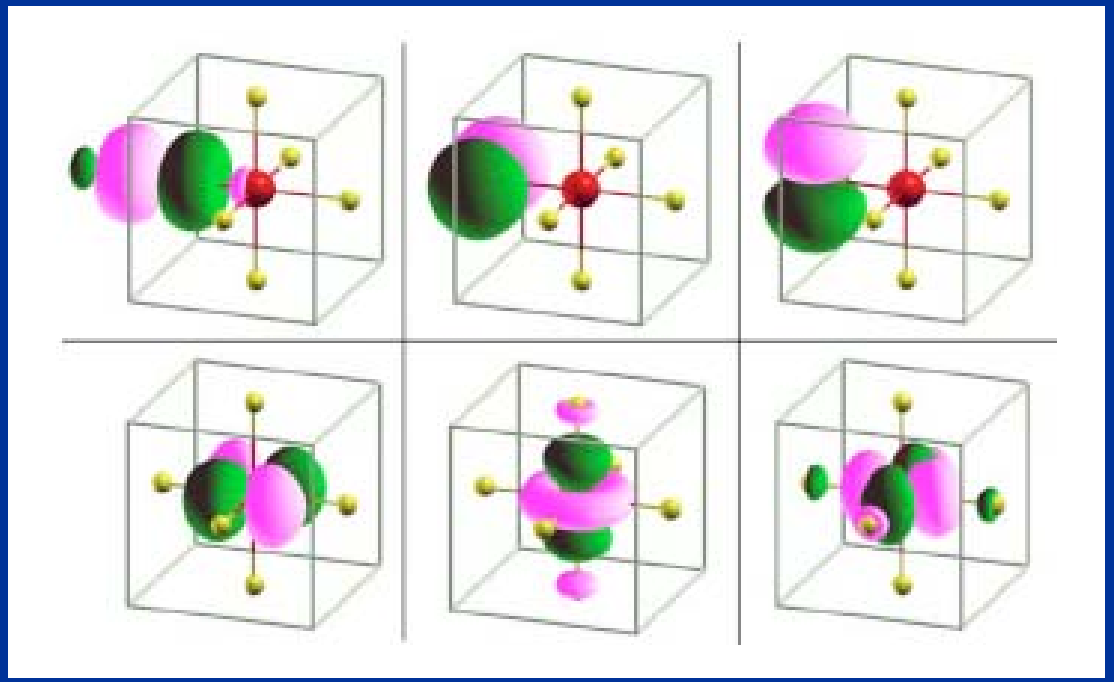
More work needed on this issue (in progress) …

Example: $SrVO_3$ Wannier functions



t2g only

O2p+Vt2g and eg



Implementation in practice: introducing a basis set

$$B_{\mathbf{k},\alpha} \;;\; \alpha = \mathbf{R}, l, m, \text{etc...}$$

Can be any preferred basis: Bloch, LMTO, mixed (FLAPW)

$$\hat{H}_{\mathrm{KS}}(\mathbf{k}) = \sum_{\alpha\alpha'} |B_{\mathbf{k}\alpha}\rangle\langle B_{\mathbf{k}\alpha'}| \left(\sum_{\nu} \varepsilon_{\mathbf{k}\nu} \langle B_{\mathbf{k}\alpha}|\psi_{\mathbf{k}\nu}\rangle\langle\psi_{\mathbf{k}\nu}|B_{\mathbf{k}\alpha'}\rangle \right)$$

$$\Delta\Sigma_{\alpha\alpha'}(\mathbf{k}, i\omega_n) = \sum_{mm'} \langle B_{\mathbf{k}\alpha}|\chi^{\mathbf{k}}_m\rangle\langle\chi^{\mathbf{k}}_{m'}|B_{\mathbf{k}\alpha'}\rangle \times [\Sigma^{\mathrm{imp}}_{mm'}(i\omega_n) - \Sigma^{\mathrm{dc}}_{mm'}]$$

DMFT self-consistency condition reads:

$$G^{\mathrm{imp}}_{mm'}(i\omega_n) = \sum_{\mathbf{k}} \sum_{\alpha\alpha'} \langle\chi^{\mathbf{k}}_m|B_{\mathbf{k}\alpha}\rangle\langle B_{\mathbf{k}\alpha'}|\chi^{\mathbf{k}}_{m'}\rangle \times \{[i\omega_n + \mu - \mathbf{H}_{\mathrm{KS}}(\mathbf{k}) - \mathbf{\Delta\Sigma}(\mathbf{k}, i\omega_n)]^{-1}\}_{\alpha\alpha'}$$

Inversion of matrix of size N_B*N_B at each k-point and each frequency !

The Wannier route

- Perform Wannier construction for some set of bands W (aka some energy window)

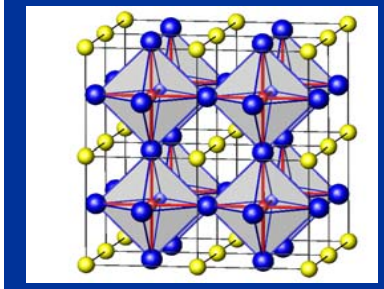
$$w_\alpha(\mathbf{r}-\mathbf{T}) = \frac{V}{(2\pi)^3}\int_{\mathrm{BZ}} d\mathbf{k} e^{-i\mathbf{k}\cdot\mathbf{T}} \sum_{\nu\in\mathcal{W}} U^{(\mathbf{k})}_{\alpha\nu}\psi_{\mathbf{k}\nu}(\mathbf{r}),$$

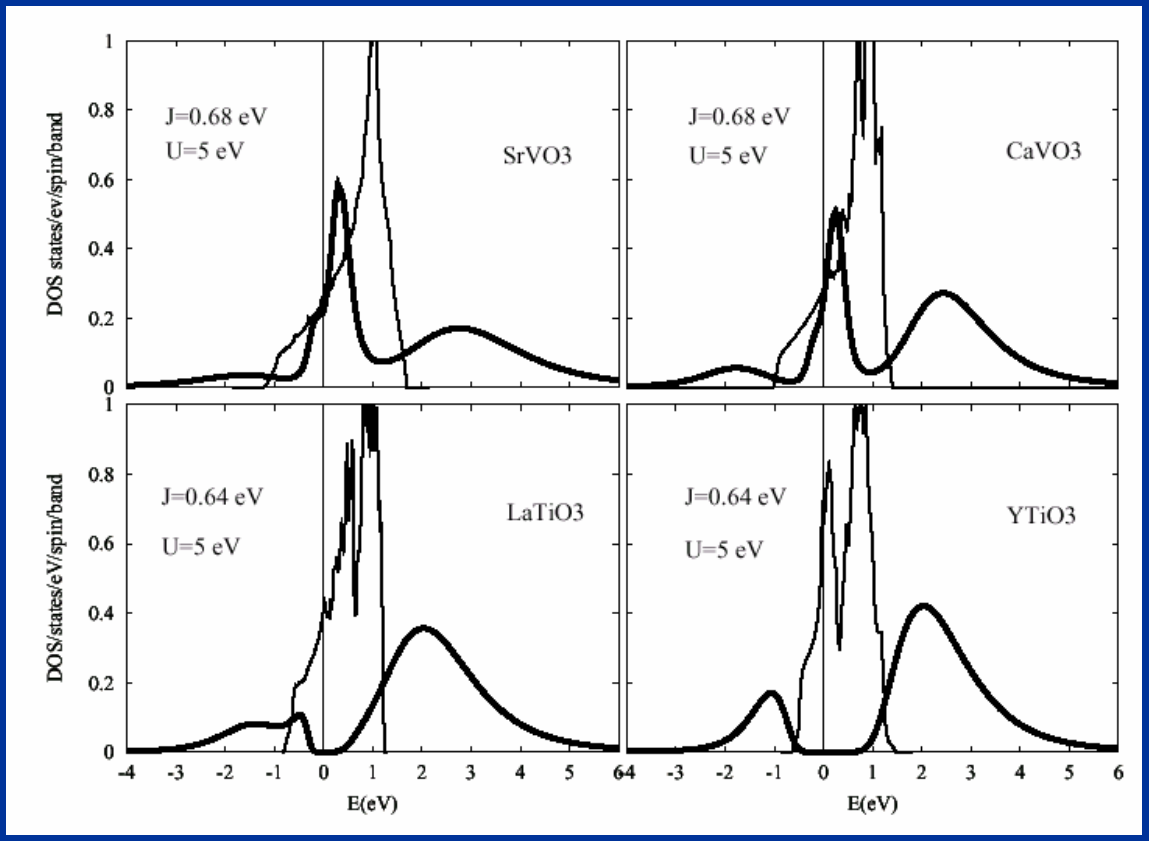
- Select a subset C of W as defining the correlated orbitals:

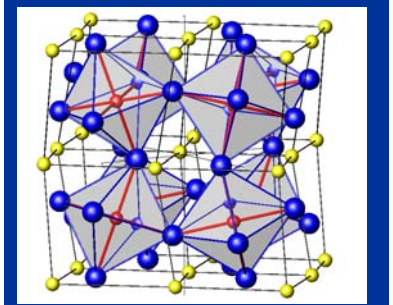
$$G^{\mathrm{imp}}_{mm'}(i\omega_n) = \sum_{\mathbf{k}} \{[(i\omega_n+\mu)\mathbb{1} - \mathbf{H}^{(\mathcal{W})}_{\mathrm{KS}}(\mathbf{k}) - \mathbf{\Delta\Sigma}^{(\mathcal{C})}(i\omega_n)]^{-1}\}_{mm'}$$

W=C most economical choice when possible (e.g isolated set of `correlated' bands), but perhaps more localised C-set preferable ??

Photoemission spectra of correlated metals and (paramagnetic) Mott insulators







E.Pavarini et al., PRL 2004

cf. also Sekiyama et al. (Ca/SrVO3) PRL 2004

3-peak structure clearly revealed in recent high-photon energy PES experiments

w/relative intensities between QP and Hubbard satellites in good agreement w/DMFT

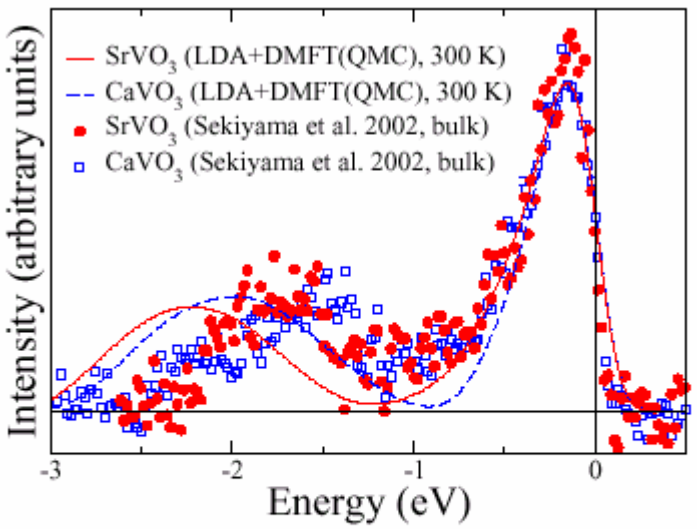
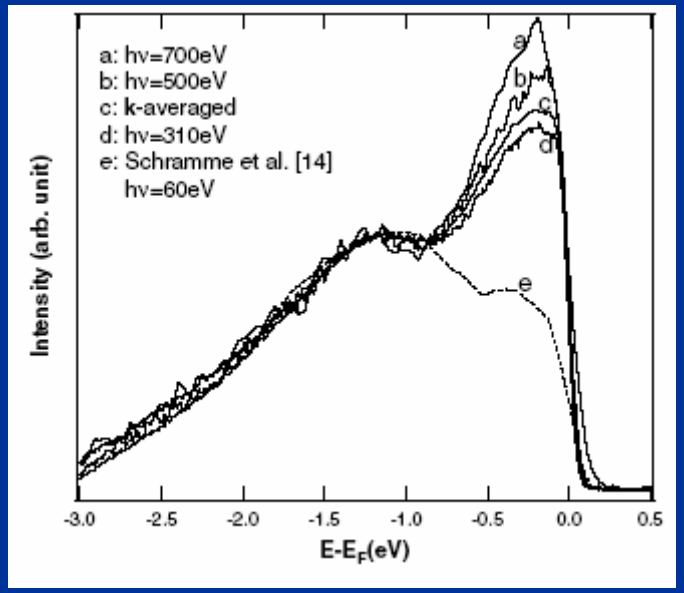


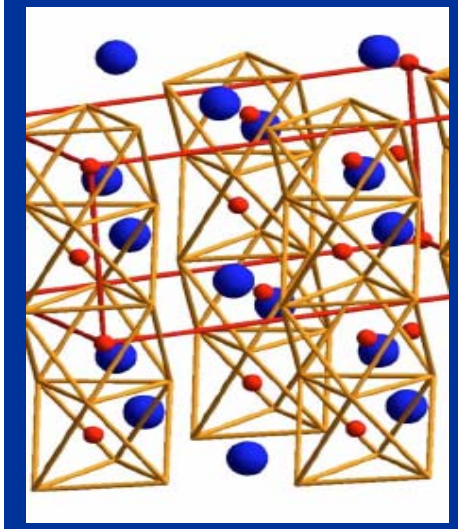
FIG. 4: Comparison of the calculated, parameter-free LDA+DMFT(QMC) spectra of $SrVO_3$ (solid line) and $CaVO_3$ (dashed line) with bulk-sensitive high-resolution PES ($SrVO_3$: circles; $CaVO_3$: rectangles) [4]. Horizontal line: experimental subtraction of the background intensity.

Sekiyama et al, Ca/SrVO3

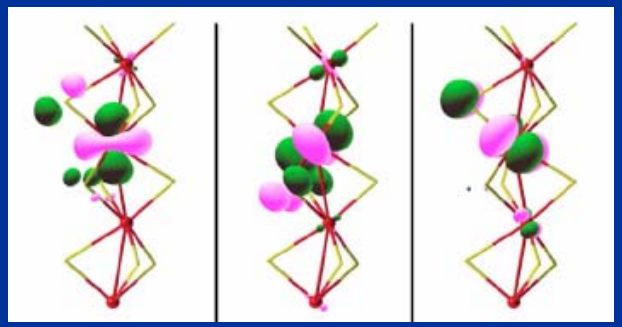


Mo et al, V2O3
(DMFT calculations by Keller, Held et al.
cf. also Poteryaev et al.

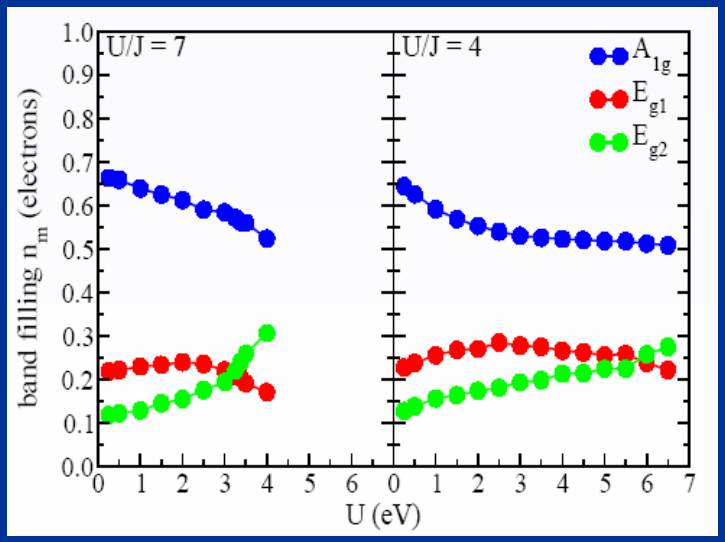
Correlation-induced inter-orbital charge transfers and modifications of the Fermi surface w.r.t LDA: the example of BaVS3

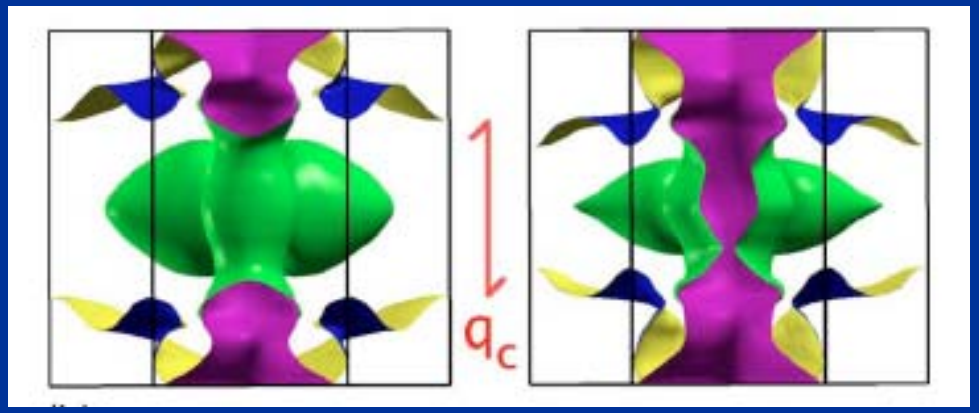


Lechermann, Biermann and A.G, PRL 2005



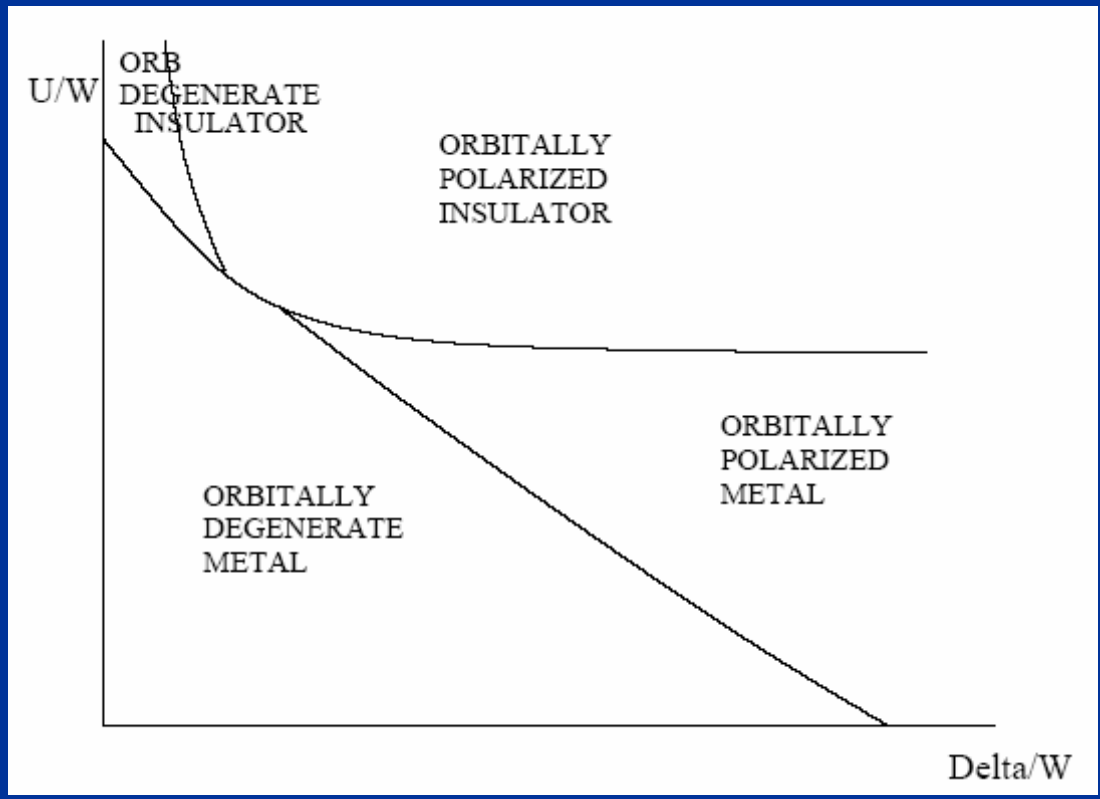
Correlation-induced nesting of the Fermi surface:





LDA Correlated

More generally, competition between:
-Crystal field splitting (considerably enhanced by correlations) >> ***orbital polarization***
- Hund's rule >> ***orbital compensation***



Cf. Manini et al. PRB 66, 115107 (2002)

Na_xCoO_2: do the hole pockets exist ?

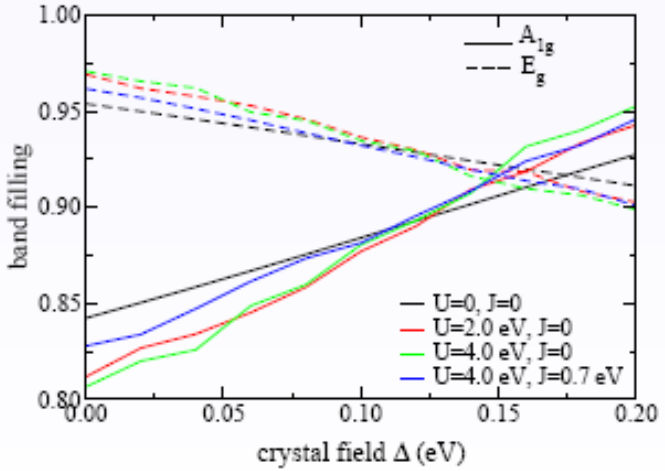
- LDA: yes
- ARPES: no

- [Zhang *et al.*, PRL **93** 236402] LDA+U calculation: no
  magnetic order, double-counting correction
- [Ishida *et al.*, PRL **94** 196401] LDA+DMFT calculation: yes
  orbital compensation effect, i.e., interorbital charge transfer from E_g to A_{1g}
- [Zhou *et al.*, PRL **94** 206401] LDA+Gutzwiller approach: no
  $U \to \infty$, J=0, Δ=0.01 eV

... to be further explored:

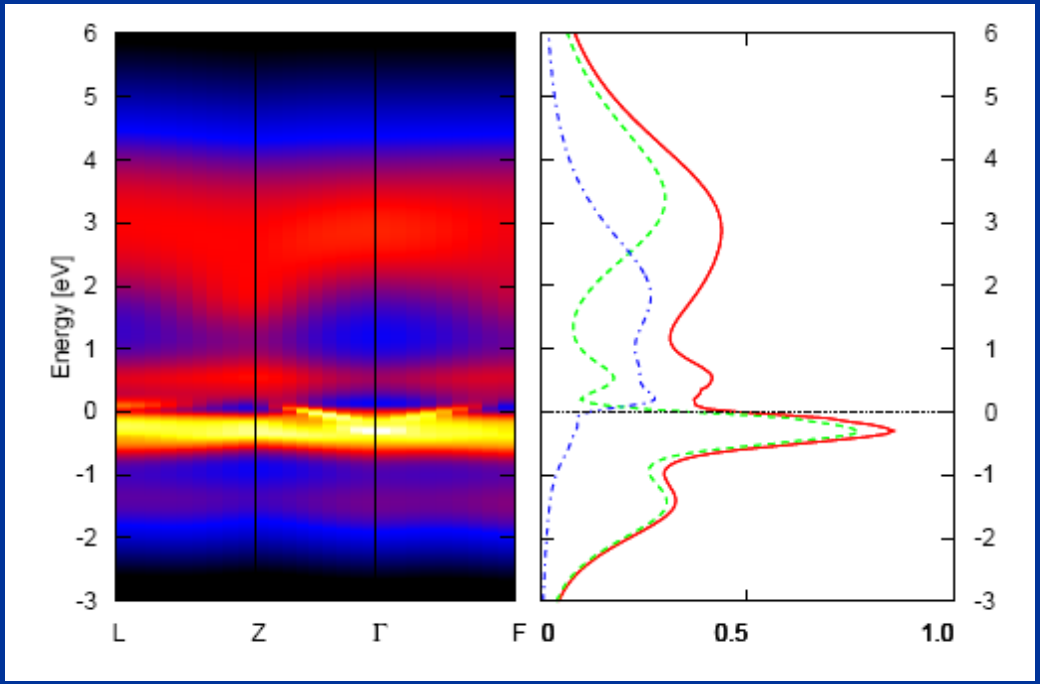
- spin-flip and pair-hopping terms in the Coulomb vertex
- importance of double counting
- non-local effects
- interatomic Coulomb interaction V
- LDA charge density update

remark on importance of crystal-field splitting ...

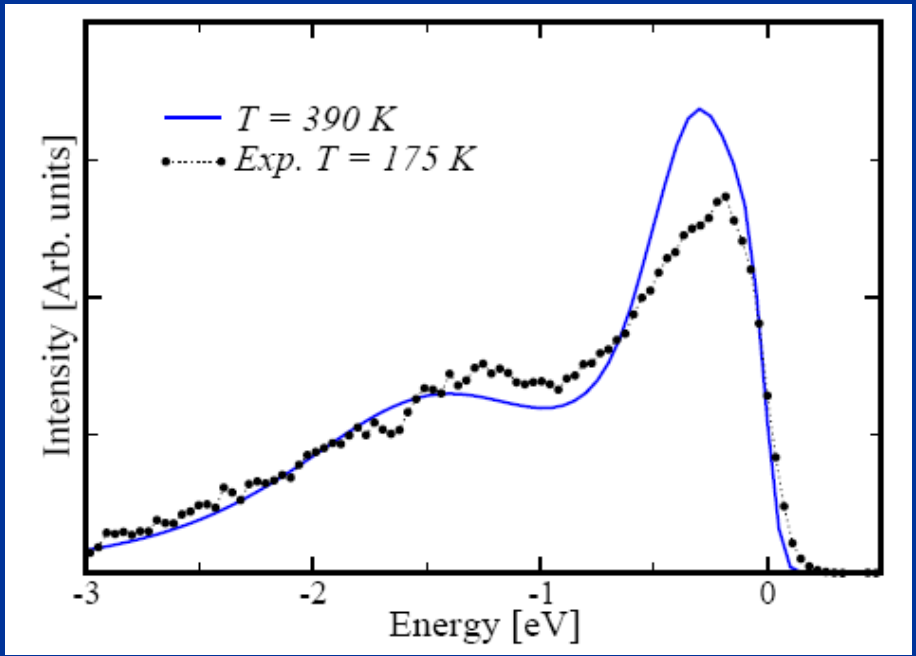


$\Delta_{A_{1g},E_g}(Na_xCoO_2) \sim 0.1$ eV

Lechermann, 2005



V2O3: correlation-enhanced Xtal field splitting and short-lived Egpi quasiparticles



Total energy: the LDA+DMFT free-energy functional

$$\Gamma[\rho, G_{mm'}] =$$
$$= T[\rho, G_{mm'}] + E_H[\rho] + E_{\mathrm{XC}}[\rho, G_{mm'}]$$

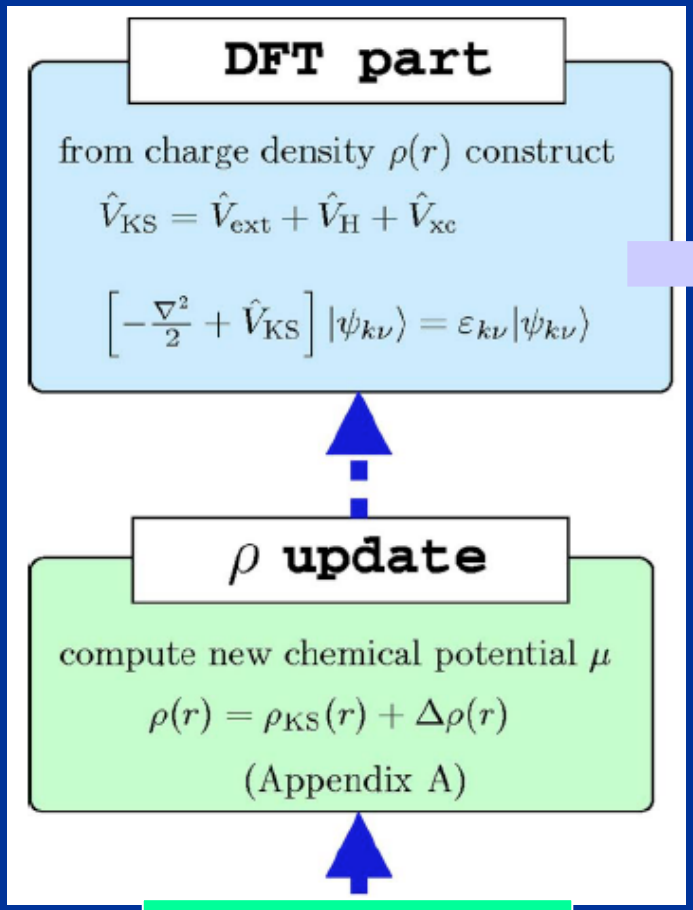
$$-\mathrm{tr}\ln[i\omega_n + \mu + \tfrac{1}{2}\nabla^2 - v_{KS}(\mathbf{r}) - \chi^*.\Delta\Sigma.\chi] - \int d\mathbf{r}\,(v_{KS} - v_c)\rho(\mathbf{r}) - \mathrm{tr}\,[G.\Delta\Sigma] +$$
$$+ \tfrac{1}{2}\int d\mathbf{r}\,d\mathbf{r}'\rho(\mathbf{r})U(\mathbf{r}-\mathbf{r}')\rho(\mathbf{r}') + E_{xc}[\rho(\mathbf{r})] + \Sigma_{\mathbf{R}}\left(\Phi_{imp}[G^{\mathbf{RR}}_{ab}] - \Phi_{DC}[G^{\mathbf{RR}}_{ab}]\right)$$

In these expressions,
V_{KS} is the Kohn-Sham potential
and $\Delta\Sigma$ is the (dc-corrected) local self-energy in ``correlated'' subset

Finally, total energy is calculated as:

$$E_{LDA+DMFT} = E_{DFT} - \Sigma'_\lambda\, \varepsilon^{KS}_\lambda + \langle H_{KS}\rangle + \langle H_U\rangle - E_{DC}$$
$$= E_{DFT} + \Sigma_{\mathbf{k},LL'}\, h^{KS}_{LL'}[\langle c^\dagger_{L\mathbf{k}} c_{L'\mathbf{k}}\rangle_{DMFT} - \langle c^\dagger_{L\mathbf{k}} c_{L'\mathbf{k}}\rangle_{KS}] + \langle H_U\rangle - E_{DC}$$

Update of charge density



From DMFT

Construct G_{KS} and back to DMFT

$$\rho(\mathbf{r}) = \sum_{\mathbf{k}\nu\nu'} D^{(\mathbf{k})}_{\nu'\nu}(\mathbf{r}) \Delta N^{(\mathbf{k})}_{\nu\nu'} + \sum_{\nu} \Theta(\mu - \varepsilon_{\mathbf{k}\nu}) D^{(\mathbf{k})}_{\nu\nu}(\mathbf{r}).$$

KS density matrix:

$$D^{(\mathbf{k})}_{\nu'\nu}(\mathbf{r}) = \psi_{\mathbf{k}\nu}(\mathbf{r}) \psi^{*}_{\mathbf{k}\nu'}(\mathbf{r}).$$

Many-body correction:

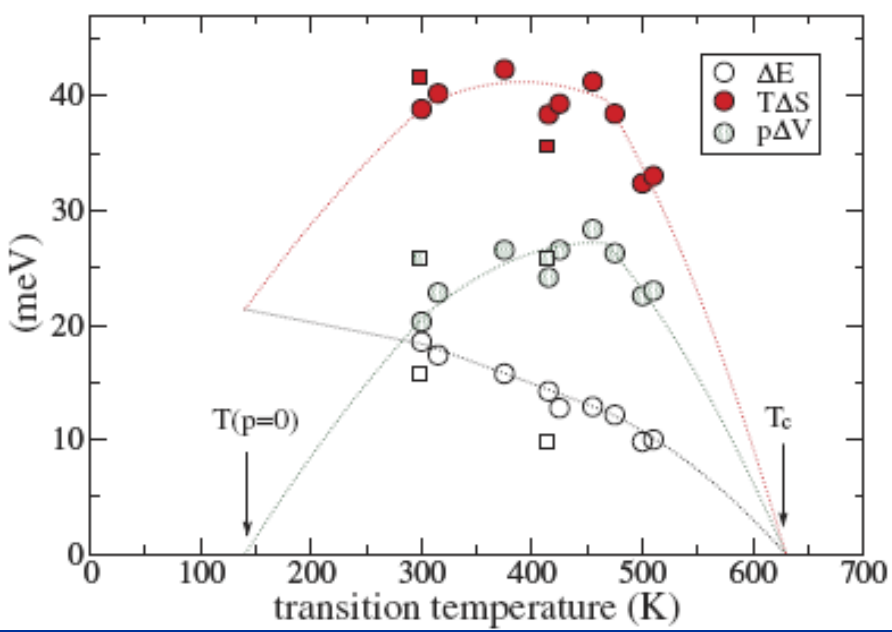
$$\Delta N^{(\mathbf{k})}_{\alpha\alpha'} \equiv \frac{1}{\beta} \sum_{nmm'} G^{\rm KS}_{\alpha m}(\mathbf{k}, i\omega_n) \Delta\Sigma_{mm'}(i\omega_n) G_{m'\alpha'}(\mathbf{k}, i\omega_n)$$

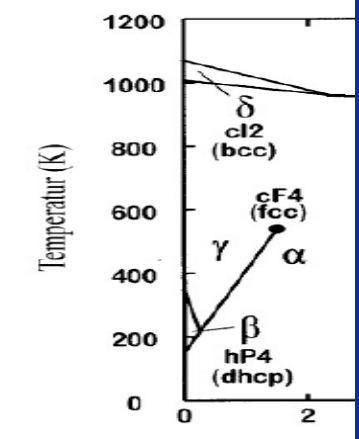
KS system is updated

and modified by many-body effects…

The α-γ transition of cerium is entropy-driven…

Amadon et al. PRL 2006



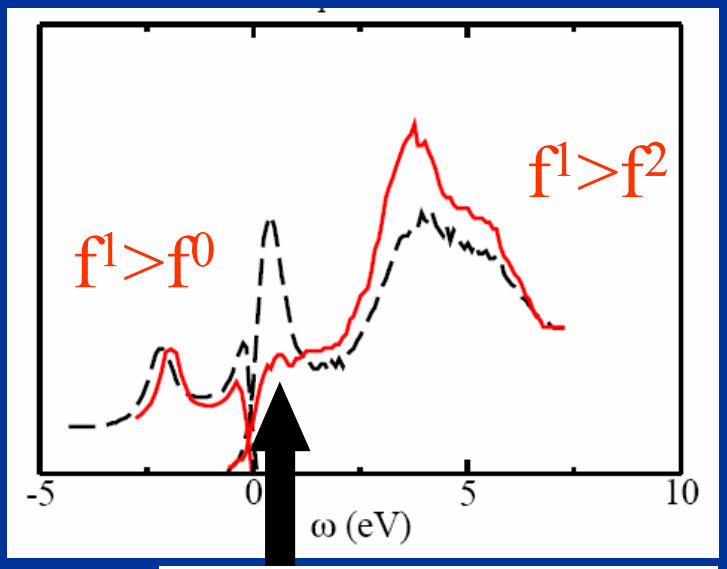


Red:
γ-cerium
(higher volume
Phase)

Entropy and energy
Across transition from
Experimental equation of state

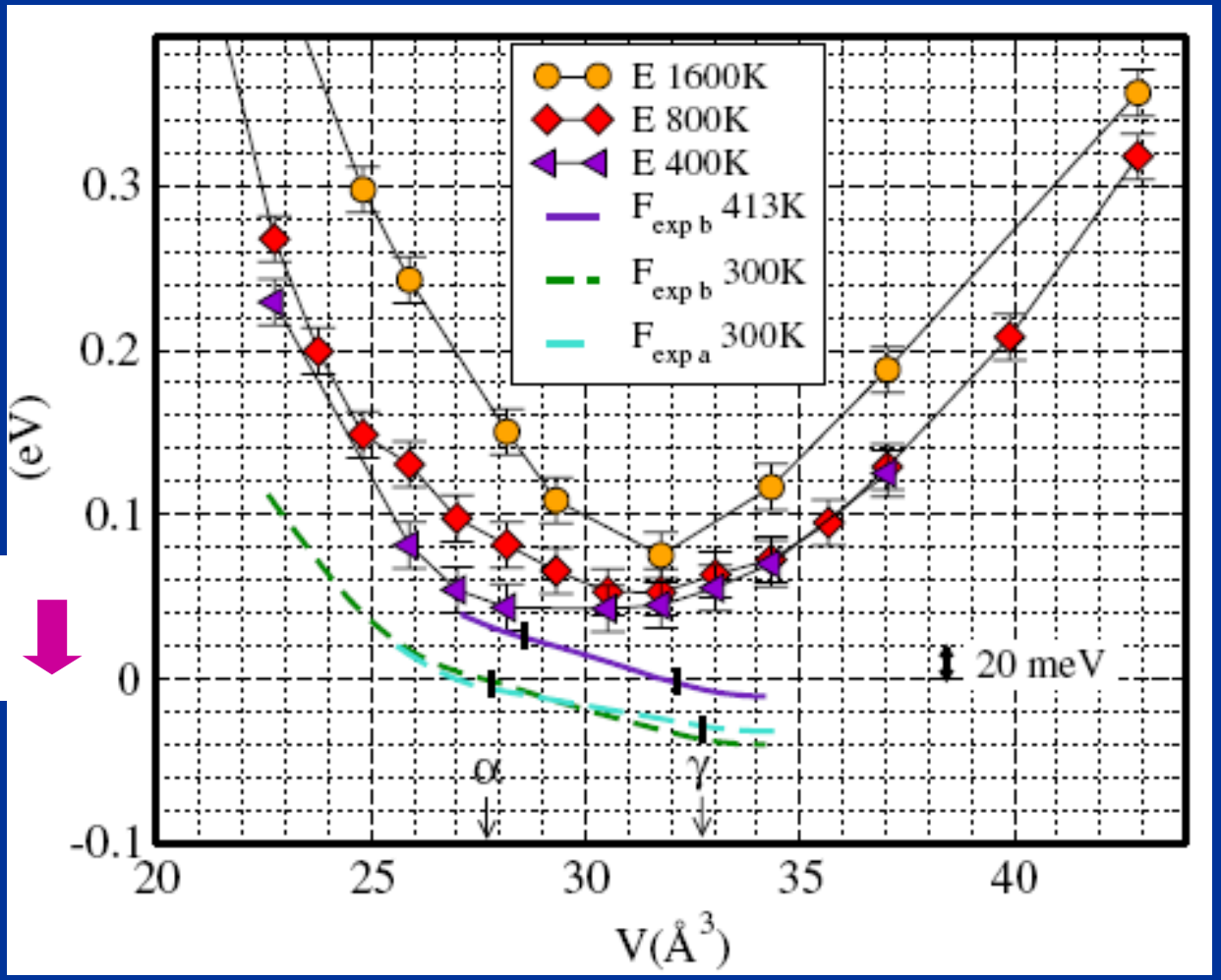
PES experiments
(Wuilloud et al,
Weliczka et al.)

Black:
α-cerium
(lower volume
Phase)

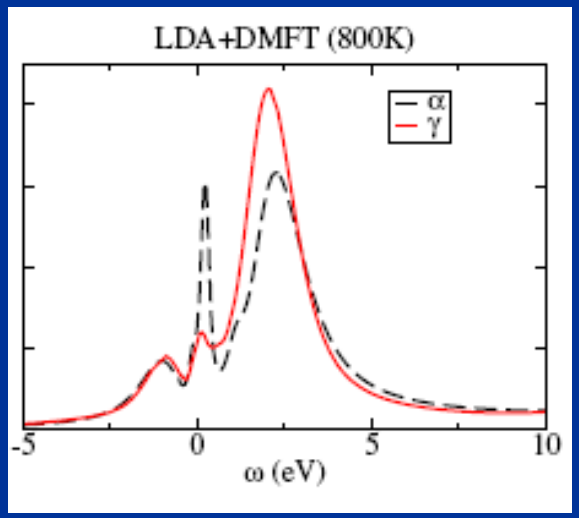


Kondo resonance

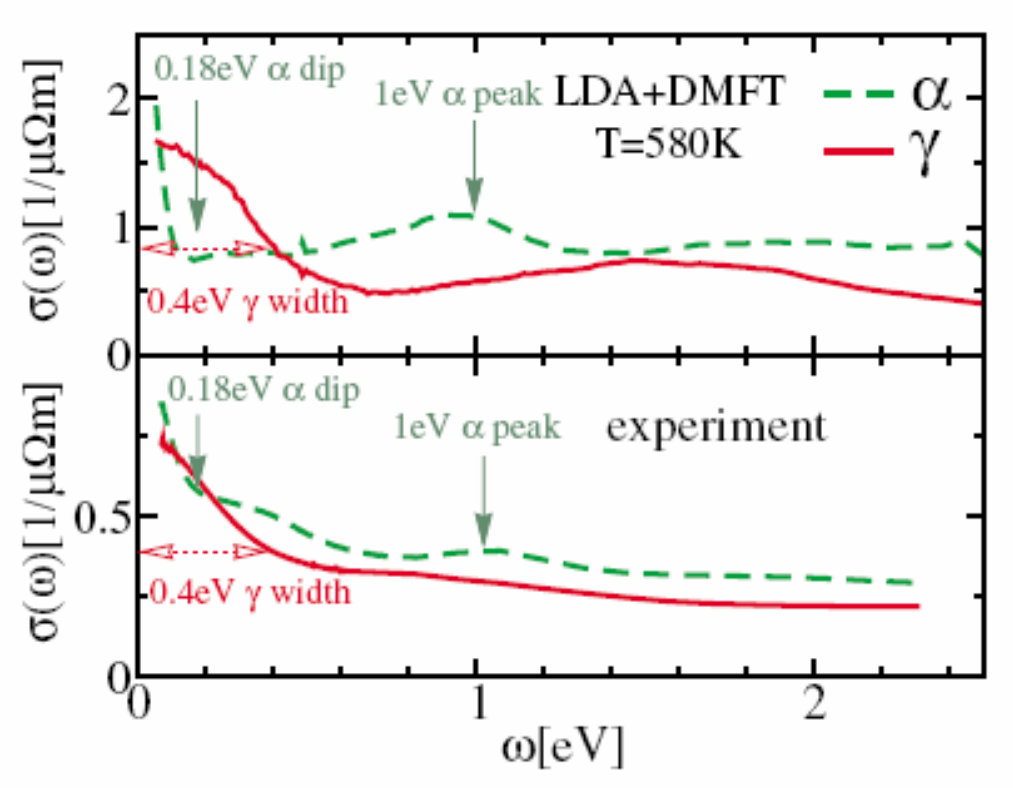
Consistent with LDA+DMFT calculations of total energy



Entropic stabilisation of gamma phase



Optical spectra from DMFT



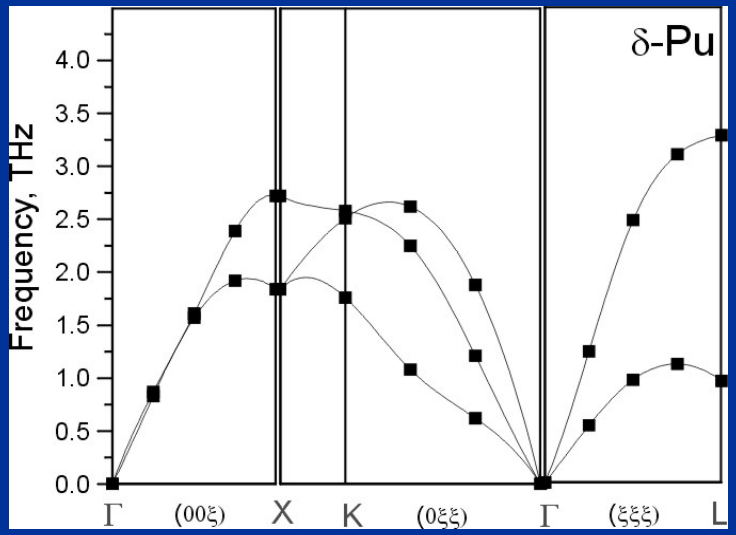
Haule et al, PRL 2005

Expts: van der Eeb, PRL 2001

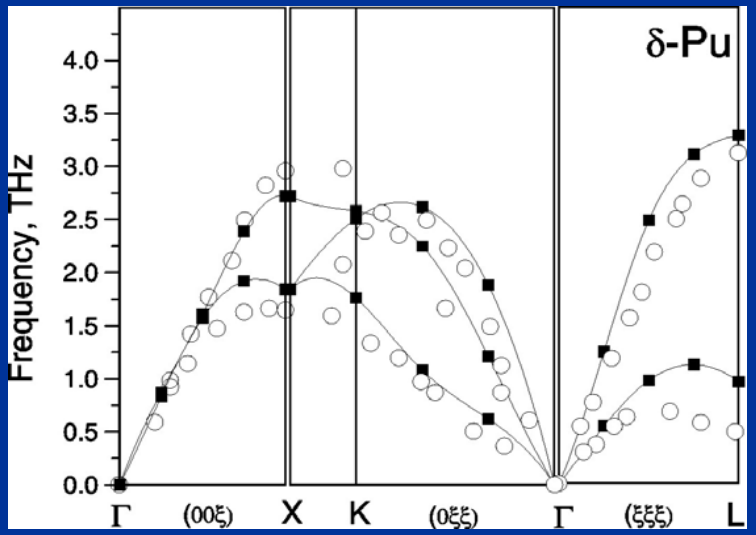
Drude peak in the α-phase, not in γ

FIG. 1 (color online). The top panel shows the calculated optical conductivity for both α and γ phase of cerium. The temperature used in calculation is 580 K while the volume of α and γ phase is 28.06 Å^3 and 34.37 Å^3, respectively. The bottom panel shows experimental results measured by the group of van der Marel [2]. The measurements for α phase were done at 5 K and for γ phase at 400 K.

Phonons in fcc δ-Pu PREDICTED from DMFT



(Dai, Savrasov, Kotliar,Ledbetter, Migliori, Abrahams, Science, 9 May 2003)



(experiments from Wong et.al, Science, 22 August 2003)

Phonons From Linear-response In DMFT: Savrasov&Kotliar, PRL 2003 [MnO,NiO]

	C_{11} (GPa)	C_{44} (GPa)	C_{12} (GPa)	C'(GPa)
Theory	34.56	33.03	26.81	3.88
Experiment	36.28	33.59	26.73	4.78

[Squares]

[Open dots]

CONCLUSION / OVERVIEW

- DMFT is an energy-dependent mean-field approach aimed at treating strong correlation effects
- The frequency-dependent on-site self-energy is calculated through an effective atomic problem embedded in a self-consistent medium
- Quasiparticle excitations (and bandwidth narrowing) as well as Hubbard satellites are treated on equal footing
- The method has been happily blended with DFT-LDA, and applied to long-standing problems in electronic structure calculations of strongly correlated materials

Frontiers (I)

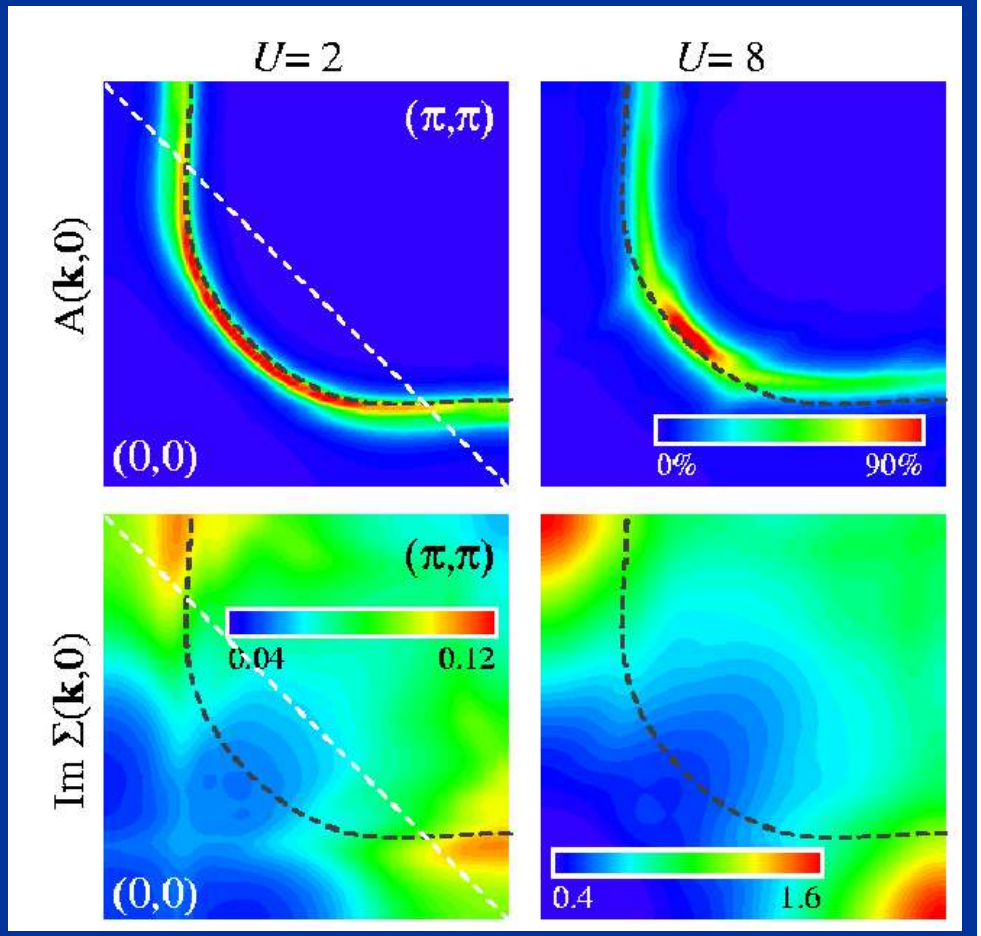
- Fully first-principle scheme: ab-initio calculation of (frequency-dependent) U, GW-functionals
- ``Optimal'' choice of correlated orbitals ?
- More flexible implementations within electronic structure codes: in progress

Frontiers (II) …

Beyond a purely-local self-energy:
restoring some momentum-dependence

>> CLUSTER extensions of DMFT: C-DMFT

This is needed both in the context of MODELS
of strongly-correlated electrons, to explain some of the
key aspects of the cuprates (differentiation of the
Fermi surface into **hot and cold regions**,
cf. work by Sherbrooke and Rutgers/Saclay/Rome group)
AND
in a realistic electronic-structure context,
for some materials e.g w/ Peierls insulator character
(cf. recent work on Ti_2O_3 and VO_2, Poteryaev, Biermann et al.)



Senechal, A.M Tremblay, PRL 2004

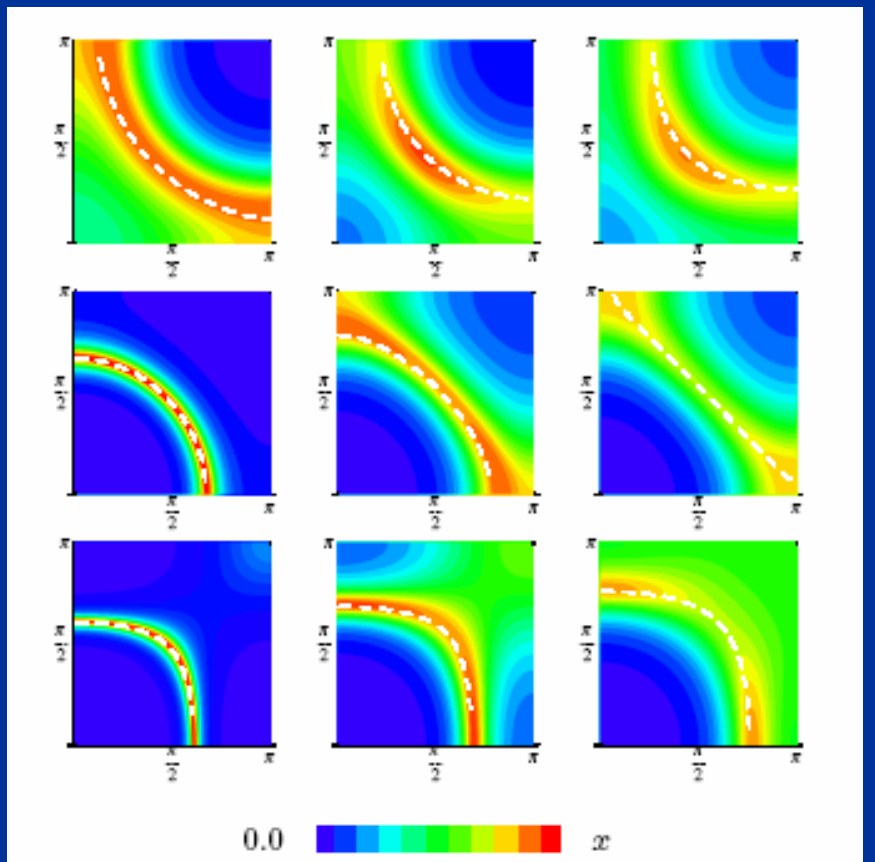


FIG. 4: $A(k,\omega = 0^+)$ in the first quadrant of the Brillouin zone. From the top: in the first row $t' = -0.3t$, $n = 0.73, 0.89, 0.96$, color scale $x = 0.28, 0.22, 0.12$; in the second $t' = +0.3t$, $n = 0.70, 0.90, 0.95$, color scale $x = 0.82, 0.34, 0.27$; in the lowest row $t' = +0.9t$, $n = 0.69, 0.92, 0.96$, color scale $x = 0.90, 0.32, 0.22$. The white dashed line is the FS given by $t_{\rm eff}(k) = \mu$.

Civelli et al., PRL 2005, Cluster-DMFT

Some general references…

- **Lecture notes (A.G) cond-mat/0403123**

  Strongly Correlated Electron Materials: Dynamical Mean-Field Theory and Electronic Structure

  [published as: Lectures on the Physics of Highly Correlated Electron Systems VIII (2004) 3, American Institute of Physics Conference Proceedings Vol. 715]

- **Review articles:** A.G, G.Kotliar, W.Krauth and M.Rozenberg, Rev.Mod.Phys. **68** (1996) 13; G.Kotliar et al. (2006), K.Held (2006)
- **Overview article**: G.Kotliar and D.Vollhardt, Physics Today, March 2004

http://www.cpht.polytechnique.fr/cpht/correl/mainpage.htm

Illustrate first on simple one-band lattice model:

$$H = -\sum_{\mathrm{RR}'\sigma} t_{\mathrm{RR}'} f^{\dagger}_{\mathrm{R}\sigma} f_{\mathrm{R}'\sigma} + \sum_{\mathrm{R}} H^{\mathrm{R}}_{\mathrm{atom}}$$

R=lattice (atomic) site

e.g Hubbard model: $H^{\mathrm{R}}_{\mathrm{atom}} = U \hat{n}^{f}_{\mathrm{R}\uparrow} \hat{n}^{f}_{\mathrm{R}\downarrow} + \epsilon_0 [\hat{n}^{f}_{\mathrm{R}\uparrow} + \hat{n}^{f}_{\mathrm{R}\downarrow}]$

Focus on key observable: on-site Green's function (of the whole lattice model): $G_{RR}(\omega)$

Introduce a **REFERENCE SYSTEM** in order to represent G_{RR}: **we are familiar with this concept from DFT** in which a reference system of non-interacting electrons is introduced, with a well-chosen (Kohn-Sham) potential such as to reproduce the local density $\rho(\vec{r})$,the key observable of DFT.

In DMFT, the REFERENCE SYSTEM is the atom coupled to a bath of (free) electrons, with appropriate energy levels E_p's and hybridization V_p's to the atomic orbital, chosen such that the Green's function of this embedded atom reproduces G_{RR}

For the simple Hubbard case, this yields:

$$H_{\mathrm{imp}} = H_{\mathrm{atom}}[f_\sigma, f_\sigma^\dagger] + \sum_{p\sigma}[V_p\, f_\sigma^\dagger a_{p\sigma} + h.c] + \sum_{p\sigma} E_p\, a_{p\sigma}^\dagger a_{p\sigma}$$

This is the Anderson model of a magnetic ``impurity'' in a solid !

Ep's and Vp's can be recast into a hybridization function:

$$\Delta(\omega) = \sum_p \frac{|V_p|^2}{\omega - E_p}$$

It plays the role of an **ENERGY-DEPENDENT mean-field**, (Weiss field, conjugate to GRR) which must be chosen such that:

$$G_{\mathrm{imp}}[\Delta(\omega)] = G_{\mathbf{RR}}(\omega)$$

On the other hand, G_{RR} is related to the self-energy of the lattice (solid) by Dyson's equation:

$$G_{\mathbf{RR}}(\omega) = \sum_{\mathbf{k}} \frac{1}{\omega + \mu - \varepsilon_{\mathbf{k}} - \Sigma(\mathbf{k}, \omega)}$$

In which ε_k is the tight-binding band (FT of the hopping $t_{RR'}$)

At this point, no approximation has been made: we have just used a reference system to represent G_{RR}

Let us now make the **APPROXIMATION** that the lattice self-energy is **k-independent** and coincides with that of the effective impurity problem:

$$\Sigma(\mathbf{k}, \omega) \simeq \Sigma_{\mathrm{imp}}(\omega)$$