# Electronic Structure Calculations using Dynamical Mean Field Theory

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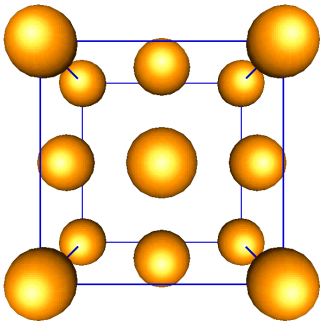
(*) DMFT = Dynamical Mean Field Theory

## The Menu

- Correlations in Condensed Matter -- Modeling Correlated Electron Behavior
- What's a mean field theory?
- Dynamical mean field theory (DMFT) and "DFT+DMFT"
- Beyond "DFT+DMFT": functional approaches, GW+DMFT …
- Conclusions/perspectives

# From your solid state physics lecture …:

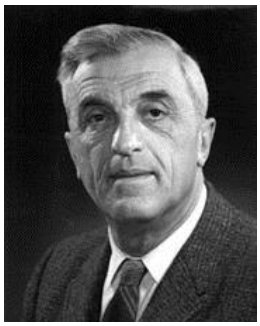
In a perfect cristal, the atoms form a periodic lattice …



… the electrons live in the periodic potential created by the ions

**Bloch's theorem:** Electronic eigenstates are plane waves modulated by periodic function

Bloch's theorem:



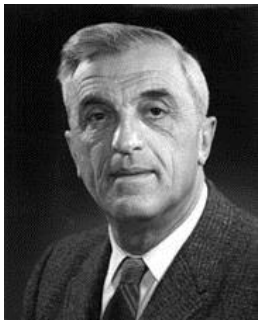
$$H = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x)$$

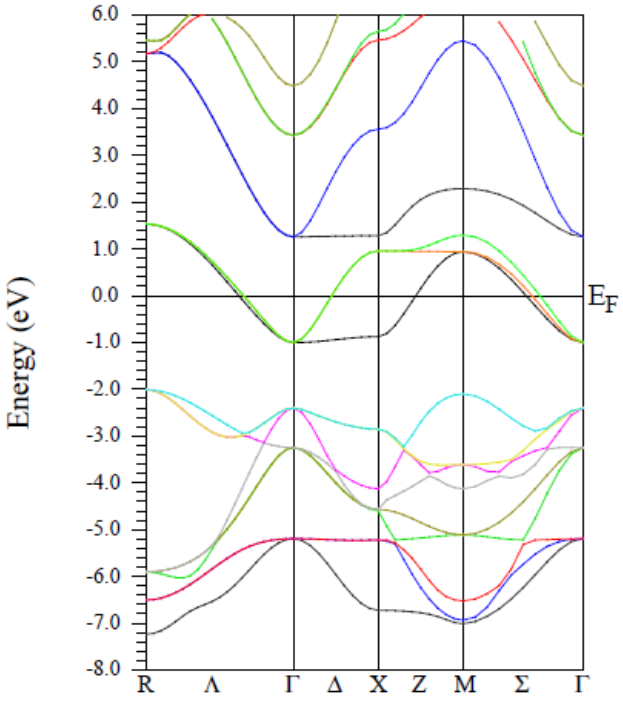
The eigenstates of an electron in a periodic potential $V(x) = V(x+a)$

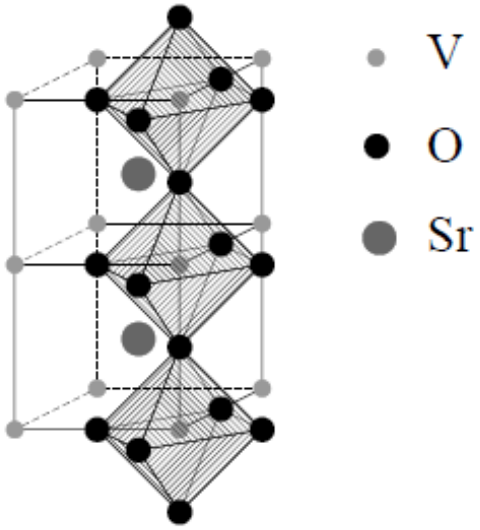
are $\Psi_k(x) = e^{ikx} u_k(x)$

with $u_k(x+a) = u_k(x)$

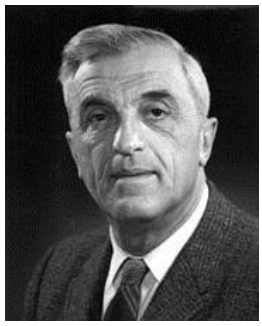
# Bloch's band picture: The example of SrVO3






Where are the electrons?



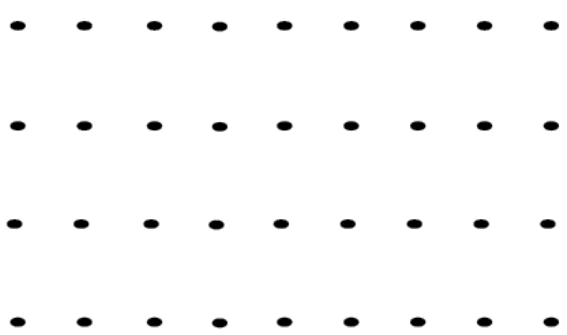
$$|\Psi_{kn}(r)|^2 = |e^{ikx}u_{kn}(r)|^2 = |u_{kn}(r)|^2$$

Everywhere in the solid !

=> Delocalisation (driven by kinetic energy)

# Question: “H-solid”

Consider an hypothetical Hydrogen solid, with H atoms occupying the sites of a 2d periodic lattice. Describe the electronic eigenstates !



[Let’s consider 1s orbital only, forget about molecule formation (ions are fixed!), magnetic solutions and assume nearest neighbor hopping only ….]

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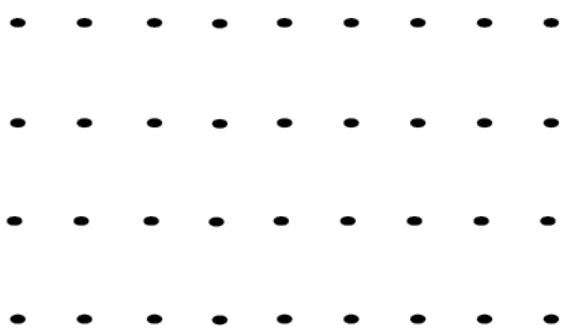

Additional information:
lattice constant a = 8 km

# The electronic Coulomb Hamiltonian

$$H = \sum_i \frac{p_i^2}{2m} + \sum_{i<j} V_{ee}(r_i - r_j) + \sum_{iJ} V_{ei}(R_J - r_i)$$

Electron-electron Coulomb interaction

Electron-ion Coulomb interaction

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$V_{eff}(r_i)$

**Independent electron picture**

# The independent electron picture – consequences:

$$H = \sum_{electrons\ i} h(i)$$

- N-electron state = Slater determinant of Bloch waves
- Momentum k of single electron a good quantum number
- Spectrum = band structure
- Products of expectation values factorize !

# Back to the H-"solid" with a=8km …

The "independent particle picture" predicts a band metal with very small but finite bandwidth of a half-filled band and electrons delocalised over hundreds of kilometers ….. In reality:

- Atoms independent
- Atomic occupations are good quantum numbers => think in real space!
- Insulator not because of interference effects opening the band gap, but Coulomb blocking
- "Double occupancy" is suppressed! -- E.g.:

$$0 = \langle n_{R\uparrow} n_{R\downarrow} \rangle \neq \langle n_{R\uparrow} \rangle \langle n_{R\downarrow} \rangle$$

# Correlations?

- "Correlatio" (lat.) = interrelation
- Two entities are "correlated" if there exists a mutual relationship ….
- Mathematically:

**Correlations:** $\langle AB \rangle \neq \langle A \rangle \langle B \rangle$

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Example: $A = n_\uparrow, B = n_\downarrow$, eigenvalues 0 or 1

Hamiltonian: $H = \epsilon(n_\uparrow + n_\downarrow) + U n_\uparrow n_\downarrow$

$$\langle n_\uparrow n_\downarrow \rangle = \frac{1}{Z} \sum_{n_\uparrow=0,1,\ n_\downarrow=0,1} n_\uparrow n_\downarrow e^{-\beta\epsilon(n_\uparrow+n_\downarrow)-\beta U n_\uparrow n_\downarrow}$$

$$\neq \langle n_\uparrow \rangle \langle n_\downarrow \rangle$$

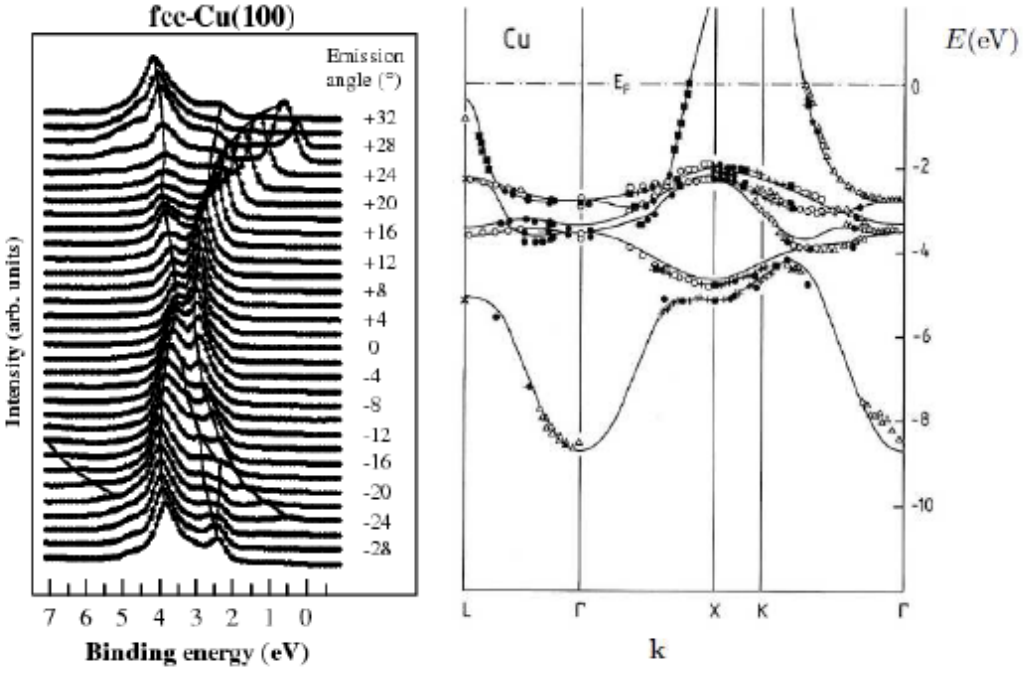
Correlations! (Hamiltonian not separable)

In general: **correlations = effects beyond mean field theory**

# Some orders of magnitude

- Kinetic energy of an electron in the solid?
- Coulomb matrix element between localised Wannier functions?

# Why does band theory work?????



# Several answers ….

- Screening reduces Coulomb interactions, typically by an order of magnitude
- Landau theory!

  [Band theory not as a single particle theory,

  but as a description of low-energy excitations

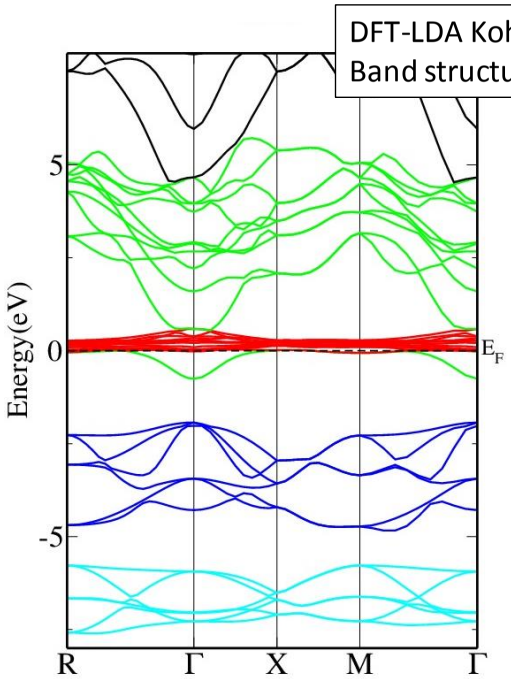
  in the solid => “Quasi-particles”]

- It does not always work ……

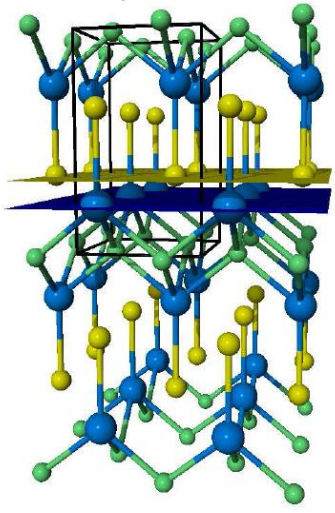
Example :

CeSF – an f-electron pigment

(cf. Rhodia’s Neolor series)




Ce: $4f^1$ configuration, paramagnetic



Tomczak, Pourosvkii, Vaugier, Georges, Biermann, PNAS (2013)

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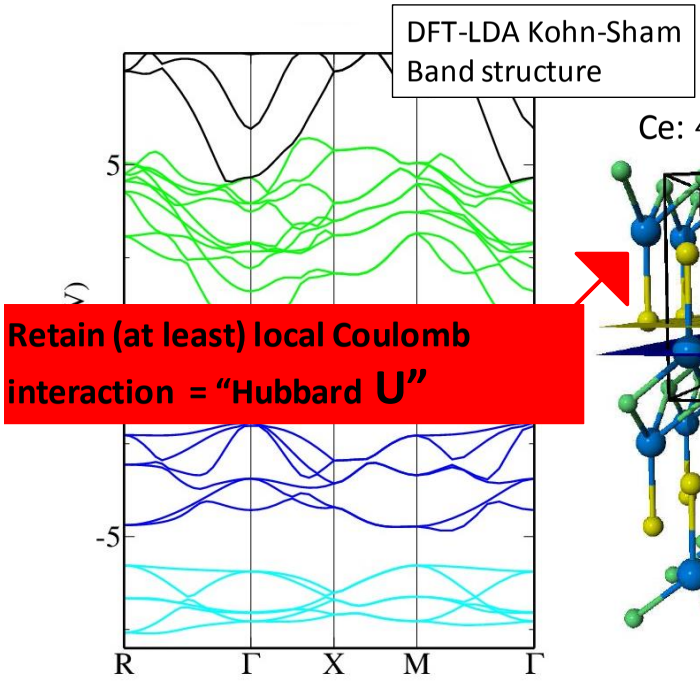


Retain (at least) local Coulomb interaction = "Hubbard U"

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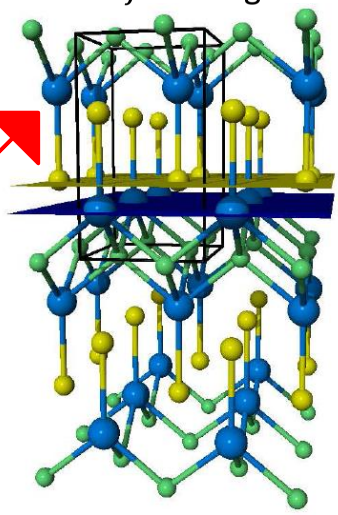

Tomczak, Pourosvkii, Vaugier, Georges, Biermann, PNAS (2013)

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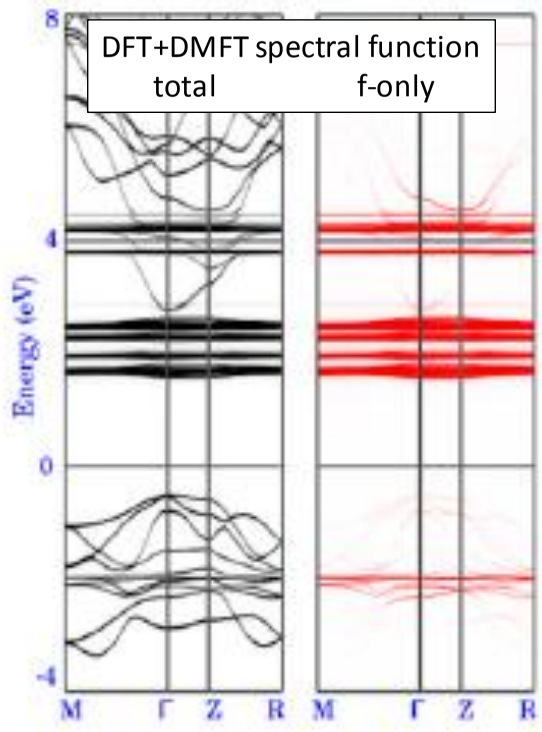


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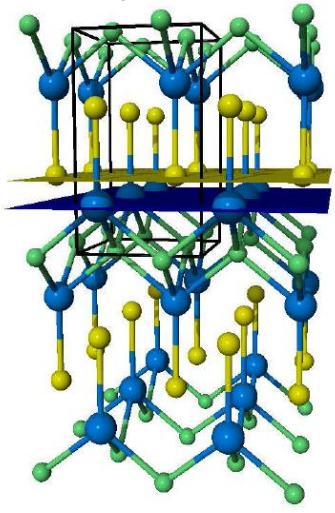


Calculated colour of CeSF:

Tomczak, Pourosvkii, Vaugier, Georges, Biermann, PNAS (2013)

# “Mott insulators”

- Examples: paramagnetic YTiO3, CeSF, Ce2O3 …. are metallic in band theory, but insulating in nature !
- Note: This is not a failure of DFT (or the specific choice of the effective single particle potential) but a failure of the single particle picture itself!
- Note: symmetry breaking helps the single particle picture, e.g. magnetism suppresses double occupation without the need for correlations!

# A note on magnetism …

- Example: ferro- or antiferromagnetic ordered solid
- At each site R either

$$0 = \langle n_{R\uparrow} \rangle \quad \text{or} \quad 0 = \langle n_{R\downarrow} \rangle$$

Then, trivially: $0 = \langle n_{R\uparrow} n_{R\downarrow} \rangle$

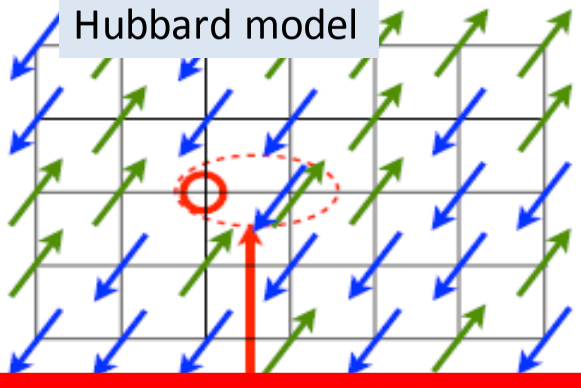
- Seemingly, no need for correlations:

$$\langle n_{R\uparrow} n_{R\downarrow} \rangle = \langle n_{R\uparrow} \rangle \langle n_{R\downarrow} \rangle$$

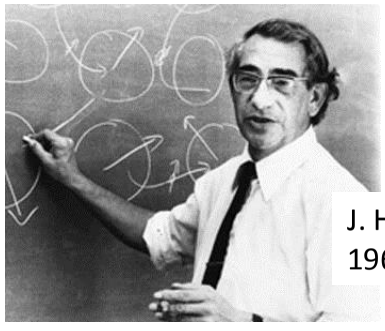
# Side remark: “LDA+U”

- Static mean field theories that apply a spin-dependent effective potential to the single-particle band structure can open the gap in the magnetic phases!
- Note however: mismatch in energy scales (Neel temperature << gap !) indicates that magnetic order is likely not the primary reason for the gap
- Needed: true finite temperature description!

# Modelling correlated electron behavior “Lattice models”




**Local Coulomb interaction = “Hubbard U”**



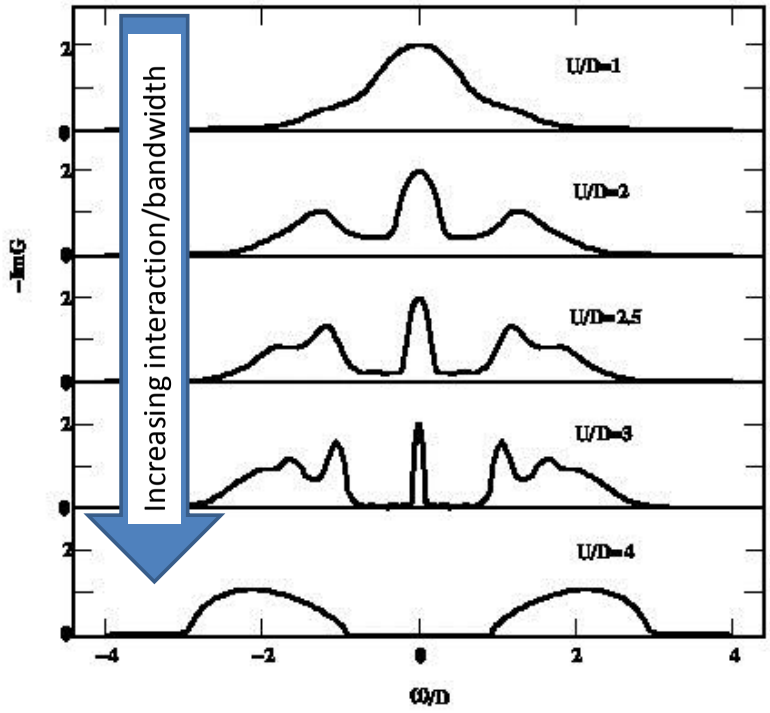
J. Hubbard, 1964

=> Minimal description of interplay between Coulomb interaction and delocalisation energy

$$H = -t \sum_{\langle ij \rangle \sigma} (c^{\dagger}_{i\sigma} c_{j\sigma} + \text{H.c.}) - \mu \sum_i n_i$$

$$+ U \sum_i n_{i\uparrow} n_{i\downarrow}$$

# The Mott transition




Spectral function of half-filled Hubbard model, paramagnetic phase

Zhang, Rozenberg, Kotliar, 1993
Georges, Kotliar, 1992

# The Menu

- Correlations in Condensed Matter -- Modeling Correlated Electron Behavior
- **What's a mean field theory?**
- Dynamical mean field theory (DMFT) and "DFT+DMFT"
- Beyond "DFT+DMFT": functional approaches, GW+DMFT …
- Conclusions/perspectives

# Example: Ising model $H = -\sum_{(ij)} J_{ij} S_i S_j$

- Map lattice model onto a single spin in an effective magnetic field

$$H_{eff} = -\sum_i h_i^{eff} S_i$$

- Determine magnetic field ("mean field") self-consistentlv

$$h_i^{eff} \simeq h + \sum_j J_{ij} m_j = h + zJm$$

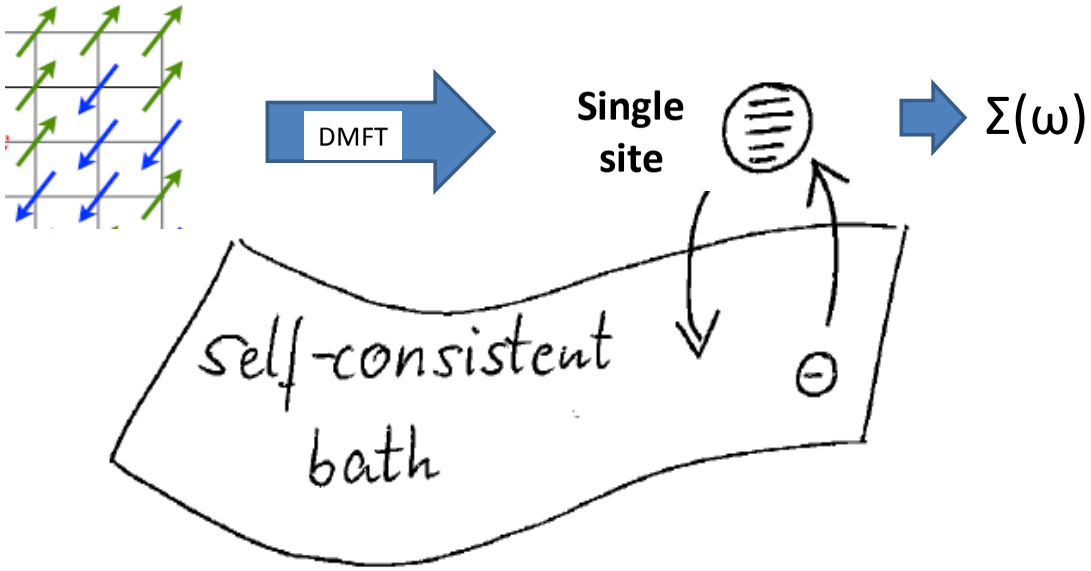
$$m = \tanh(\beta h + z\beta Jm)$$

## What's a mean field theory?

Two ingredients:

- **Auxiliary system ("reference system")**, that can be solved
- **Self-consistency condition** for the mean field to restore symmetries of the original problem

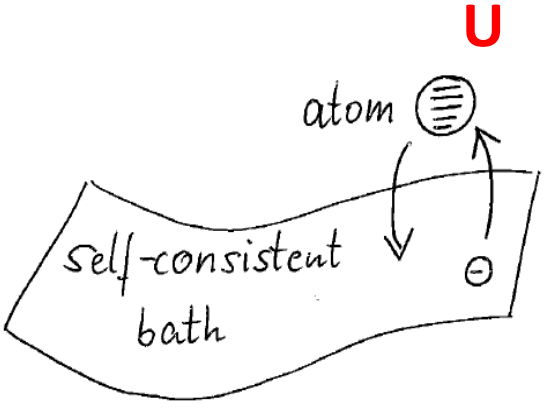
# Dynamical mean field theory (DMFT)




For a review, see Georges, Kotliar, Krauth, Rozenberg, Rev. Mod. Phys. 1996

## DMFT

Calculate $G_{loc}$ from an impurity problem (that is, a single site coupled to a bath):




$$H_{AIM} = H_{atom} + H_{bath} + H_{coupling}$$

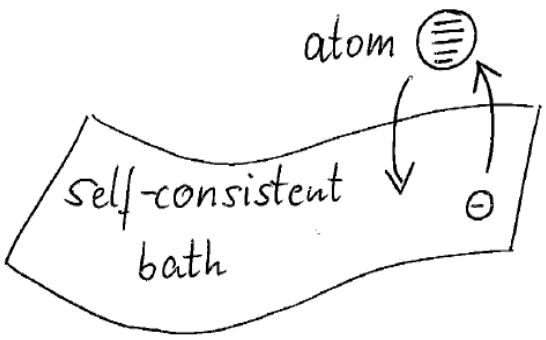
$$H_{atom} = U\, n_{\uparrow}^{c} n_{\downarrow}^{c} + (\varepsilon_0 - \mu)\,(n_{\uparrow}^{c} + n_{\downarrow}^{c})$$

$$H_{bath} = \sum_{l\sigma} \tilde{\varepsilon}_l\, a_{l\sigma}^{\dagger} a_{l\sigma}$$

$$H_{coupling} = \sum_{l\sigma} V_l\,(a_{l\sigma}^{\dagger} c_{\sigma} + c_{\sigma}^{\dagger} a_{l\sigma})$$

Determine bath (the dynamical mean field) self-consistently

# Anderson impurity problem:

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$$H_{coupling} = \sum_{l\sigma} V_l\,(a_{l\sigma}^{\dagger} c_{\sigma} + c_{\sigma}^{\dagger} a_{l\sigma})$$

Integration over bath degrees of freedom gives hybridisation function

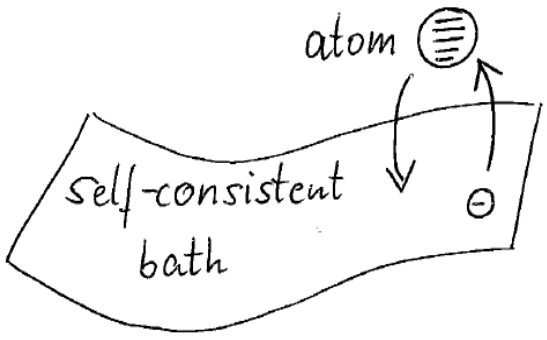
$$\Delta(i\omega_n) = \sum_l \frac{|V_l|^2}{i\omega_n - \widetilde{\varepsilon}_l}$$

# Equivalent formulation of Andersen impurity problem:

Impurity action:

$$S_{eff} = -\int_0^{\beta} d\tau \int_0^{\beta} d\tau' \sum_{\sigma} c_{\sigma}^{+}(\tau)\mathcal{G}_0^{-1}(\tau - \tau')c_{\sigma}(\tau') + U\int_0^{\beta} d\tau\, n_{\uparrow}(\tau)n_{\downarrow}(\tau)$$

$$\mathcal{G}_0^{-1}(i\omega_n) = i\omega_n + \mu - \varepsilon_0 - \Delta(i\omega_n)$$



# DMFT – one slide for experts …

Impurity action:

$$S_{eff} = -\int_0^\beta d\tau \int_0^\beta d\tau' \sum_\sigma c_\sigma^+(\tau)\mathcal{G}_0^{-1}(\tau-\tau')c_\sigma(\tau') + U\int_0^\beta d\tau\, n_\uparrow(\tau)n_\downarrow(\tau)$$

$$\mathcal{G}_0^{-1}(i\omega_n) = i\omega_n + \mu - \varepsilon_0 - \Delta(i\omega_n)$$

Calculate Green's function G and deduce self-energy:

$$\Sigma_{imp}(i\omega_n) \equiv \mathcal{G}_0^{-1}(i\omega_n) - G^{-1}(i\omega_n)$$

DMFT approximation: $\Sigma_{ii} \simeq \Sigma_{imp}\ ,\ \Sigma_{i\neq j} \simeq 0$

$$G(\mathbf{k}, i\omega_n) = \frac{1}{i\omega_n + \mu - \varepsilon_0 - \varepsilon_{\mathbf{k}} - \Sigma(\mathbf{k}, i\omega_n)}$$

and self-consist …

# Standard MFT vs. DFT vs. DMFT

| | Standard Mean Field Theory – ex.: Ising Model | DFT | DMFT |
|---|---|---|---|
| Physical quantity | Magnetisation | Density | Local Green's function |
| Auxiliary System | Spin in effective field | Electrons in effective potential | Quantum impurity problem **(interacting!)** |
| "Weiss field" | Effective magnetic field | Kohn-Sham potential | **Dynamical** mean field (effective hybridisation) |

# DMFT in a nutshell …

- Non-perturbative.
- Captures weak and strong coupling limits on equal footing; gives a picture of the Mott transition
- Incorporates “atomic physics” of localised degrees of freedom into the itinerant band picture
- Describes correlation effects on different energy scales (=> coexistence of quasi-particle excitations and Hubbard bands in the correlated metallic state)
- Self-energy is taken to be purely local – for non-local fluctuations cluster extensions required
- Finite temperatures well described

# DMFT as the infinite dimensional solution

- Hubbard model in the limit of infinite coordination number stays non-trivial model (Metzner and Vollhardt, 1989)
- In that limit, perturbation theory simplifies, self-energy purely local (Mueller-Hartmann, 1989)
- A constructive solution can be obtained from mapping onto impurity problem (Georges, Kotliar, 1992)
- Further contributions by: Ohkawa, Brandt, Mielsch, Keiter, … For bibliography see Georges et al., Rev. Mod. Phys. 1996

# “Ab initio” modeling of materials …?

Combine
**ab initio techniques**
with
**many-body theory**

*Cf. Matthias Scheffler’s lecture*

## Density Functional Theory

**Nobel Price in Chemistry, 1998**

Interacting electron gas

Mapping

Non-interacting electrons in effective potential

such that the ground state density is the same for the two systems

P. Hohenberg, W. Kohn, 1964,
W. Kohn, L. Sham, 1965

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**DFT used here as a means to generate the one-body part of a many-body Hamiltonian**

# Multi-orbital Hubbard-Hamiltonian

**One-particle part of Hamiltonian from DFT-LDA**

$$H = \sum_{\{im\sigma\}} (H^{LDA}_{im,i'm'} - H^{double\ counting}_{im,i'm'}) a^{+}_{im\sigma} a_{i'm'\sigma}$$

$$+ \frac{1}{2} \sum_{imm'\sigma\ (\text{correl. orb.})} U^{i}_{mm'} n_{im\sigma} n_{im'-\sigma}$$

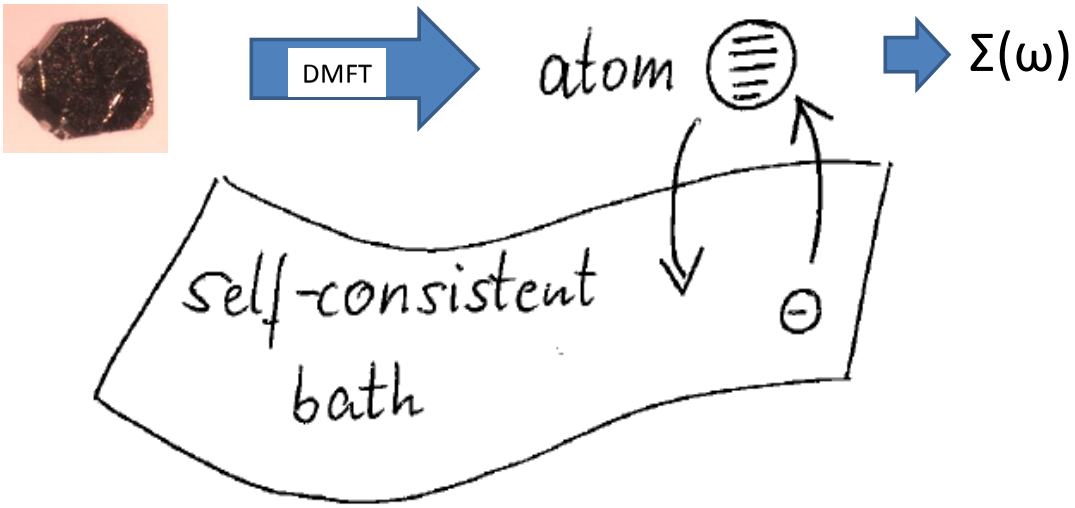
**Hubbard interaction for "correlated shell"**

$$+ \frac{1}{2} \sum_{im\neq m'\sigma\ (\text{correl. orb.})} (U^{i}_{mm'} - J^{i}_{mm'}) n_{im\sigma} n_{im'\sigma}$$

**Hund's rule coupling**

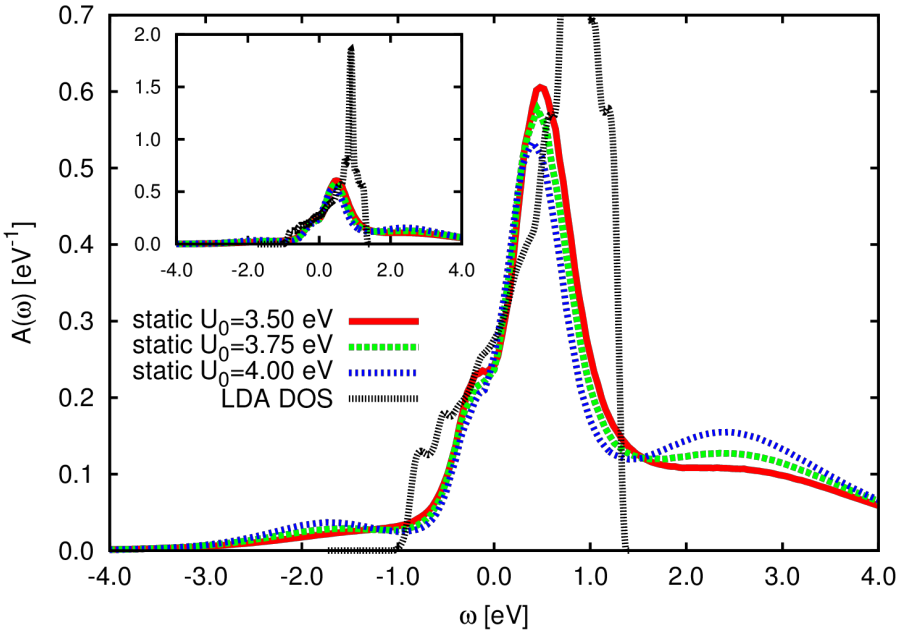
- Solve within Dynamical Mean Field Theory (DMFT)
- => "LDA+DMFT" (Ansimov et al., Lichtenstein et al., 1997/98)

# Dynamical mean field theory within realistic electronic structure calculations: “DFT+DMFT”



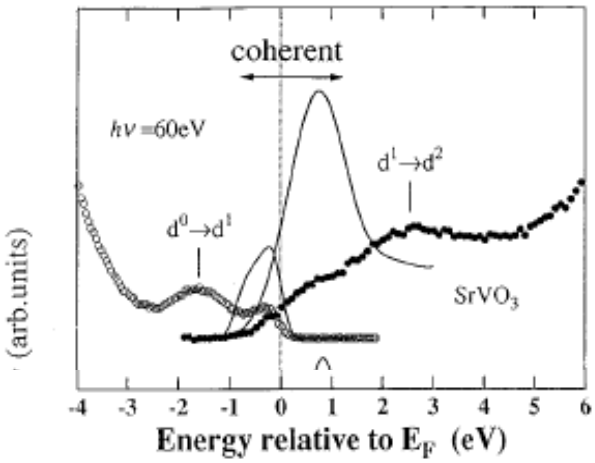

Lichtenstein, Katsnelson, 1998
Anisimov, … Kotliar, 1997

# DFT+DMFT for SrVO3

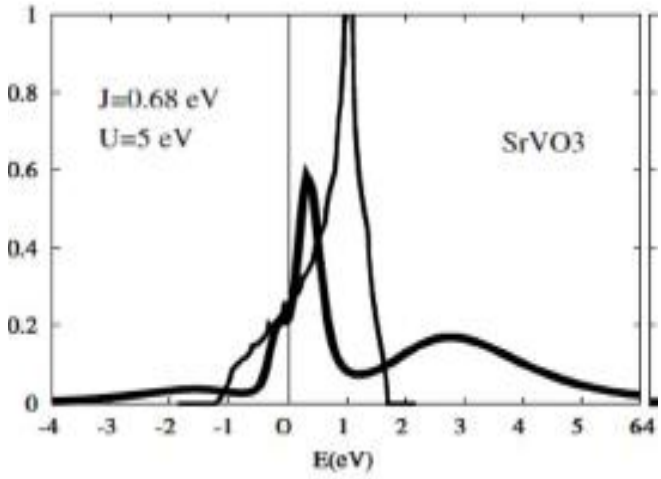



From: Tomczak, Casula, Miyake, Biermann, arXiv 2013.
See also: various authors, Pavarini et al, 2004, Nekrasov et al. 2005, Lechermann, et al. PRB 2006

# Lower Hubbard band seen in photoemission of SrVO3 !




(Inverse) Photoemission spectrum
From: Morikawa et al. 1995




DFT+DMFT calculation
From: Pavarini, SB, Poteryaev, Lichtenstein, Georges, PRL 2004

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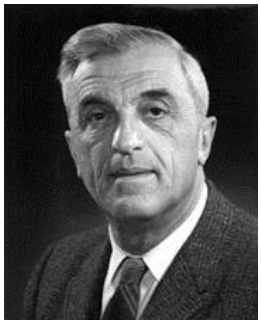
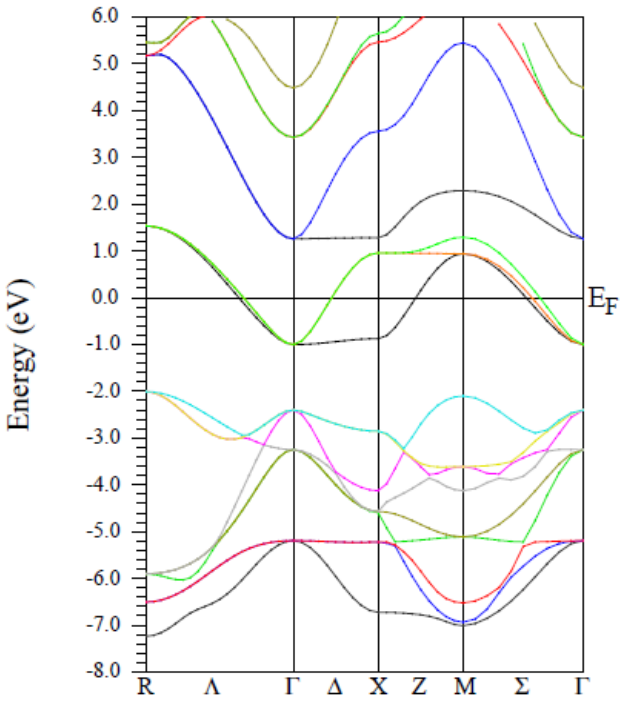
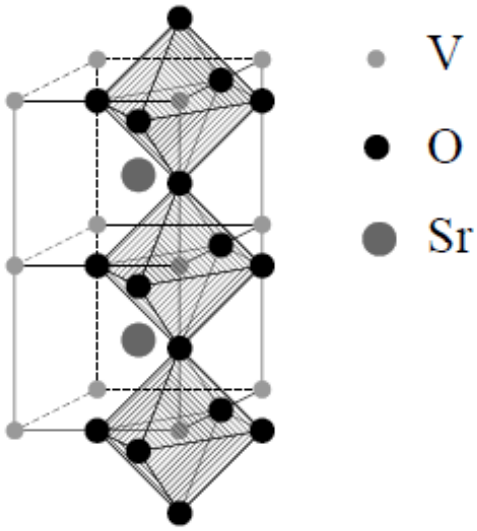
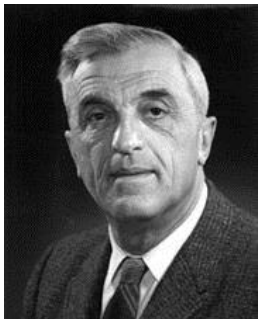
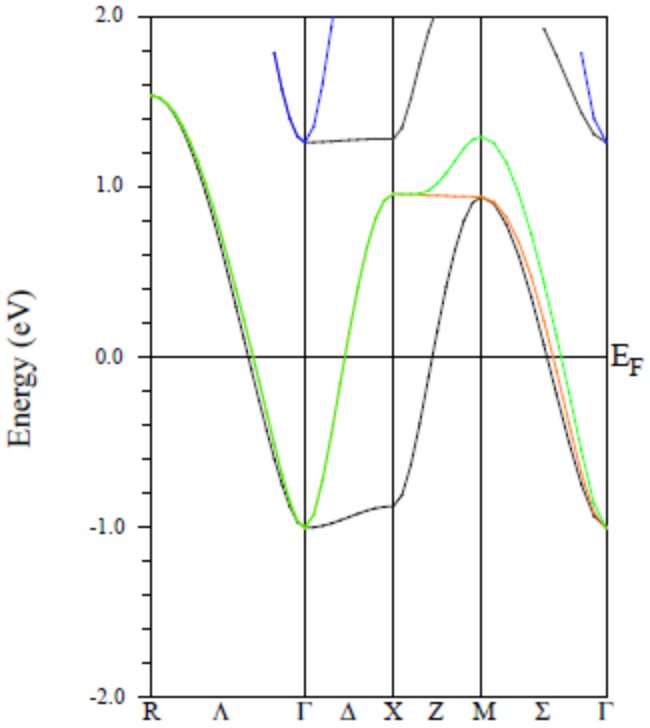


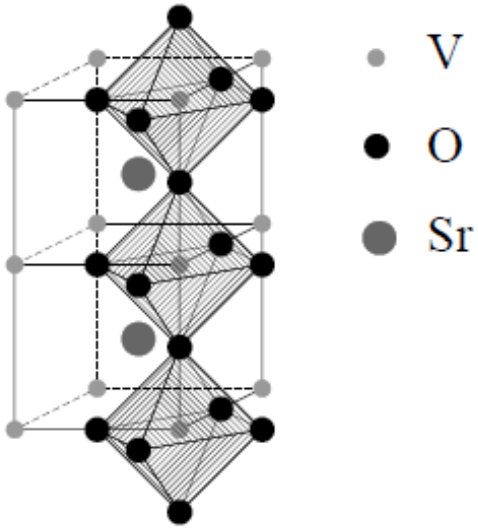


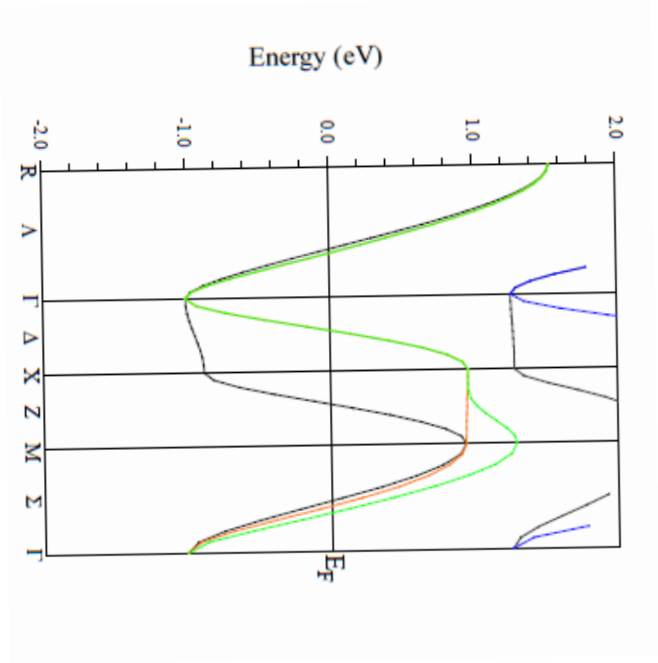
# LDA band structure of SrVO3

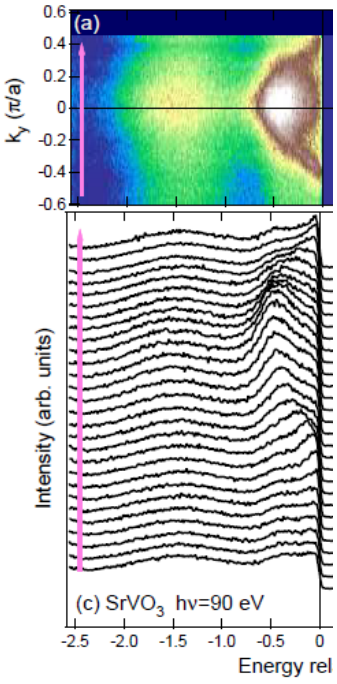




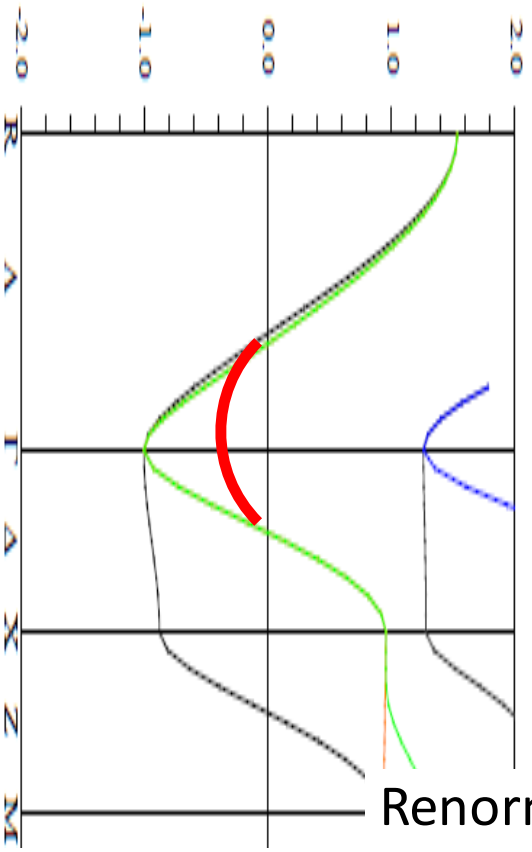

# Comparison to Angle-Resolved Photoemission: the case of SrVO3

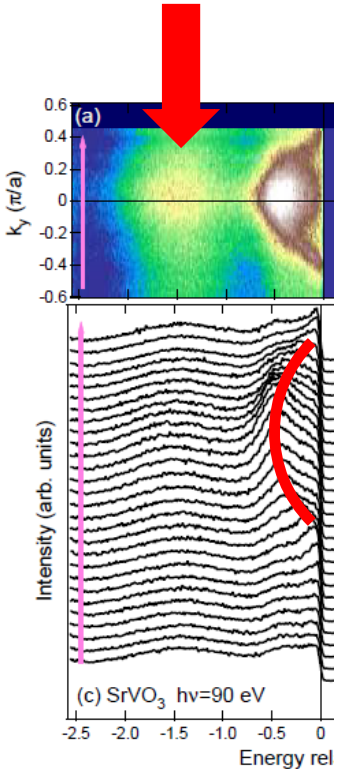



Aizaki et al., PRB 2011

“Hubbard band”



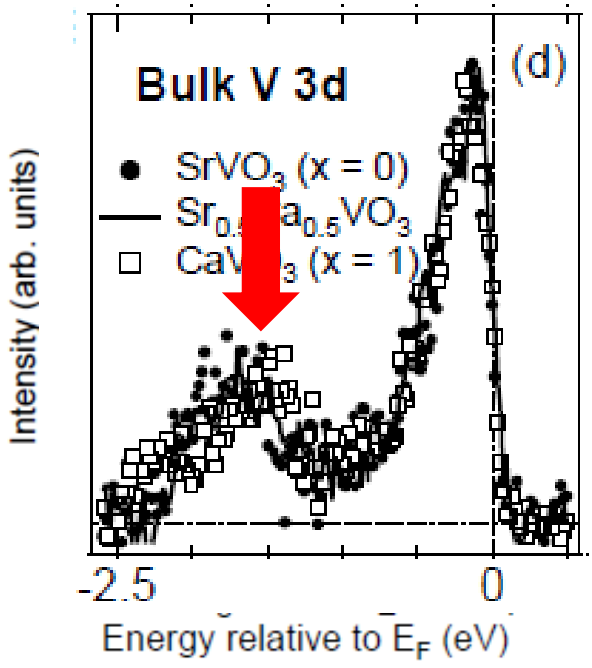



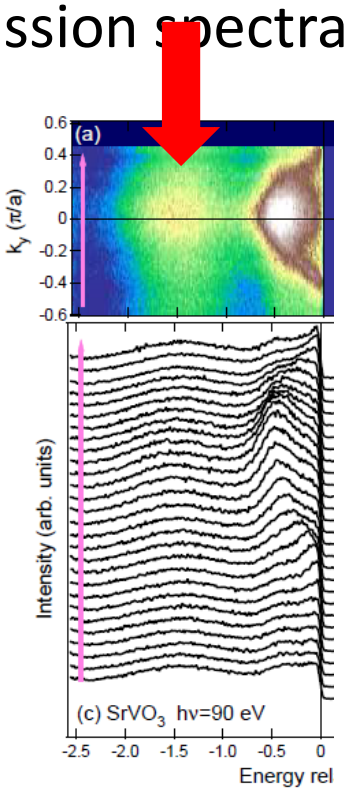

Renormalisation by factor 0.5

Aizaki et al., PRB 2011

# SrVO3:

## angle-integrated photoemission spectra



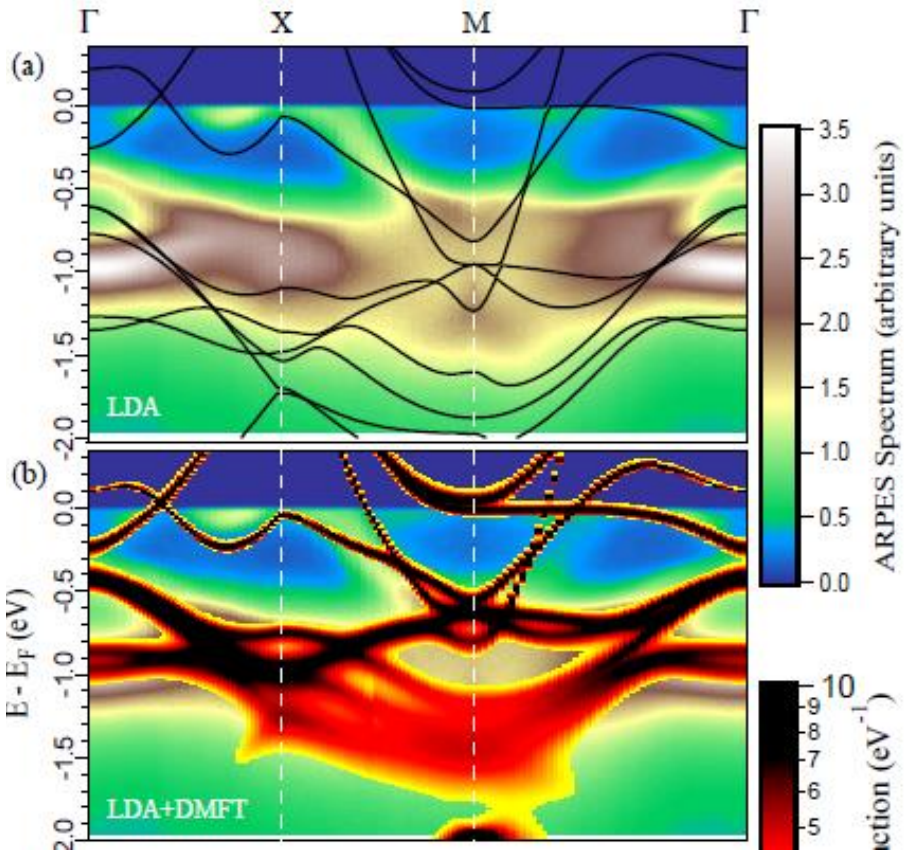

Sekiyama et al., PRL 2004

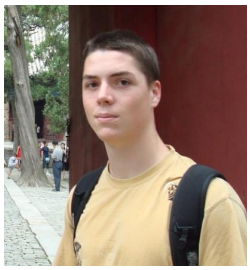
# DFT+DMFT … a story of success!

Applications to

- 3d transition metal oxides, sulphides
  [CaVO3, LaTiO3, YTiO3, VO2, V2O3, BaVS3, …]
- Transition metals [Mn, Ni, …]
- f-electron elements and compounds [Ce, CeSF, RE2O3]
- Iron Pnictides [LaFeAsO, FeSe, BaFe2As2, BaCo2As2]
- Spin-orbit materials [Sr2IrO4, Sr2RhO4]
- Low-dimensional systems (organics)
- ….

## Photoemission vs. theory: BaCo2As2



A. Van Roekeghem
IOP-CAS & Ecole Polytechnique

Xu et al., PRX (2013) &
A. van Roekeghem et al., PRL 2014

See also:
PES by Dhaka et al.

# The Menu

- Correlations in Condensed Matter -- Modeling Correlated Electron Behavior
- What's a mean field theory?
- Dynamical mean field theory (DMFT) and "DFT+DMFT"
- **Beyond "DFT+DMFT": functional approaches, GW+DMFT …**
- Conclusions/perspectives

# Towards a first-principles scheme for correlated materials: GW+DMFT

- Formulated in functional language:

Free energy of a solid as a functional Γ[G,W] of

1) the Green's function G and

2) the screened Coulomb interaction W.

[Almbladh et al., Int J. Qu. Chem. 1999]

- Γ[G,W] = Hartree part + Ψ[G,W]
- $$\Psi \approx \Psi^{\mathrm{EDMFT}}[G_{ii}, W_{ii}] + \Psi^{GW}_{\mathrm{nonloc}}[G_{ij}, W_{ij}],$$

$$\text{where } \Psi^{GW}_{\mathrm{nonloc}} = \Psi^{GW} - \Psi^{GW}_{\mathrm{loc}}.$$

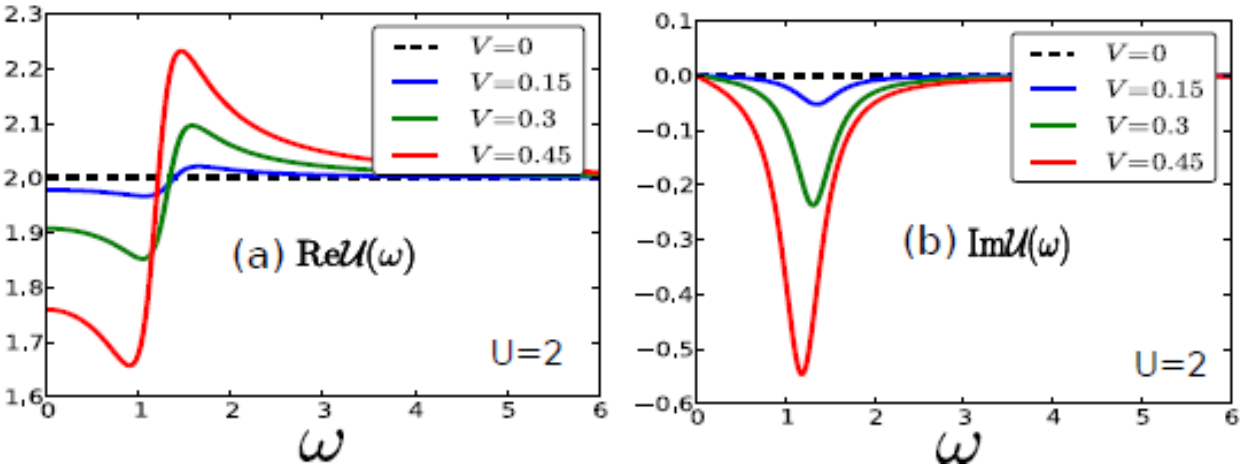
Biermann, Aryasetiawan, Georges, PRL 2003

# GW+DMFT Eqs.

$$
\begin{array}{c}
\text{Impurity model :} \\
\mathcal{G}(\tau), \mathcal{U}(\tau) \\
G_{imp} \equiv -\langle T_\tau\, cc^\dagger \rangle_S \;\rightarrow\; \Sigma^{xc}_{imp} = \mathcal{G}^{-1} - G^{-1}_{imp} \\
W_{imp} = \mathcal{U} - \mathcal{U}\chi\mathcal{U} \qquad P_{imp} = \mathcal{U}^{-1} - W^{-1}_{imp} \\
\uparrow \qquad\qquad\qquad \downarrow \\
\text{Update} \qquad\qquad \text{Combine :} \\
\mathcal{G}^{-1} = G^{-1}_{loc} + \Sigma_{imp} \qquad \Sigma = \Sigma_{imp} + \Sigma^{nonlocal}_{GW} \\
\mathcal{U}^{-1} = W^{-1}_{loc} + P_{imp} \qquad P = P_{imp} + P^{nonlocal}_{GW} \\
\uparrow \qquad\qquad\qquad \downarrow \\
\text{Self} - \text{consistency} \\
G_{loc} = \sum_{\mathbf{k}} [{G_H}^{-1} - \Sigma^{xc}]^{-1} \\
W_{loc} = \sum_{\mathbf{q}} [V^{-1}_{\mathbf{q}} - P]^{-1}
\end{array}
$$

**+ outer loop:** self-consistency over GW calculation: update P_nonlocal and $\Sigma_{nonlocal}$

"GW+DMFT" as a bridge between Coulomb interaction in the continuum and Hubbard physics:




Hubbard U becomes an auxiliary quantity that is self-consistently determined!

# What GW+DMFT is supposed to do for you …

- Describe correlated states with arbitrary local correlation strength
- Include exchange beyond DFT-LDA (!)
- Make the link between 1/|r-r'| and an auxiliary quantity U(w) (not a parameter any more!) – screening from first principles!
- Charge ordering instabilities [cf. Ayral et al., PRL 2012]
- Describe "uncorrelated states" beyond DFT
- Get rid off double counting (Caveat: in orbital-separated scheme, need to take care of "$\Sigma_{pd}$")
- Solve issue of self-consistency/starting point of GW

For applications to real solids, see eg. Hansmann et al, PRL 2013, Tomczak et al, EPL 2012, PRB 2014.
For extended model stuides, see: Ayral et al., PRL 2012, PRB 2013, Li et al., PRB 2014.

# Conclusions

- Electronic correlations

$$\langle n_{R\uparrow} n_{R\downarrow} \rangle \neq \langle n_{R\uparrow} \rangle \langle n_{R\downarrow} \rangle$$

$\Rightarrow$ need to incorporate "atomic-like" physics

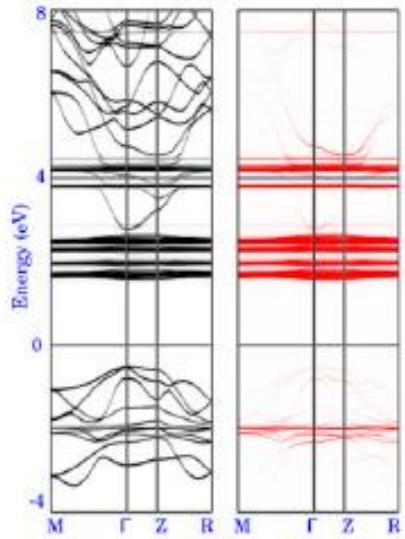
- General concepts of mean field theories: auxiliary system, self-consistency

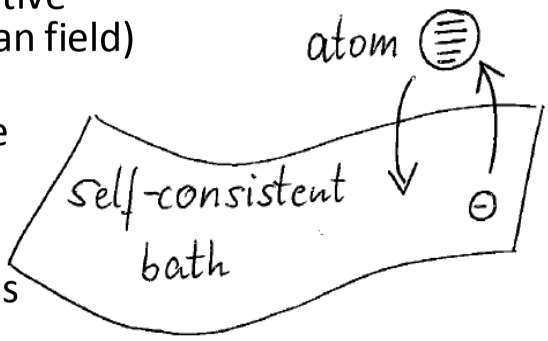
$\Rightarrow$ Examples: Ising, DFT, DMFT

- DMFT: mapping of the solid onto interacting quantum impurity problem with effective hybridisation function (dynamical mean field)

$\Rightarrow$ suitable for strong/weak coupling & intermediate correlated metal regime

- Successful to describe spectroscopic properties of a wide range of materials



# Perspectives

- Non-local extensions of DMFT ("Cluster-DMFT")
- Improved interfacing of DMFT and electronic structure techniques (GW, basis sets …)
- More quantities: transport, forces …
- Bigger systems …

# Electron addition ...

... – theoretician's point of view

Consider many-body ground state $|\Psi^N_{GS}\rangle$ and add an electron with quantum numbers $m, \sigma$:

$$c^\dagger_{m\sigma}|\Psi^N_{GS}\rangle \qquad (1)$$

# Electron addition ...

## ... – theoretician's point of view

Consider many-body ground state $|\Psi^N_{GS}\rangle$ and add an electron with quantum numbers $m, \sigma$:

$$c^\dagger_{m\sigma}|\Psi^N_{GS}\rangle \tag{2}$$

Let state evolve in time:

$$e^{iHt}\ c^\dagger_{m\sigma}|\Psi^N_{GS}\rangle \tag{3}$$



At time $t$, does the state still ressemble the initial state

$$c^\dagger_{m\sigma}|\Psi^N_{GS}\rangle \ \ ? \tag{4}$$

Consider overlap

$$\langle\Psi^N_{GS}|c_{m\sigma}\ e^{iHt}\ c^\dagger_{m\sigma}|\Psi^N_{GS}\rangle \tag{5}$$

At time $t$, does the state still ressemble the initial state

$$c^\dagger_{m\sigma}|\Psi^N_{GS}\rangle \quad ? \tag{6}$$

Consider overlap

$$\langle\Psi^N_{GS}|c_{m\sigma}\ e^{iHt}\ c^\dagger_{m\sigma}|\Psi^N_{GS}\rangle \tag{7}$$

In the case of a non-interacting system: $\sim \exp(i\ \text{Energy}\ t)$.
In an interacting system: electron decays ...



# Green's function – survival kit

Definition of (zero-temperature) Green's function:

$$G(k,t) = -\langle\hat{T}c_k(t)c^\dagger_k(0)\rangle$$

with

$$c_k(t) = exp(-iHt)c_k exp(iHt)$$

and the time-ordering operator $\hat{T}$.

$\langle ...\rangle$ denotes the expectation value in the ground state.

*NB. k from Fourier transform with respect to Bravais lattice.*
*Additional quantum numbers* $\rightarrow G$ *matrix in orbital space*

# Green's function – properties

$$A(k,\omega) = -\frac{1}{\pi} Tr \Im G(k,\omega)$$

Non-interacting case:

$$G_0(k,\omega) = \frac{1}{\omega + \mu - \epsilon_o(k) + i\eta}$$

General case: define self-energy $\Sigma$ such that

$$G(k,\omega) = \frac{1}{\omega + \mu - \epsilon_o(k) - \Sigma(k,\omega)}$$

All interaction effects are hidden in the *self-energy*:

$$\Sigma(k,\omega) = G_0^{-1}(k,\omega) - G^{-1}(k,\omega)$$



# Green's functions – properties

One-particle excitations $\leftrightarrow$ poles of $G(k,\omega)$

$$A(k,\omega) = \frac{1}{\pi} \frac{-\Im\Sigma(k,\omega)}{\left(\omega - \epsilon_0(k)\right)^2 + \left(-\Im\Sigma(\omega)\right)^2}$$

Well-defined band-like states if $\Im\Sigma$ small.

# Fermi liquids

In a Fermi liquid (local (i.e. k-independent) self-energy and $\mu = 0$, for simplicity ...):

$$\begin{aligned} Im\Sigma(\omega) &= -\Gamma\omega^2 + O(\omega^3) \\ Re\Sigma(\omega) &= Re\Sigma(0) + (1 - Z^{-1})\omega + O(\omega^2) \end{aligned}$$

$$A(k,\omega) = \frac{Z^2}{\pi} \frac{-\Im\Sigma(\omega)}{(\omega - Z\epsilon_0(k))^2 + (-Z\Im\Sigma(\omega))^2} + A_{inkoh}$$

For small Im $\Sigma$ (i.e. well-defined quasi-particles): Lorentzian of width ZIm $\Sigma$,
Poles at renormalized quasi-particle bands Z$\epsilon_0(k)$,
Weight Z (instead of 1 in non-interacting case)



# What about finite temperatures?

Define thermal Green's function!

Idea: thermal weight $exp(-\beta H)/Z$ ressembles $exp(-iHt)$
$\rightarrow$ Notion of "imaginary time"

# What about finite temperatures?

Definition of Green's function:

$$G(k,\tau) = -\langle \hat{T}_\tau c_k(\tau) c_k^\dagger(0) \rangle$$

with

$$c_k(\tau) = exp(-\tau H) c_k exp(\tau H)$$

and the time-ordering operator $\hat{T}_\tau$ in imaginary time.
$\langle ... \rangle$ denotes the thermal expectation value at temperature T, related to $\beta$ by $\beta = 1/k_B T$.



# In practice:

Obtain $G(k, i\omega_n)$ by Fourier transform from $G(k,\tau)$.
(where $\omega_n = (2n+1)\pi/\beta$ are the "fermionic Matsubara frequencies")

Need to make "analytic continuation" of $G(k, i\omega_n)$ to obtain $G(k,\omega)$ for real frequencies, and calculate spectra.

# Temperature dependence ...

... of electronic properties can be strong in correlated materials!

Not only through Fermi factor (thermal occupation of states), but also through the spectral function itself !!

Note: $\Sigma$ is temperature-dependent.
Example: In a Fermi liquid

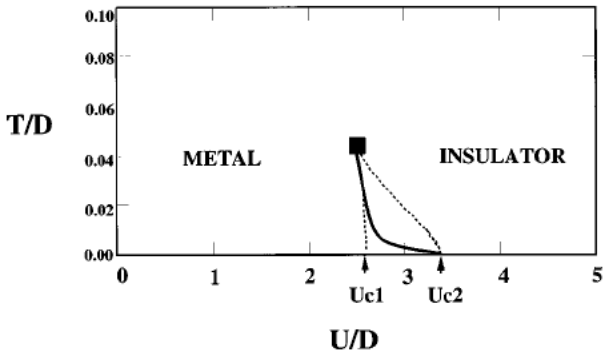
$$Im\Sigma(\omega) \quad = \quad -\Gamma(\omega^2 + \pi T^2)$$

at low energies and low temperatures
$\rightarrow$ Notion of coherence temperature (below which Fermi liquid properties are observed)



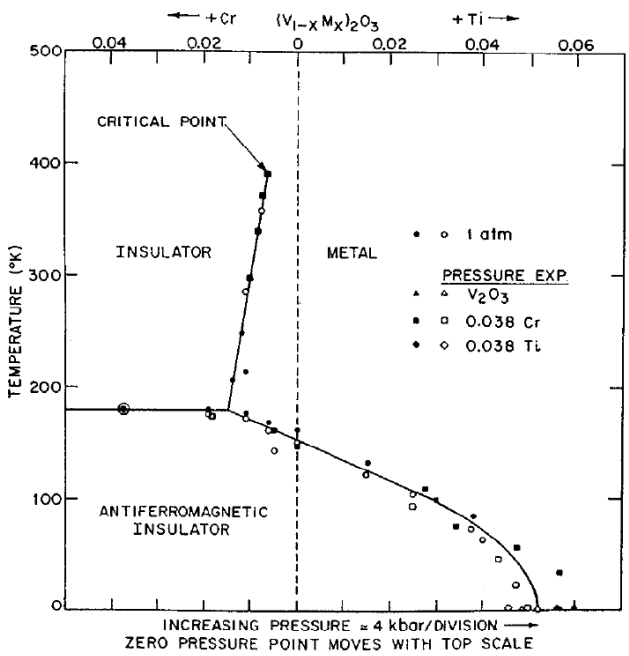
# Finite temperatures

Paramagnetic phase diagram of half-filled Hubbard model within DMFT:




First order transition (ending in 2nd order critical points) with coexistence region of metallic and insulating solutions!

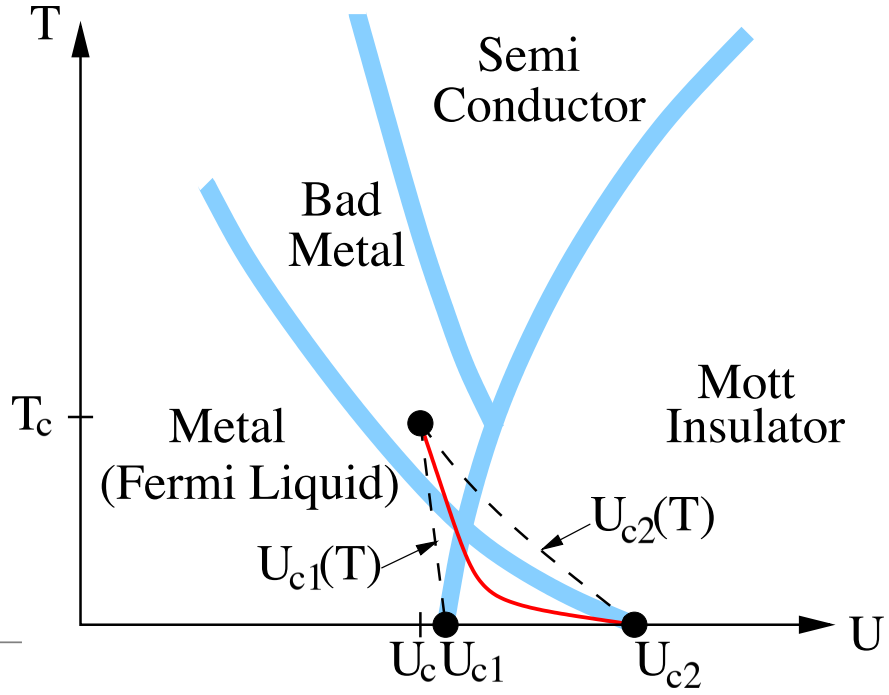
# Real materials ... : $V_2O_3$



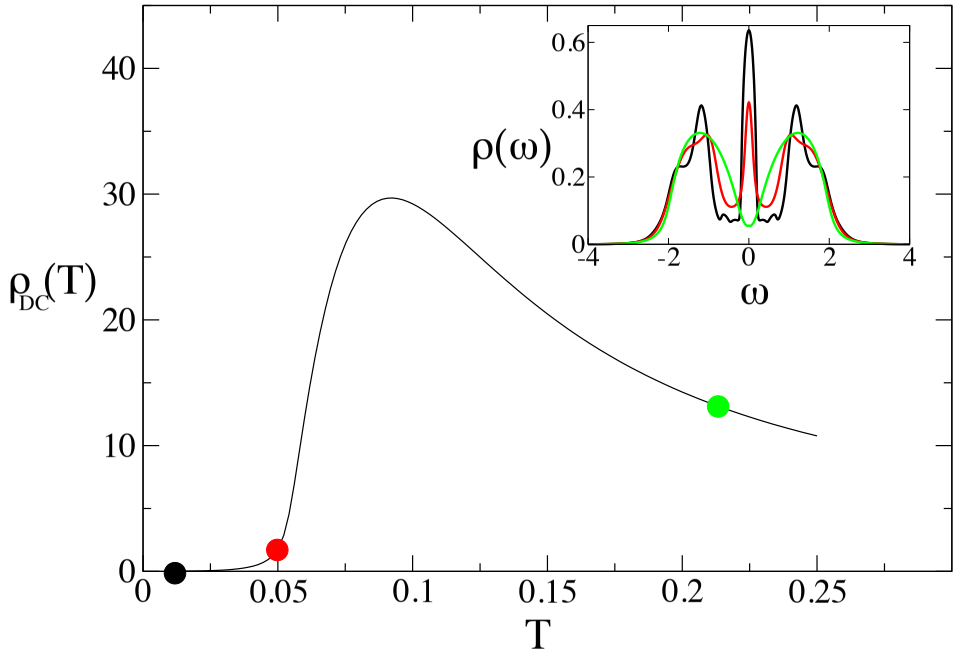



# High temperatures ?

Paramagnetic phase diagram of half-filled model within DMFT:



# High temperatures ?

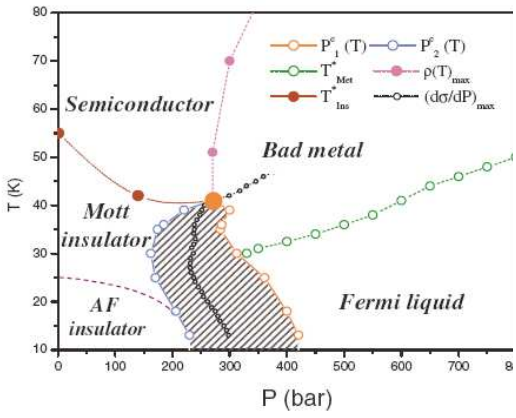


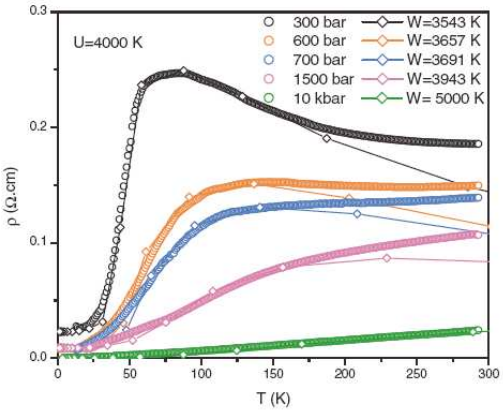

Fermi liquid, bad metal and semiconducting regime



# Real materials ...

2D Organic BEDT compound




Limelette et al., PRL 2003