From LDA++ to X+DMFT:

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Strategies for interfacing electronic structure and many-body theory

Silke Biermann

Centre de Physique Théorique,
Ecole Polytechnique, Palaiseau, France

Collaborators and Funding

Ceria	**J. Tomczak**, L. Pourovskii, L. Vaugier, A. Georges
Sr2RhO4	**C. Martins,** M. Aichhorn, L. Vaugier, S. Biermann
BaFe2As2	**P. Werner**, M. Casula, T. Miyake, F. Aryasetiawan, A. Millis ARPES: Veronique Brouet
BaCo2As2	**A. Van Roekeghem**, J. Tomczak, M. Casula, T. Ayral, H. Jiang, F. Ferrero, O. Parcollet ARPES: Hong Ding's group
SrVO3/SrTiO3	**A. Van Roekeghem**
SrVO3 within GW+DMFT	**J.Tomczak,** M. Casula, T. Miyake
Sn/Si(111)	**P. Hansmann, T. Ayral**

Spectral properties of materials …

… beyond the band picture ?

Combine

ab initio techniques

with

many-body theory

Here: **Dynamical Mean Field Theory**

Spectral properties of materials …

… beyond the band picture ?

Combine

ab initio techniques

with

many-body theory

Which ones? How?

PHYSICAL REVIEW B VOLUME 57, NUMBER 12 15 MARCH 1998-II

Ab initio calculations of quasiparticle band structure in correlated systems: LDA++ approach

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Institute of Metal Physics, Ekaterinburg 620219, Russia

(Received 11 July 1997)

We discuss a general approach to a realistic theory of the electronic structure in materials containing correlated *d* or *f* electrons. The main feature of this approach is the taking into account of the energy dependence of the electron self-energy with the momentum dependence being neglected (local approximation).

Ab initio calculations of quasiparticle band structure in correlated systems: LDA++ approach

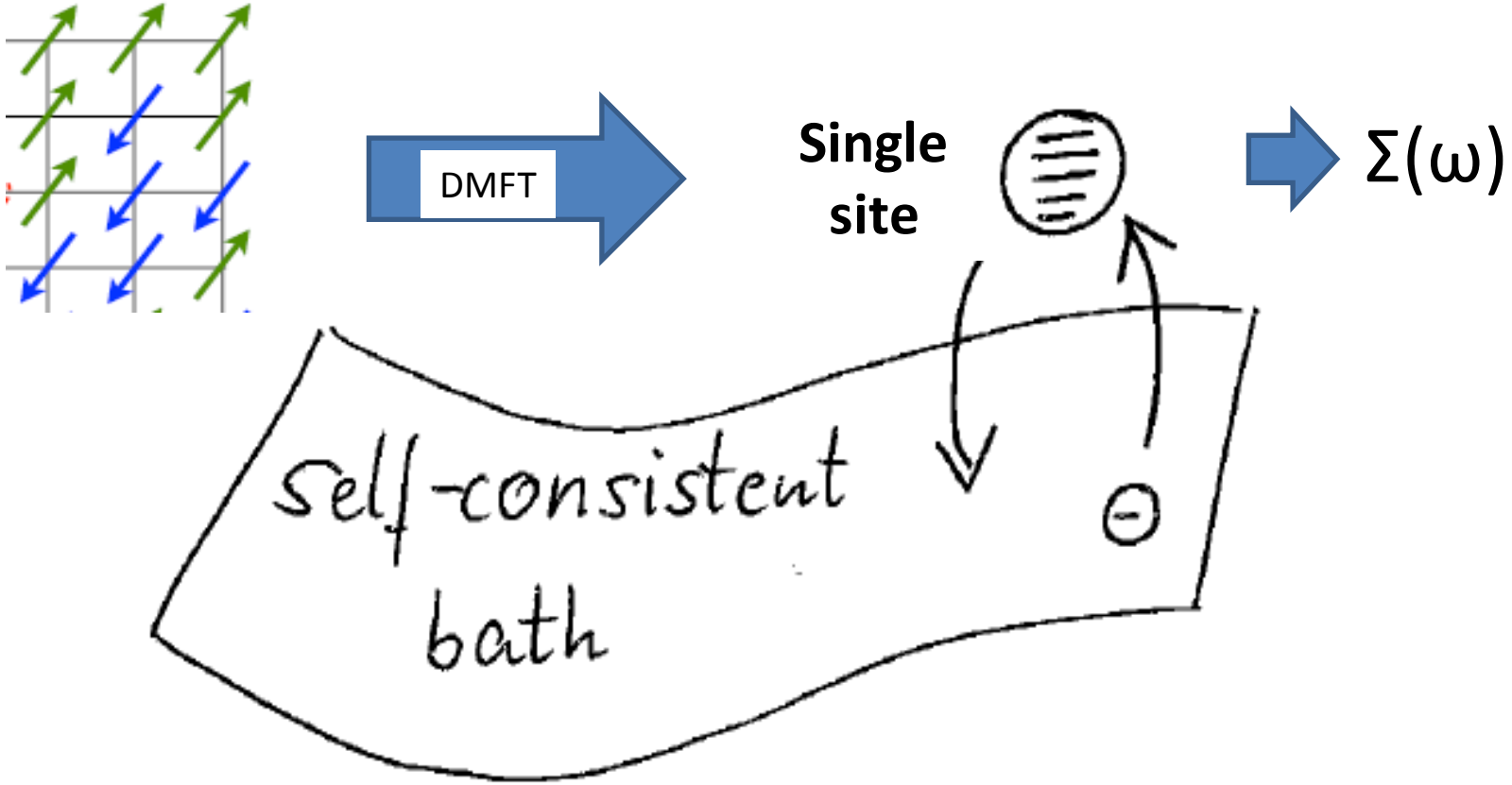
$$H=\sum_{ij\sigma\{m\}} t^{ij}_{m_1m_2} c^{+}_{im_1\sigma} c_{jm_2\sigma} + \frac{1}{2}\sum_{i\{\sigma m\}} U^{i}_{m_1m_2m_1'm_2'} c^{+}_{im_1\sigma} c^{+}_{im_2\sigma'} c_{im_2'\sigma'} c_{im_1'\sigma}, \quad (1)$$

where (i,j) represents different crystal sites, $\{m\}$ labels different orbitals, and the $\{\sigma\}$ are spin indices. Coulomb matrix elements are defined in the usual way:

$$U_{m_1m_2m_1'm_2'}=\int\int d\mathbf{r}d\mathbf{r}'\,\psi^{*}_{m_1}(\mathbf{r})\psi^{*}_{m_2}(\mathbf{r}') \times V_{ee}(\mathbf{r}-\mathbf{r}')\psi_{m_1'}(\mathbf{r})\psi_{m_2'}(\mathbf{r}'); \quad (2)$$

here $V_{ee}(\mathbf{r}-\mathbf{r}')$ is the screened Coulomb interactions and $\psi_m(\mathbf{r})$ are localized on-site basis functions (the site index being suppressed).

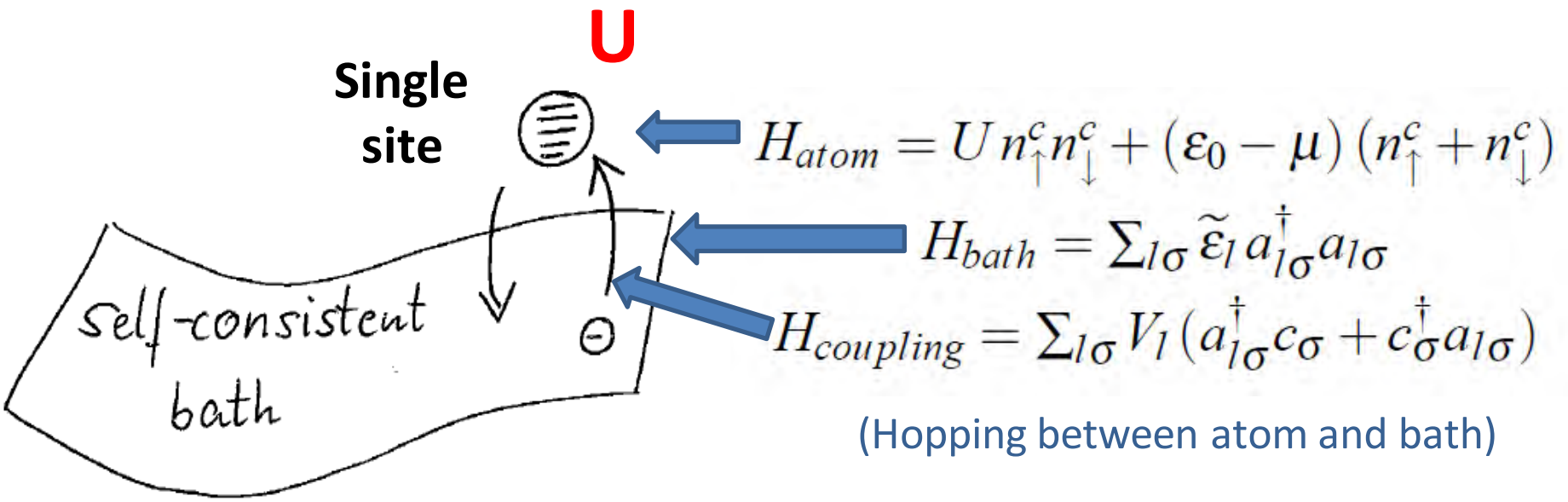
Dynamical mean field theory



Georges, Kotliar, Krauth, Rozenberg, Rev. Mod. Phys. 1996

DMFT

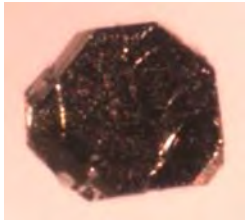
Calculate G_{loc} from an impurity problem (that is, a single site with Hubbard interaction U coupled to a bath):

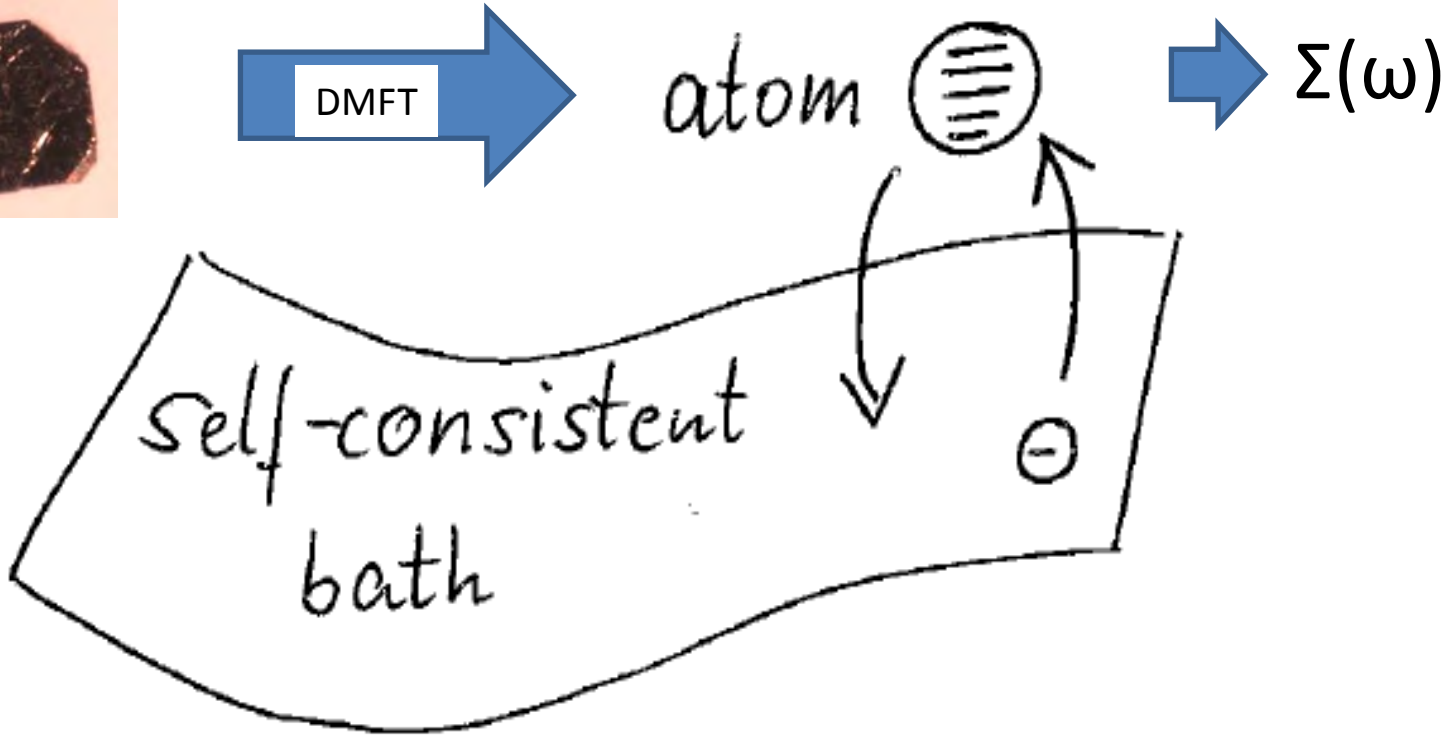


Determine bath (the dynamical mean field) self-consistently

Georges, Kotliar, Krauth, Rozenberg, Rev. Mod. Phys. 1996

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





Lichtenstein, Katsnelson, 1998
Anisimov, … Kotliar, 1997

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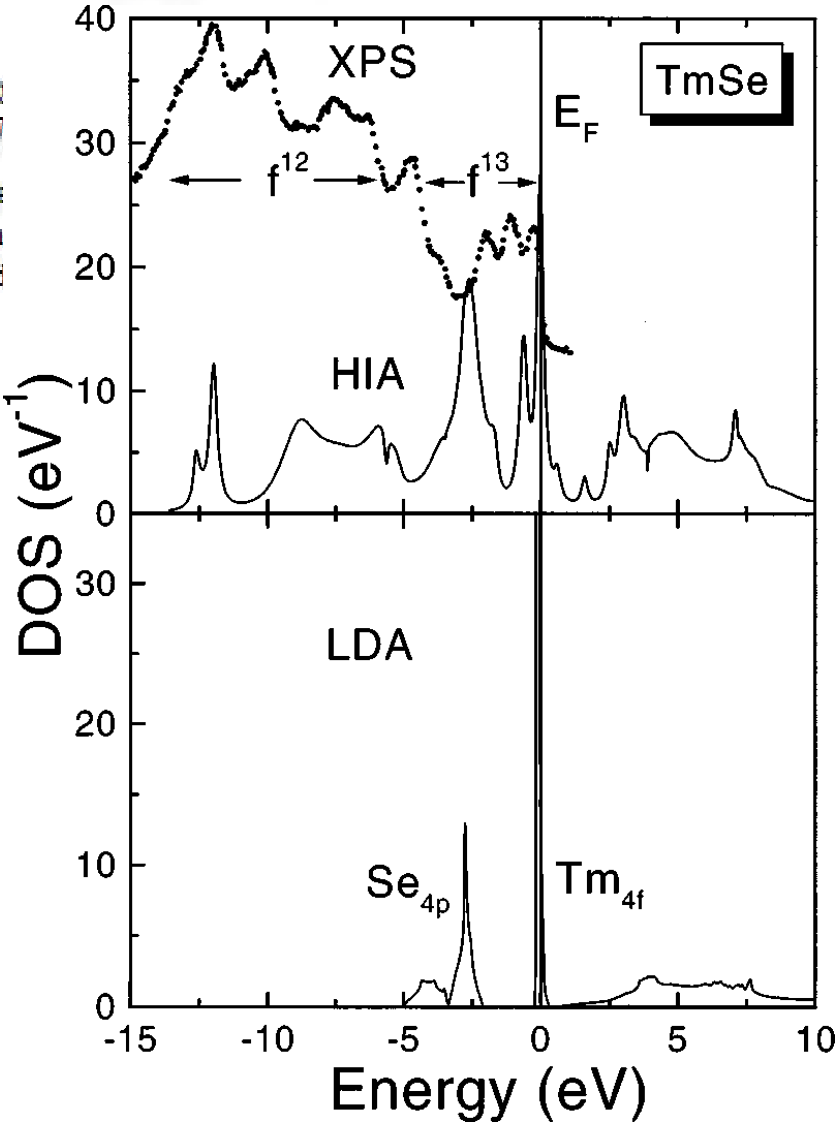


Outline

- Density functional theory + dynamical mean field theory ("DFT+DMFT")
  - Examples: CeSF, Sr2RhO4, BaCo2As2
- DFT+DMFT revisited
  - How to get rid off U?
  - How to get rid off DFT?
- Screened Exchange Dynamical Mean Field Theory
  - Concepts and relation to GW+DMFT
  - Examples: BaCo2As2, SrVO3
  - Relation to DFT? – Example: SrTiO3
- GW+DMFT
  - Examples: Adatoms on surfaces, SrVO3
- Summary/perspectives

Appetizer: it works!

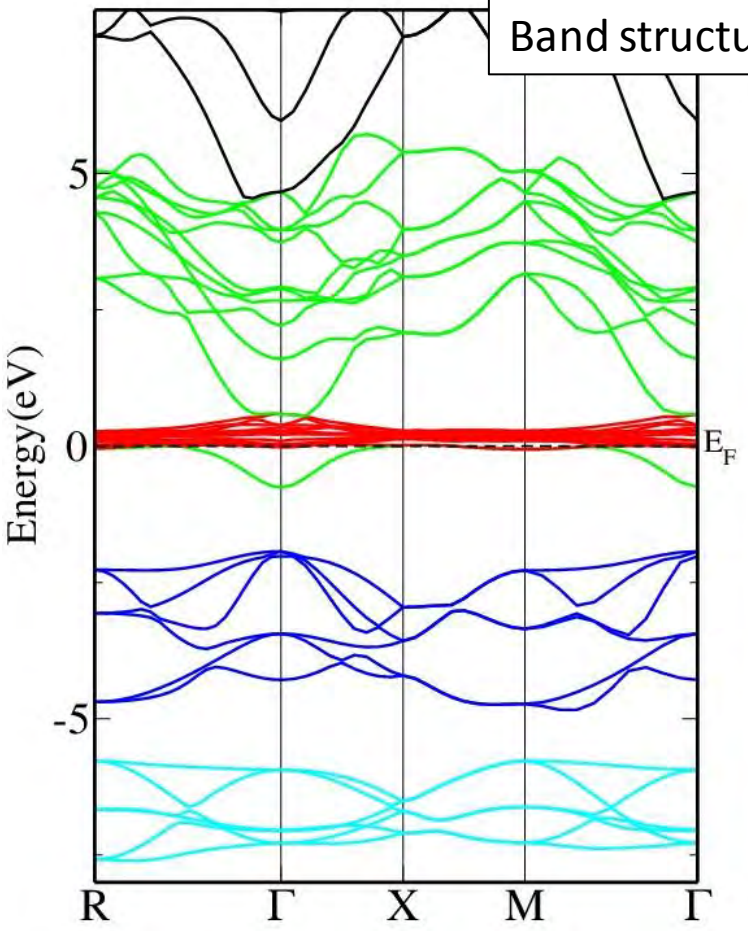
But it shouldn't ….

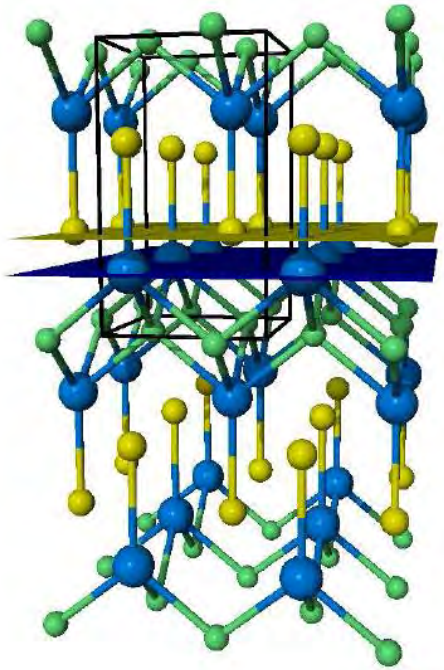
Why it works … !
(in which situations…)

How to go beyond …

Example 1:
CeSF – an f-electron pigment
(cf. Rhodia's Neolor series)

DFT-LDA Kohn-Sham
Band structure





Ce: $4f^1$ configuration,
paramagnetic

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

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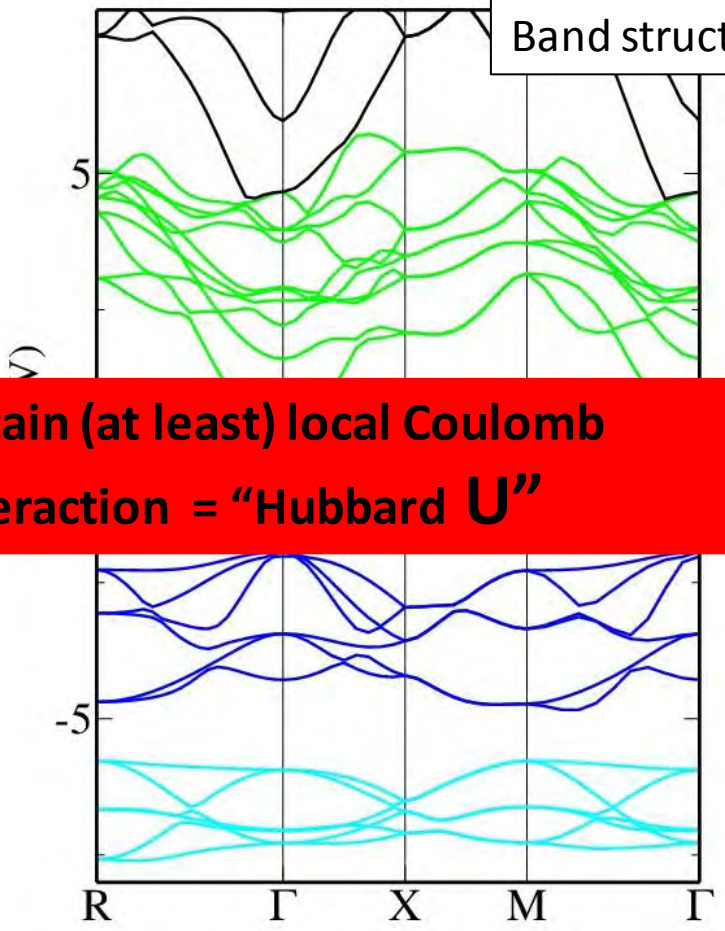
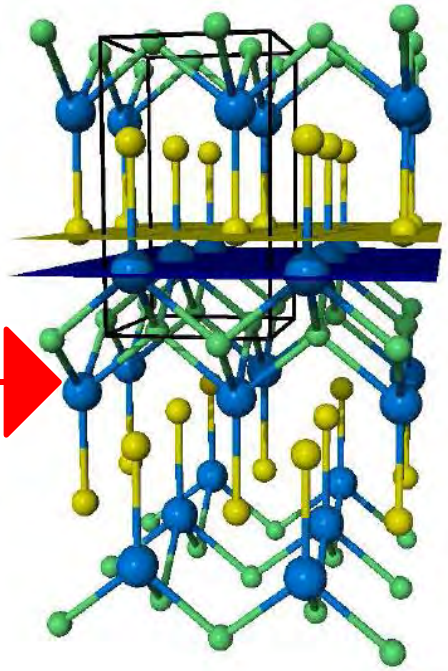


Retain (at least) local Coulomb interaction = "Hubbard U"



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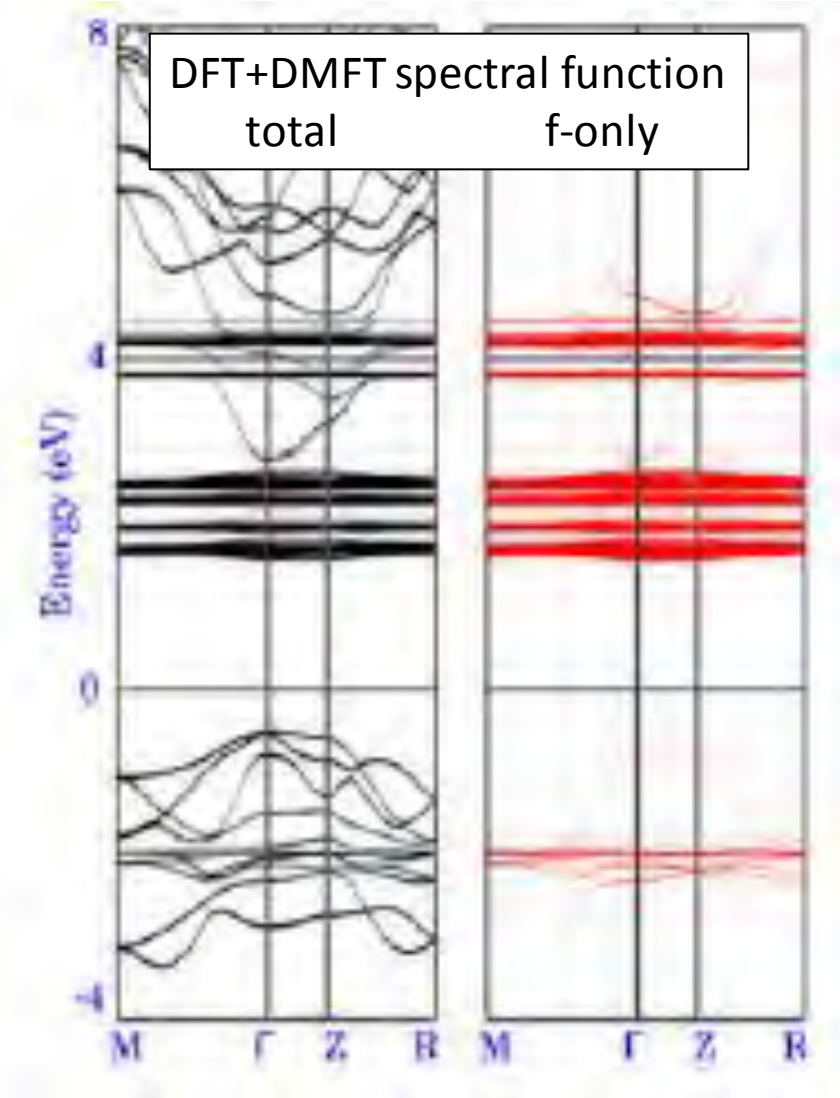
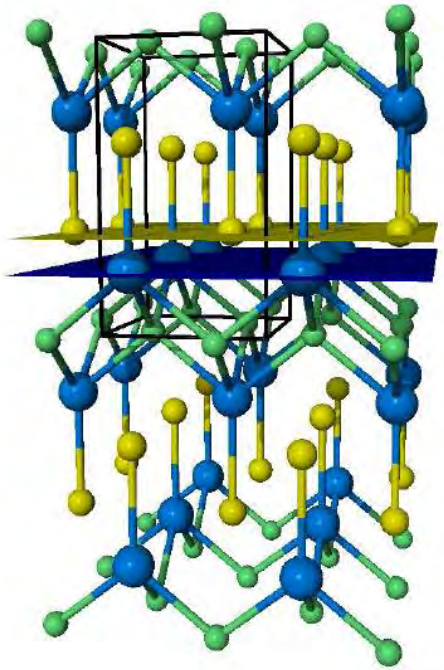


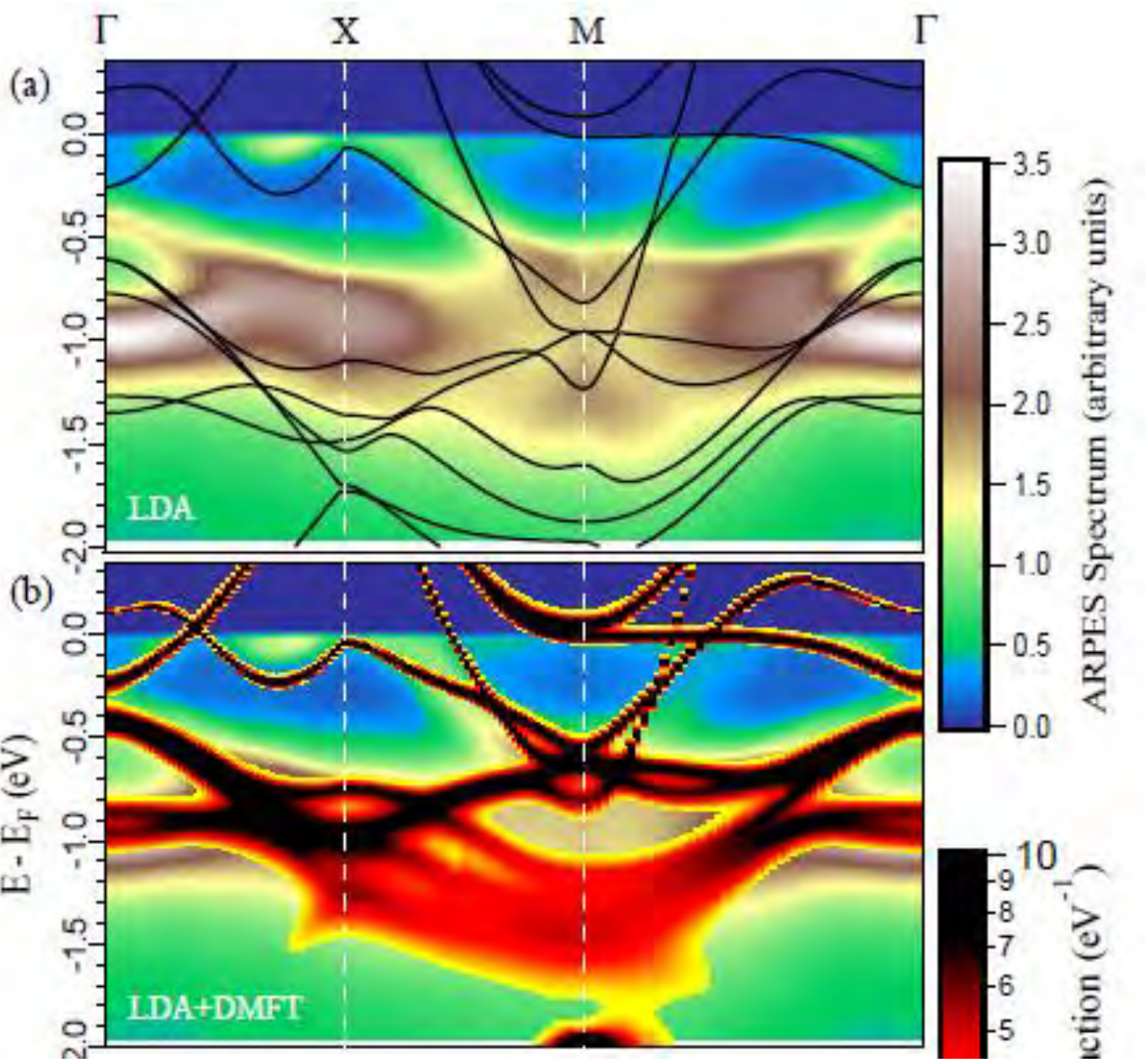


Ce: $4f^1$ configuration, paramagnetic

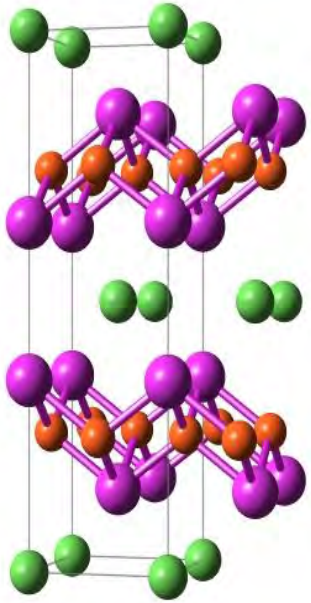
Calculated colour of CeSF:

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

Example 2: BaCo2As2

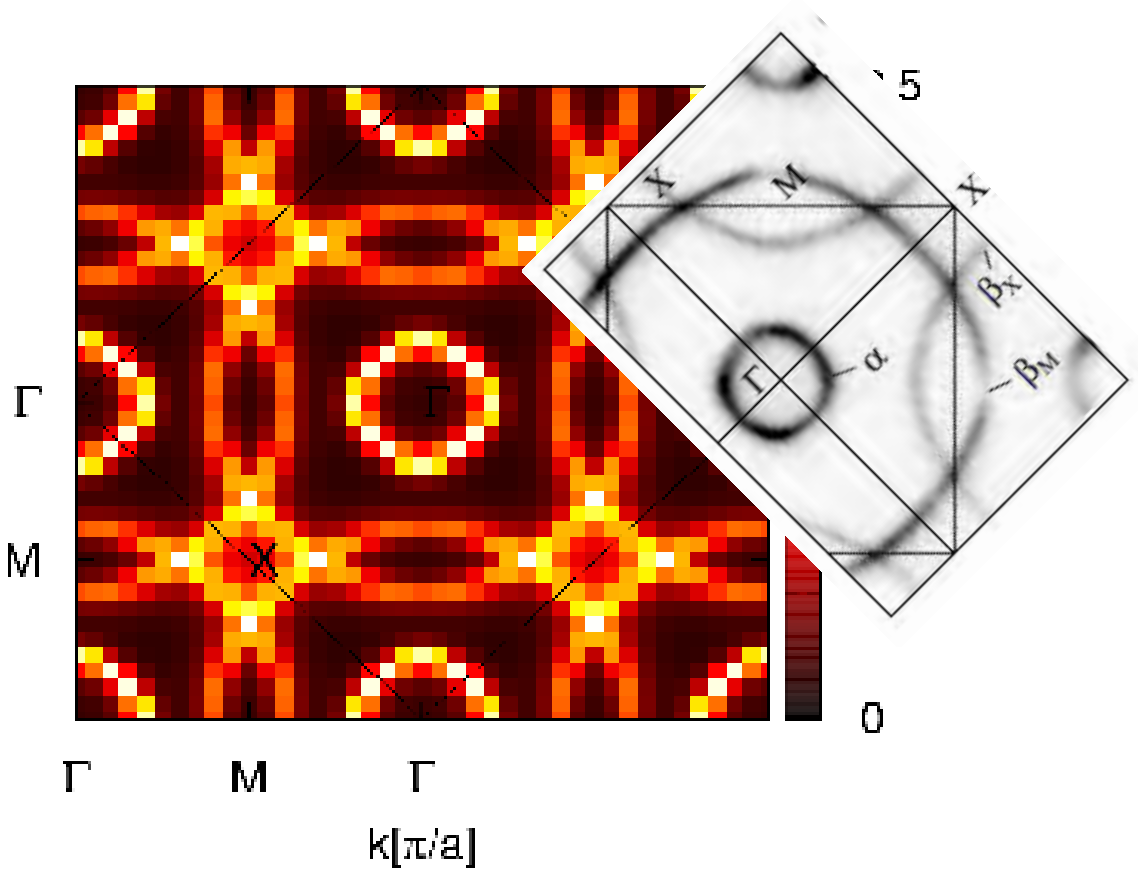


A. Van Roekeghem



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

Example 3:
Fermi surface of Sr2RhO4



Martins et al, Phys. Rev. Lett. (2011) and in preparation
Cf. Liu et al, PRL 2008.

DFT+DMFT … a story of success!

Applications to

- 3d transition metal oxides, sulphides
  [SrVO3, CaVO3, LaTiO3, YTiO3, VO2, V2O3, BaVS3, …]
- Transition metals [Mn, Ni, …]
- f-electron elements and compounds [Ce, CeSF, RE2O3]
- Iron Pnictides [LaFeAsO, FeSe, BaFe2As2, BaCo2As2, Ba2Ti2Fe2As4O …]
- Spin-orbit materials [Sr2IrO4, Sr2RhO4]
- Low-dimensional systems (organics)
- ….

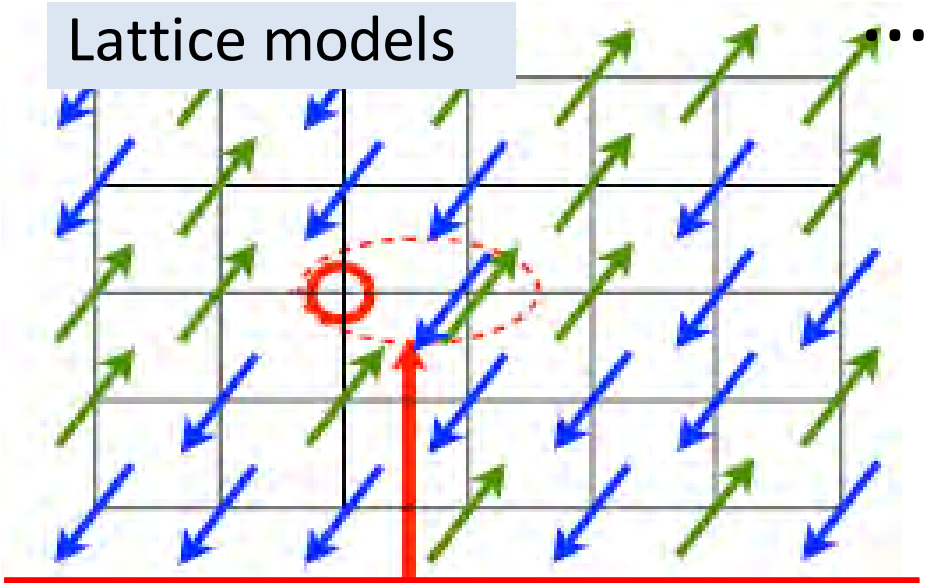
However:

- What's U in the solid?
- Why start from Kohn-Sham Hamiltonian?
- How to avoid double counting of interactions? Of screening?

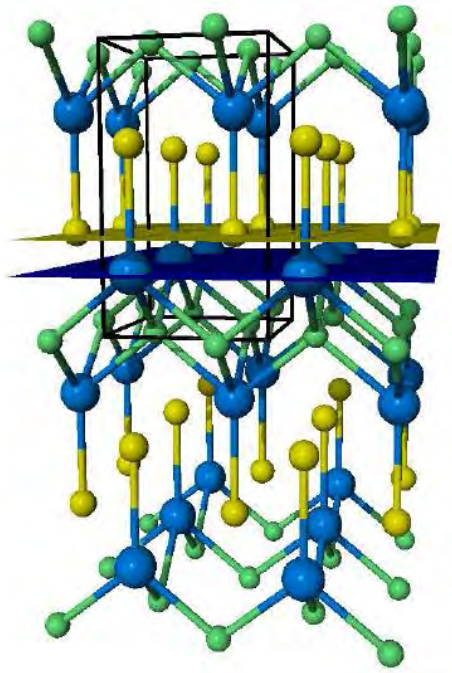
Central question: **How to "downfold" to an effective reduced Hilbert space?**

Wanted: Low-energy effective Hamiltonian

Lattice models



Local Coulomb interaction
= "Hubbard U"



Microscopic link between model and material ?

In practice: "DFT+DMFT" calculates hoppings from density functional theory

One-particle part of Hamiltonian from DFT-LDA

$$H = \sum_{ij\sigma\{m\}} t^{ij}_{m_1 m_2} c^{+}_{i m_1 \sigma} c_{j m_2 \sigma}$$

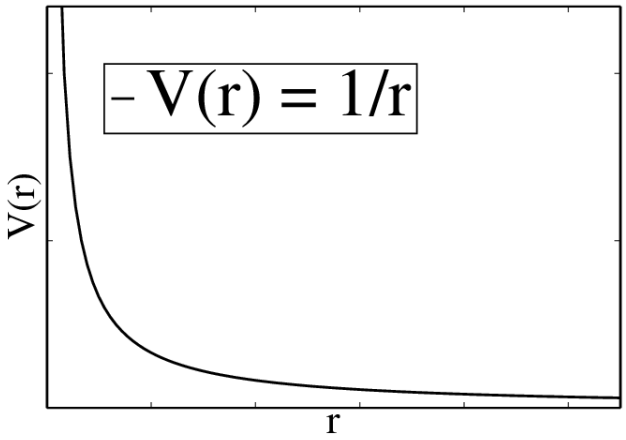
$$+ \frac{1}{2} \sum_{i\{\sigma m\}} U^{i}_{m_1 m_2 m_1' m_2'} c^{+}_{i m_1 \sigma} c^{+}_{i m_2 \sigma'} c_{i m_2' \sigma'} c_{i m_1' \sigma}$$

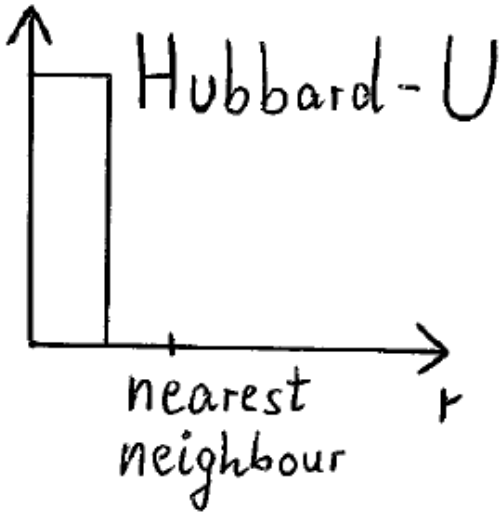
Hubbard interactions (and possibly Hund's coupling) for "correlated shell"

But what about U?

How to bridge between …

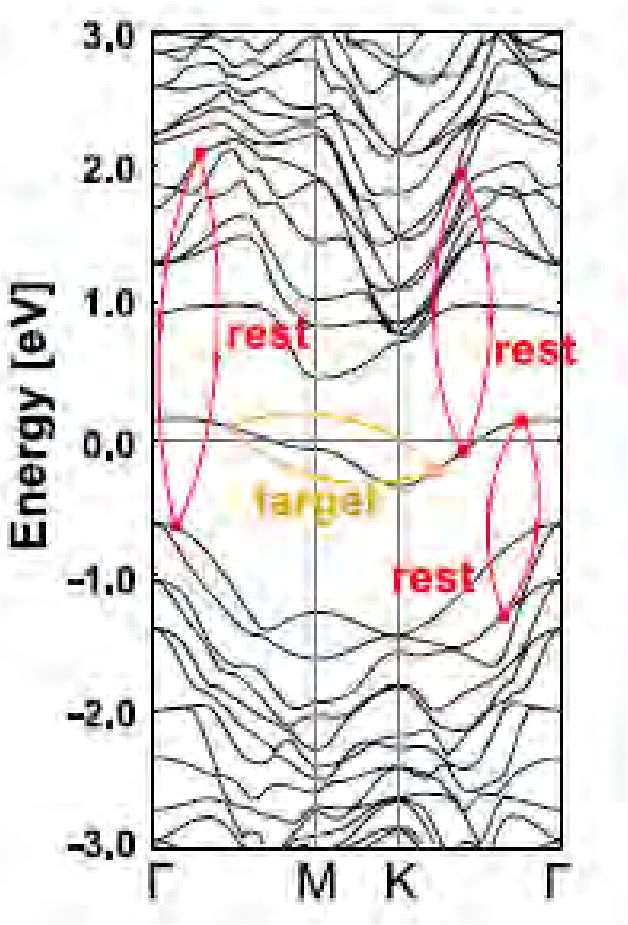
1/r Coulomb interaction & its description as “+U” ?





Description of screening?

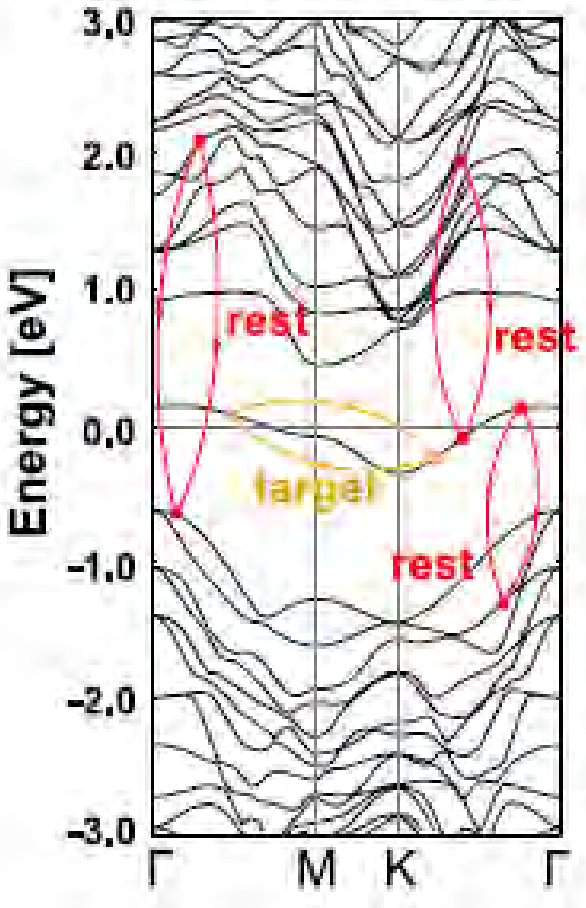
Hubbard U …

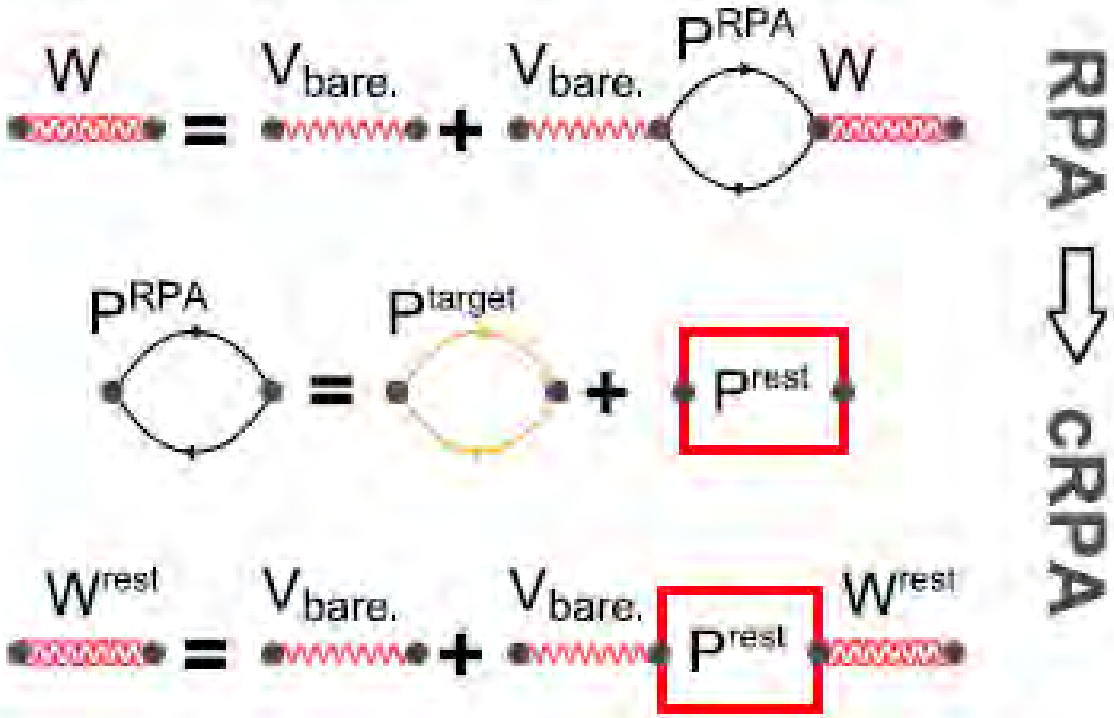


- the bare interaction within a low-energy subspace
- a partially screened interaction in the full space
- How can we calculate partial screening by higher-energy degrees of freedom?

Aryasetiawan, Imada, Georges, Kotliar, Biermann, Lichtenstein, PRB 2004.
[Figure from Hansmann et al., JPCM 2013]

Constrained Random Phase Approximation





$$U^{cRPA}_{lmno} = \langle \varphi_l \varphi_m | W^{rest} | \varphi_n \varphi_o \rangle$$

Aryasetiawan, Imada, Georges, Kotliar, Biermann, Lichtenstein, PRB 2004.

[Figure from Hansmann et al., JPCM 2013]

Hubbard U – take home messages:

- Can be calculated *ab initio* within cRPA
- Matrix element of a *partially screened interaction*

[NB. Interatomic interactions also calculable!]

- Two consequences:

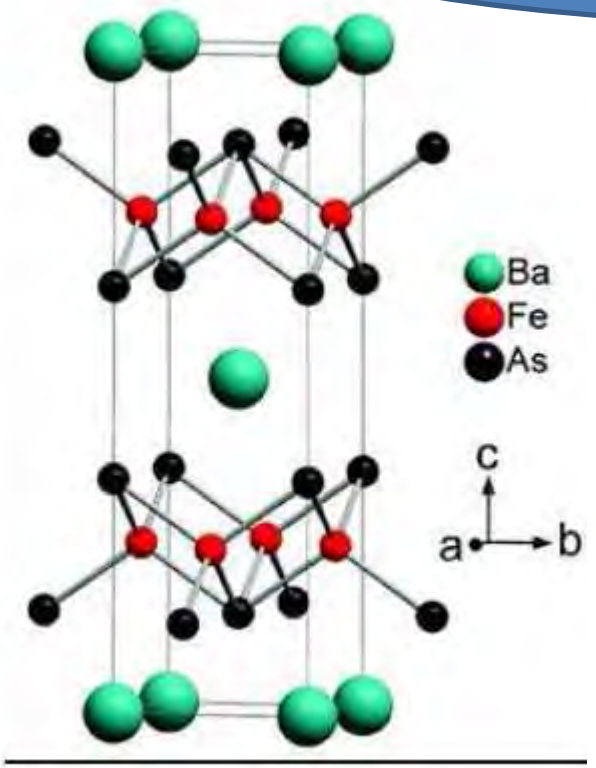
➢ U depends on subspace and orbitals

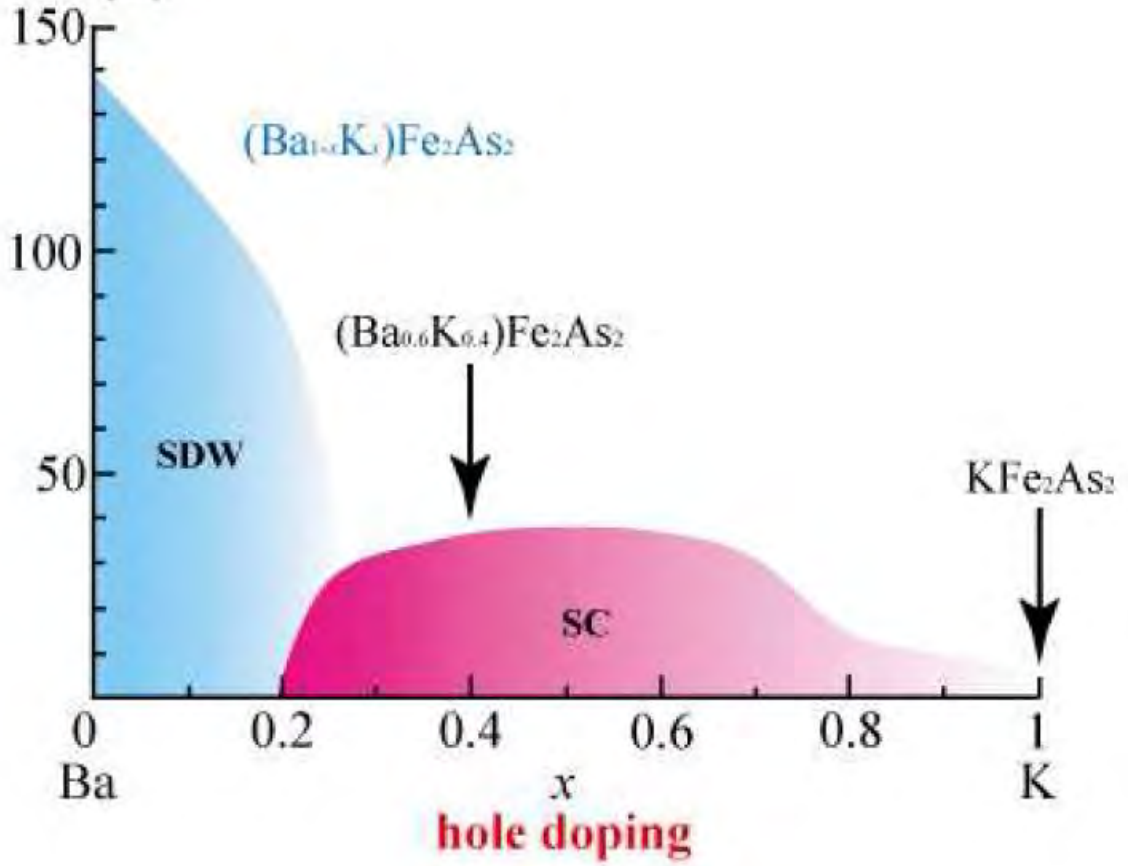
➢ U is *frequency-dependent* ("dynamically screened")

Aryasetiawan, Imada, Georges, Kotliar, Biermann, Lichtenstein, PRB 2004.
[Implementation into Wien2k: Vaugier, Jiang, Biermann, PRB 2012]
See also work by: Imada and Solovyev, Miyake, Nakamura …

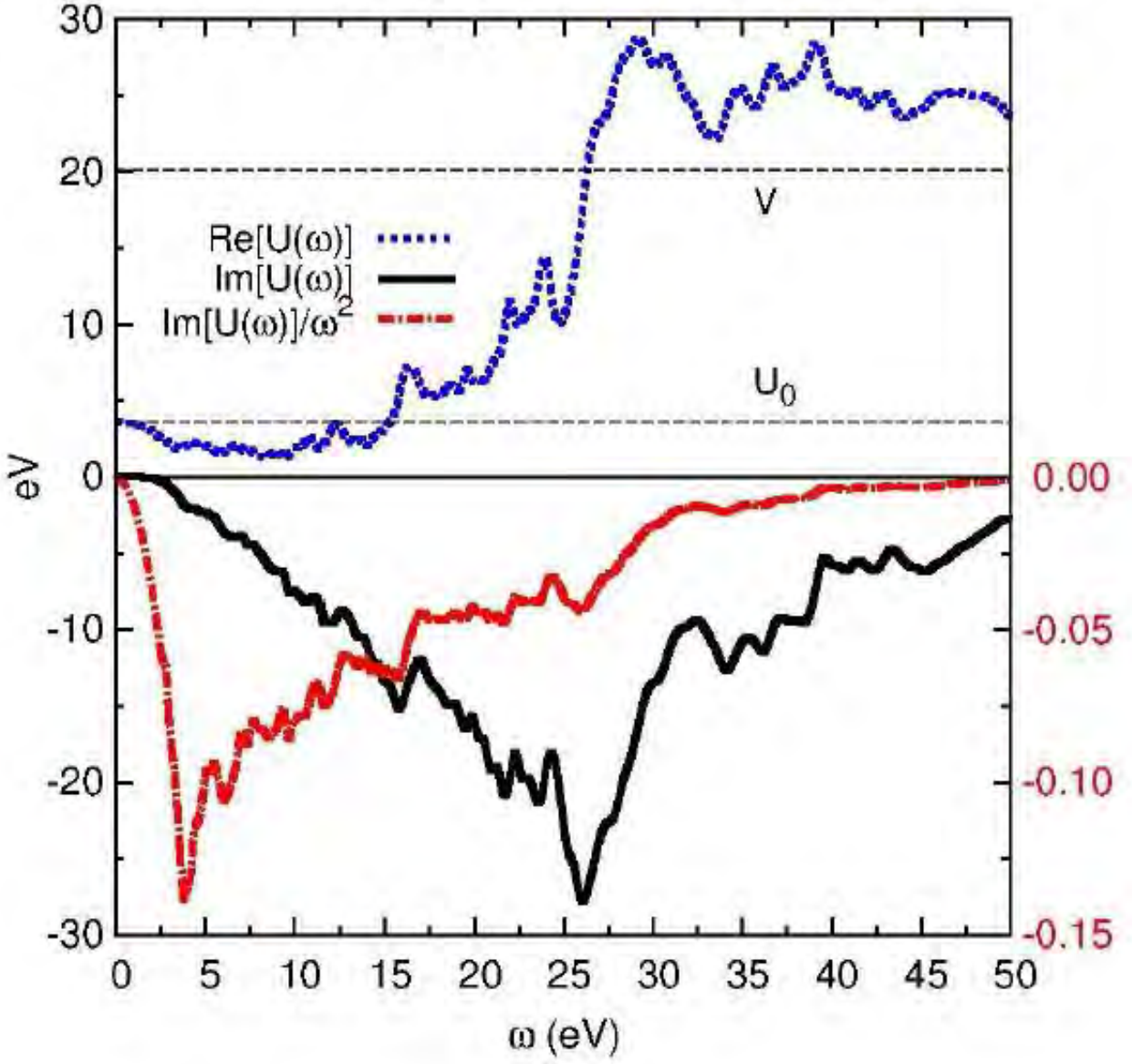
BaFe2As2

Our focus …



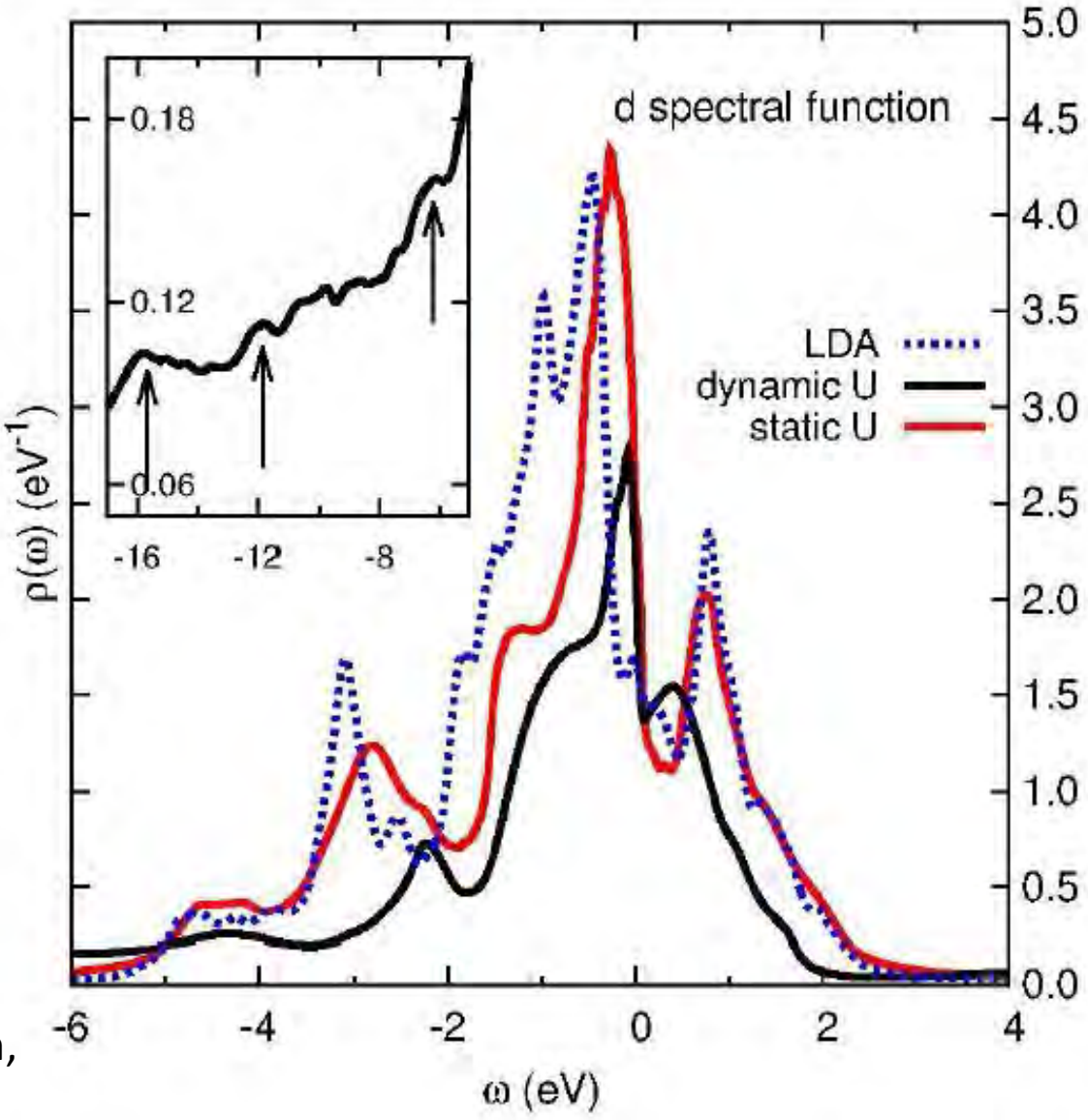


U(ω) for BaFe2As2



Werner, Casula, Miyake, Aryasetiawan, Millis, SB, Nature Phys. 2012

BaFe2As2



Werner, Casula, Miyake, Aryasetiawan, Millis, SB, Nature Physics 2012

See also: "electronic polaron effect" Casula, Werner, Miyake, Aryasetiawan, Millis, SB, PRL 2012

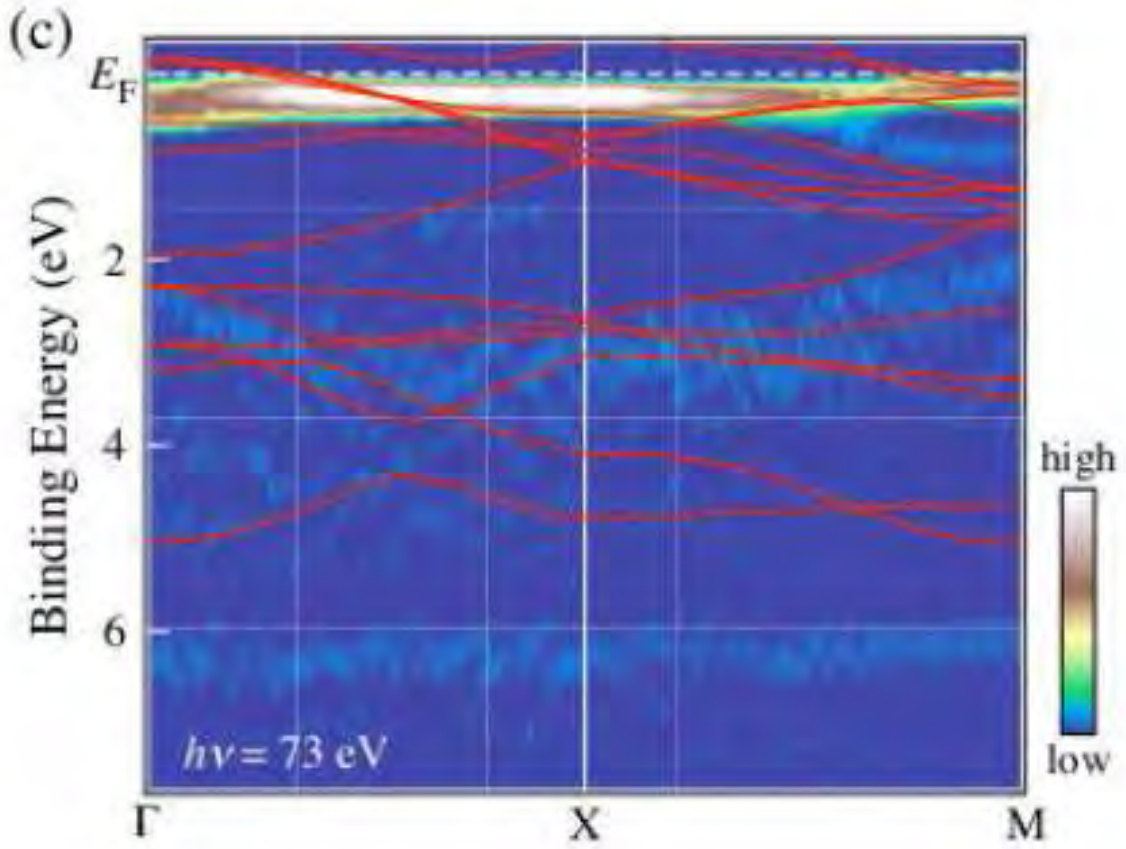
Origin of spectral weight loss?

- Problem with dynamical interactions ⇔ static problem with ***screening bosons***
- Diagonalisation of fermion-boson problem leads to ***"electronic polarons"***
- Spectral function contains ***plasmon replicae***
- **Weight** of main peak reduced to

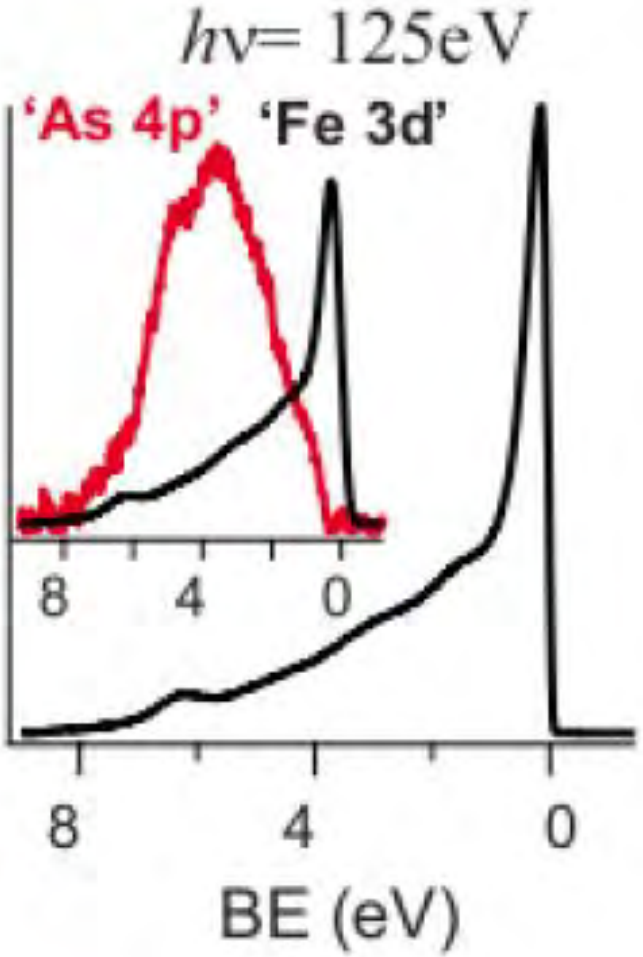
$$Z_B = e^{\frac{1}{\pi}\int_0^\infty d\omega \frac{Im\, U(\omega)}{\omega^2}}$$

[Casula, Werner, Miyake, Aryasetiawan,Millis, SB, PRL 2012]

BaFe2As2 Photoemission



Ding et al



Yi et al.

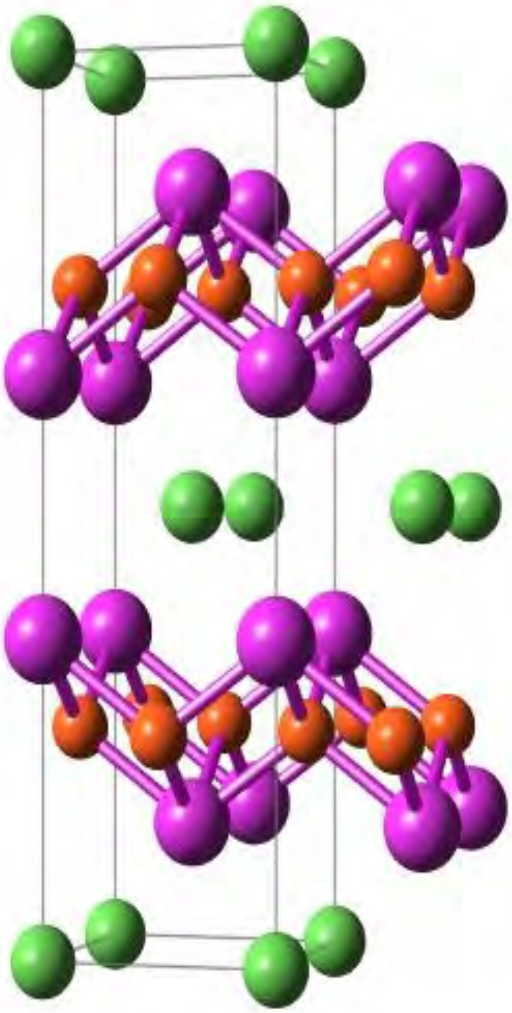
Side remark

- DMFT with dynamical U(w) closely related to cumulant approach: approximate DMFT solver for dynamical impurity problem (Casula et al., PRB 2012) can be understood as a generalized cumulant ansatz
- See also: “slave rotor” method for dynamical impurity problems: Krivenko & SB, PRB 2015
- Cf. description of plasmons with GW+cumulant approaches (cf. work by L. Hedin, F. Aryasetiawan, S. Louie, L. Reining, J. Rehr …)

Effects of dynamical interactions:

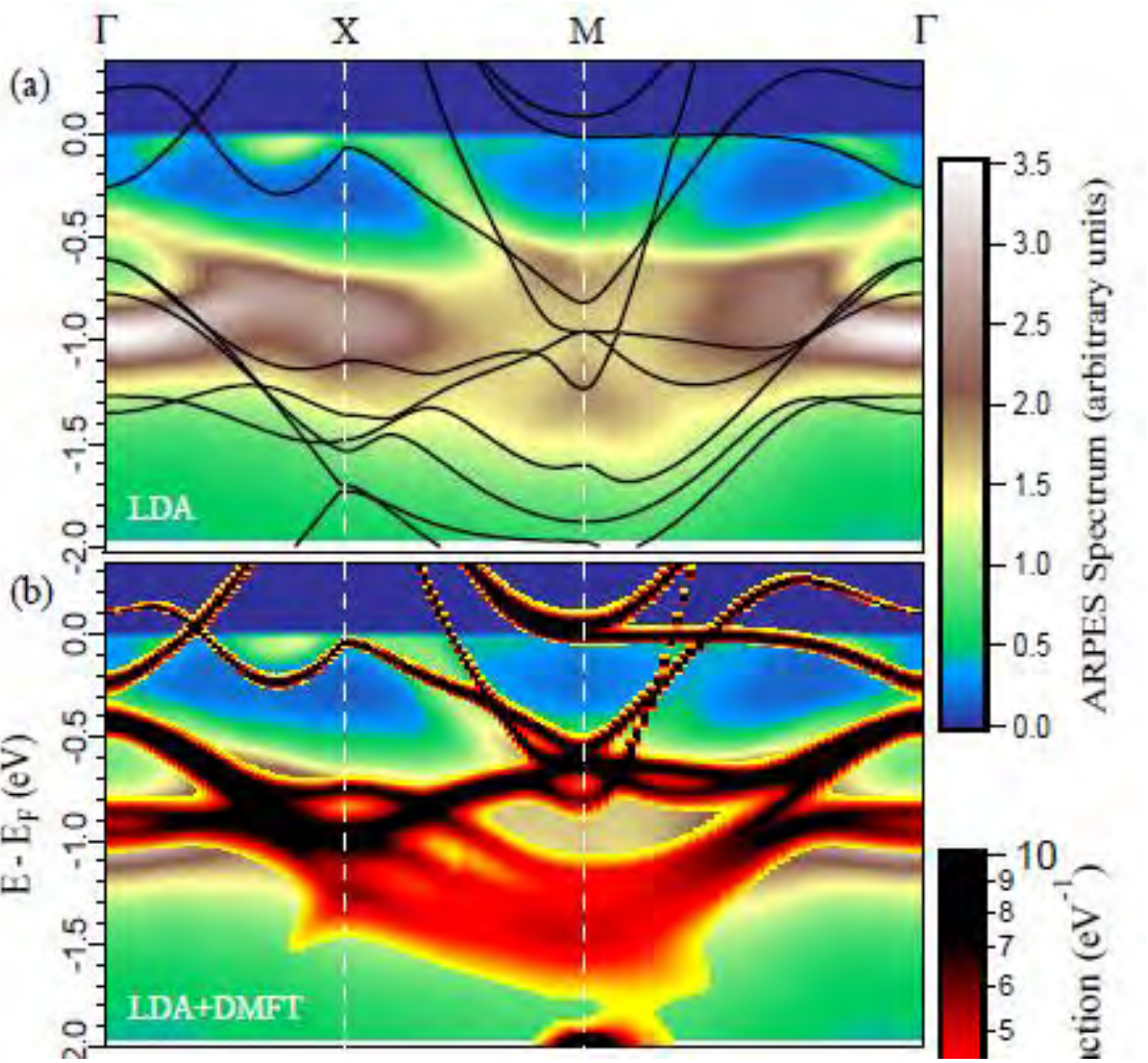
- Replicae and spectral weight transfers 
- Additional renormalisations 
  - (with respect to what starting electronic structure?)

Cobalt Pnictide: BaCo2As2



Fe-d7 configuration
=> weakly correlated

Cobalt Pnictide: BaCo2As2

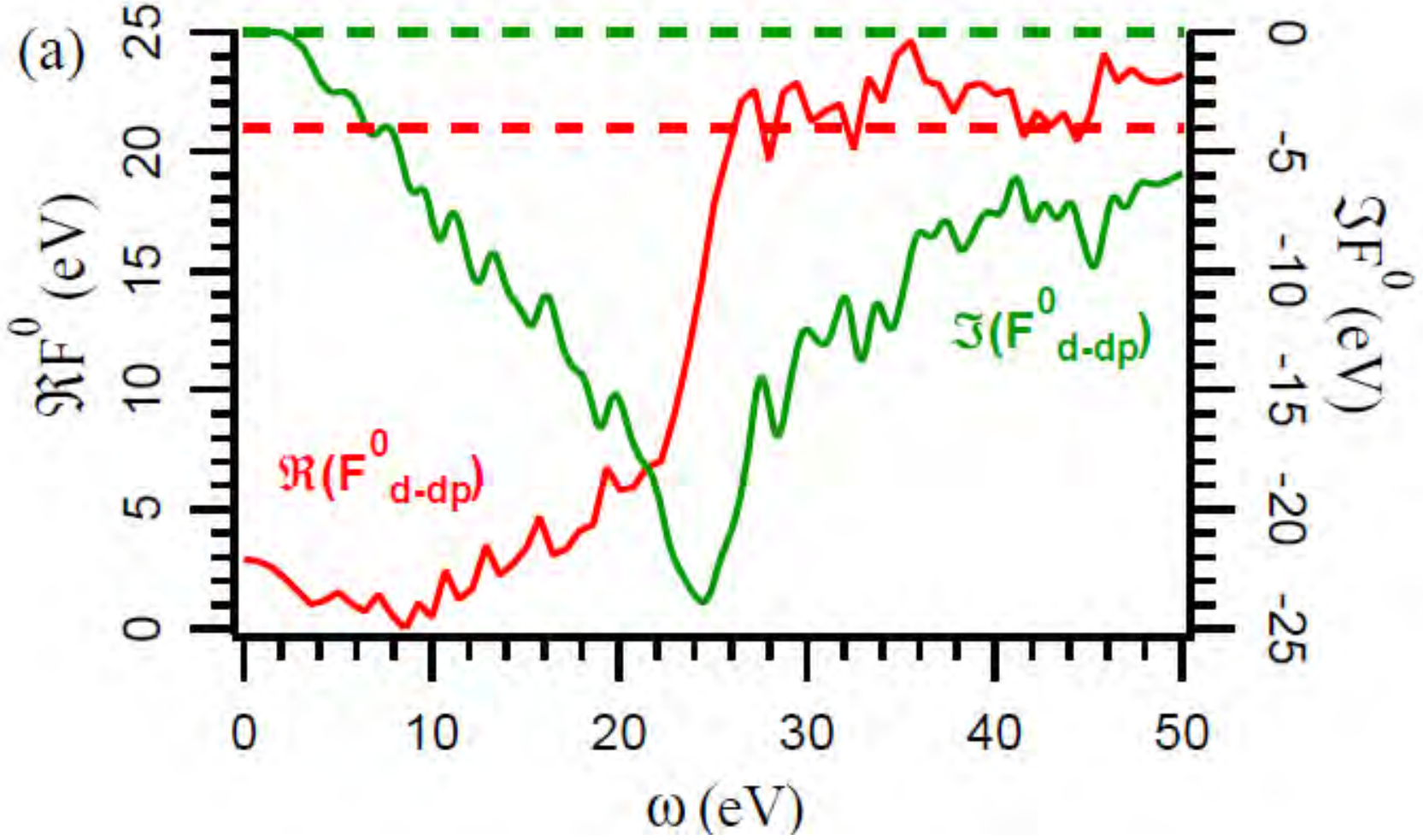


A. Van Roekeghem
IOP-CAS & Ecole Polytechnique

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

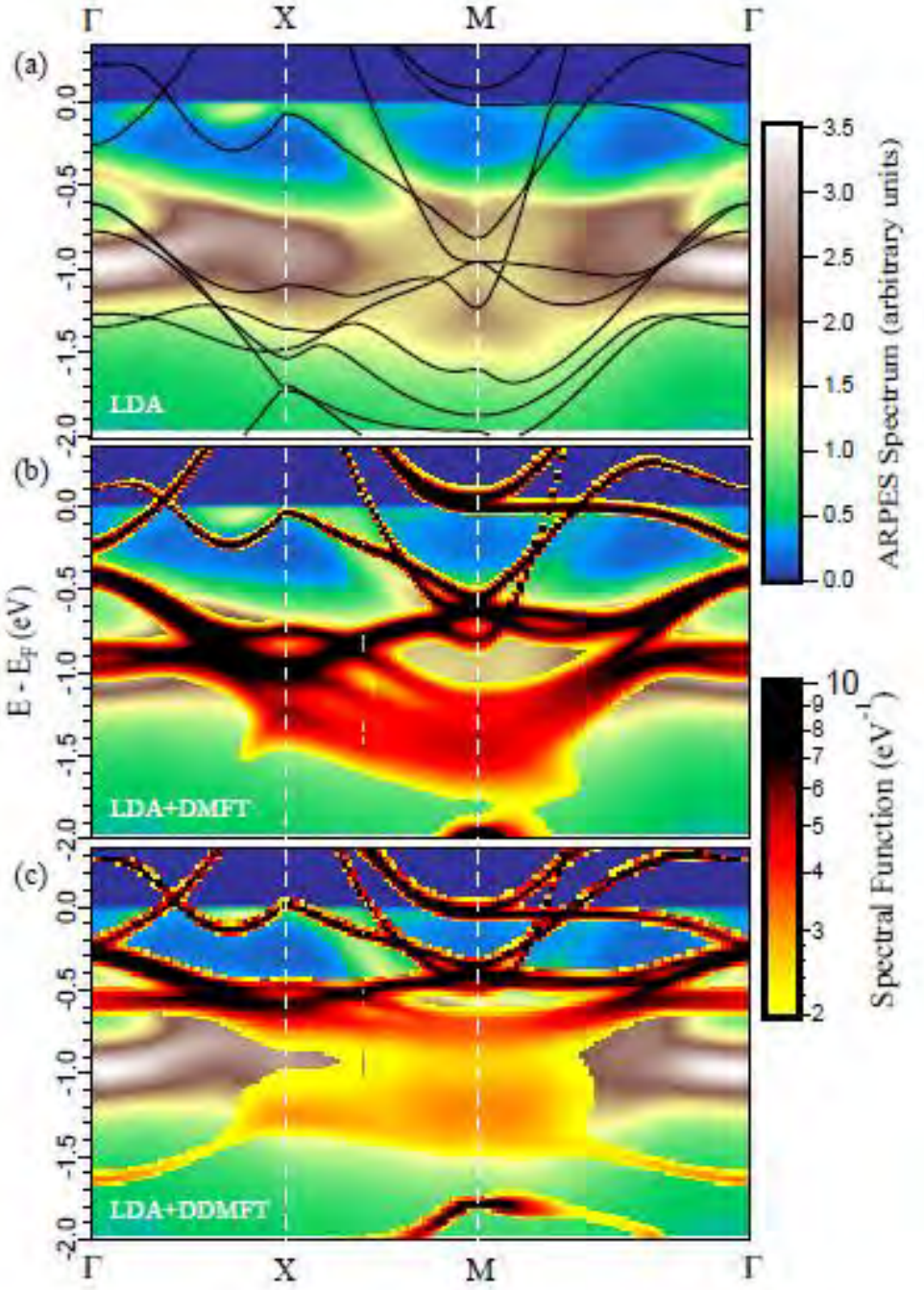
See also:
PES by Dhaka et al.

Dynamical interaction for BaCo2As2 (from cRPA)



With dynamical effects ….

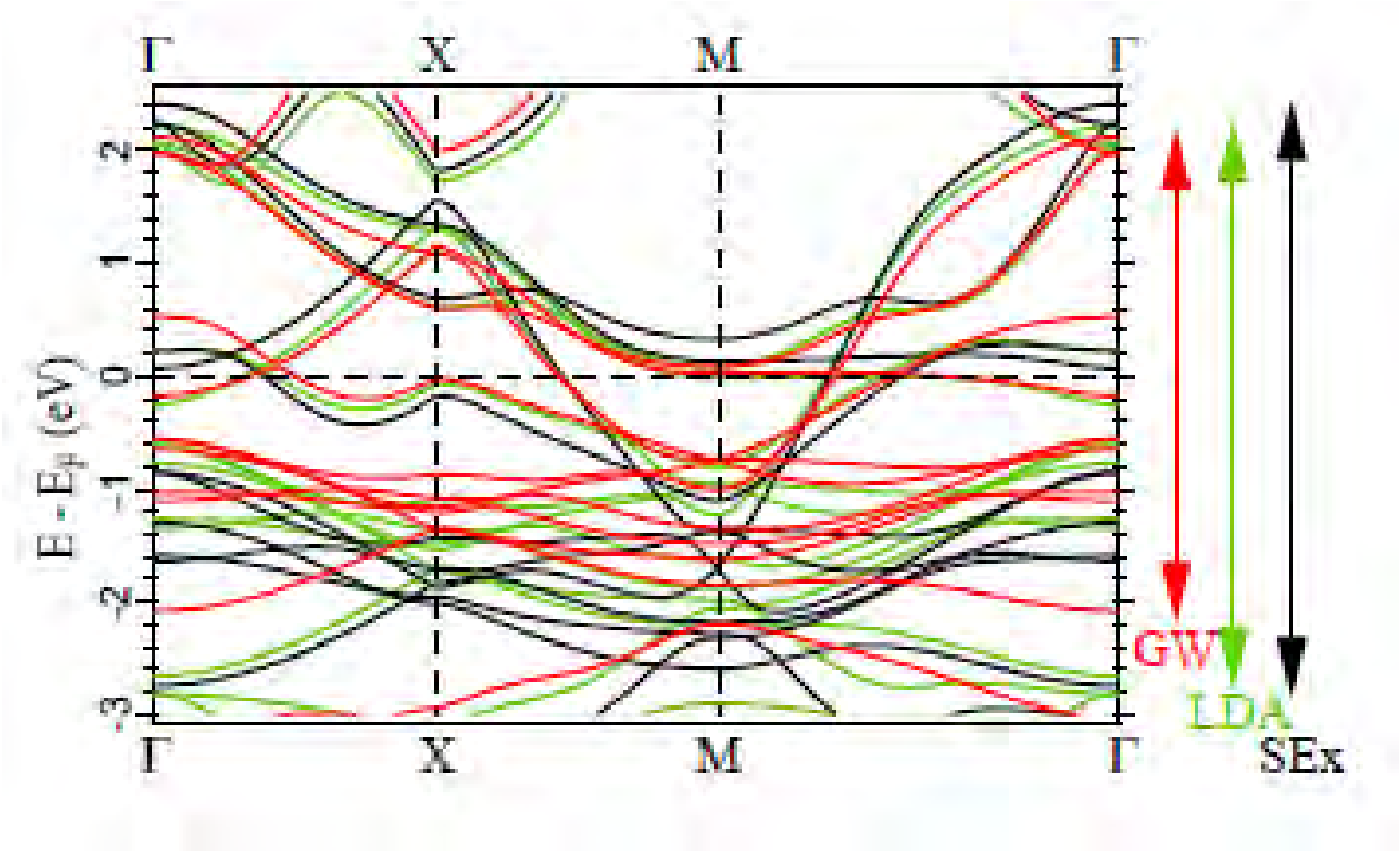
A. van Roekeghem et al., PRL 2014



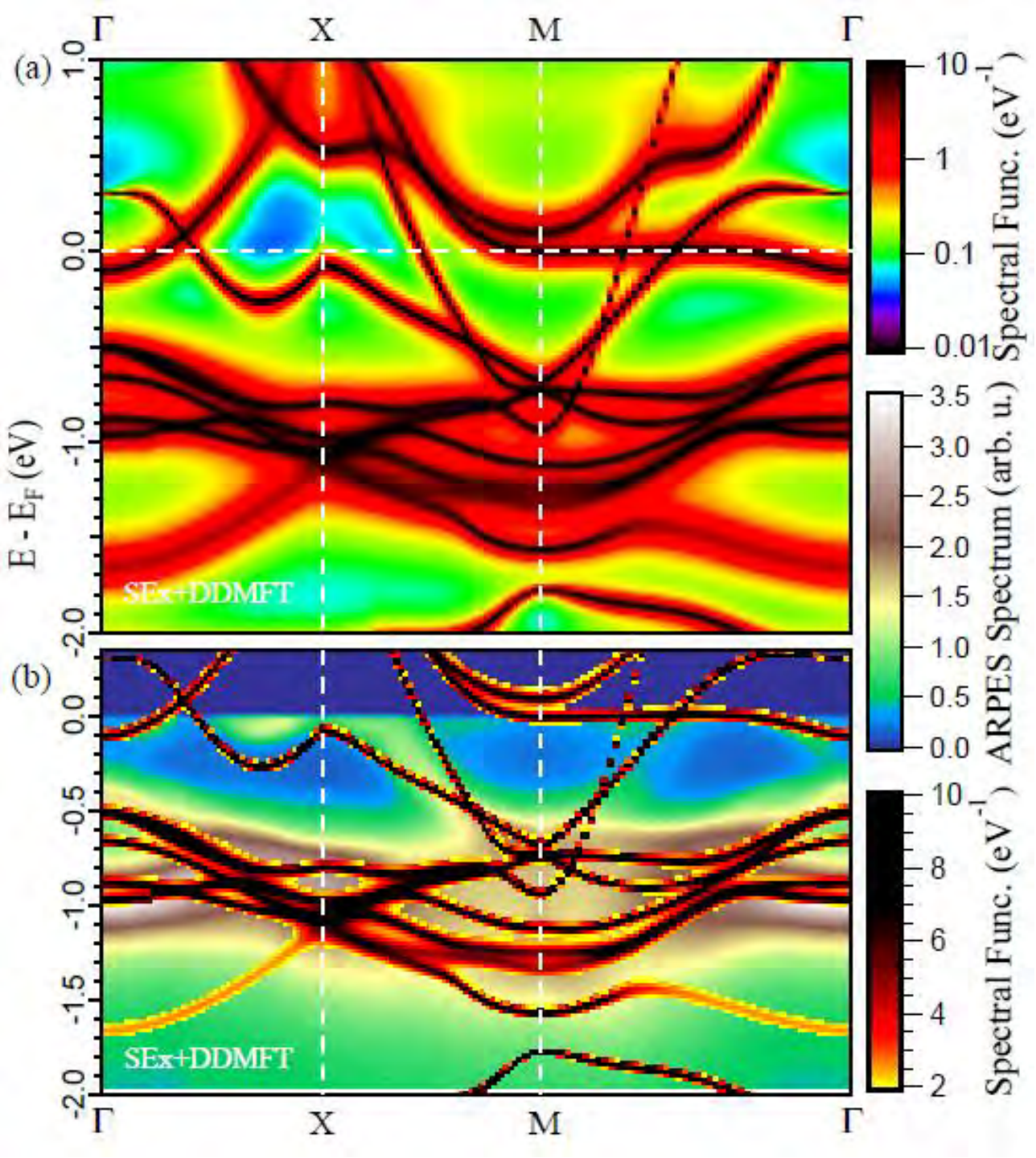
Have we worked too much ….?

No! Not enough!

Nonlocal corrections: Screened exchange vs LDA



A. van Roekeghem et al., Phys. Rev. Lett. 2014



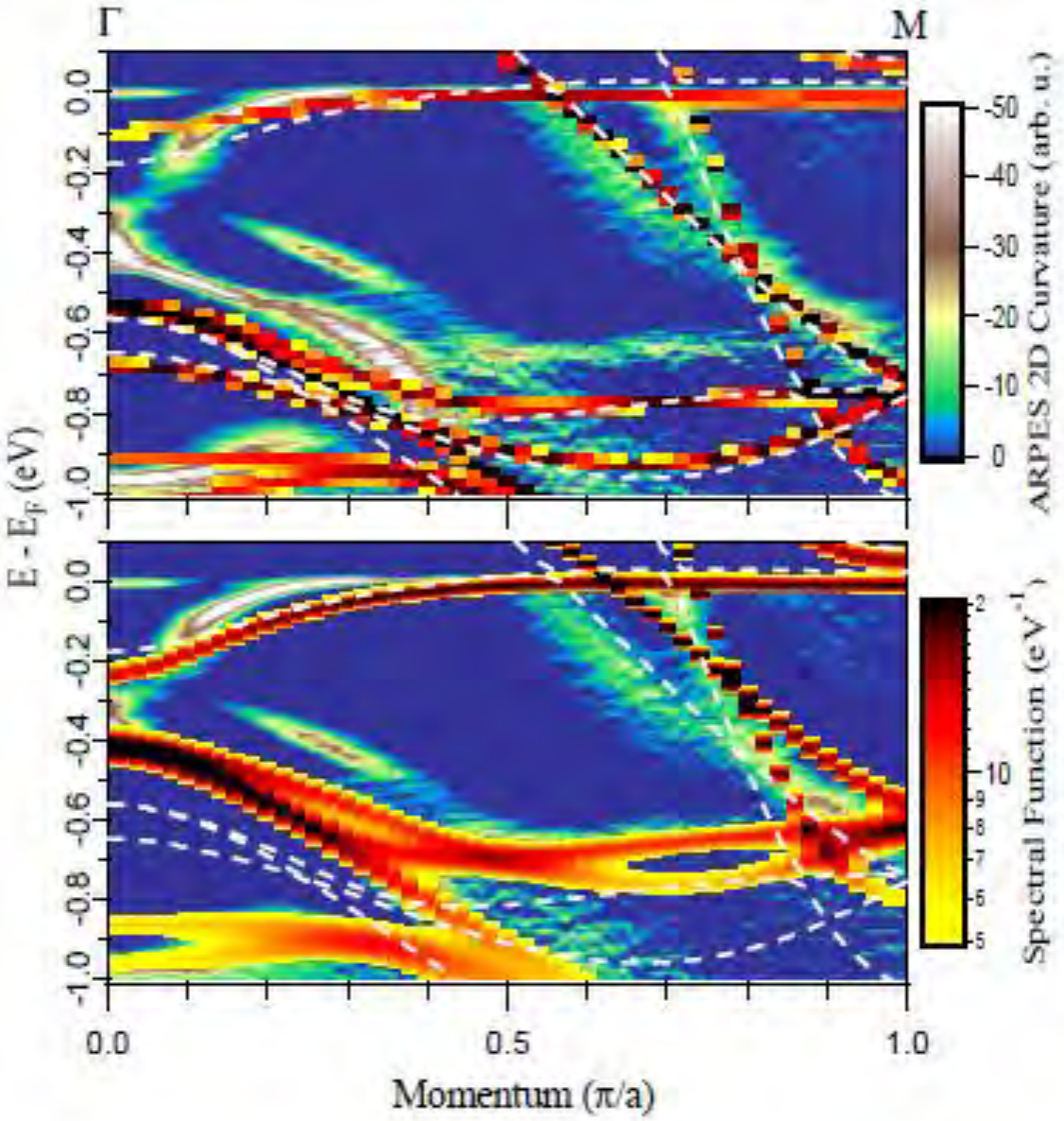
Screened Exchange + DMFT

A. van Roekeghem et al., Phys. Rev. Lett. 2014

"Screened exchange+DMFT"

vs.

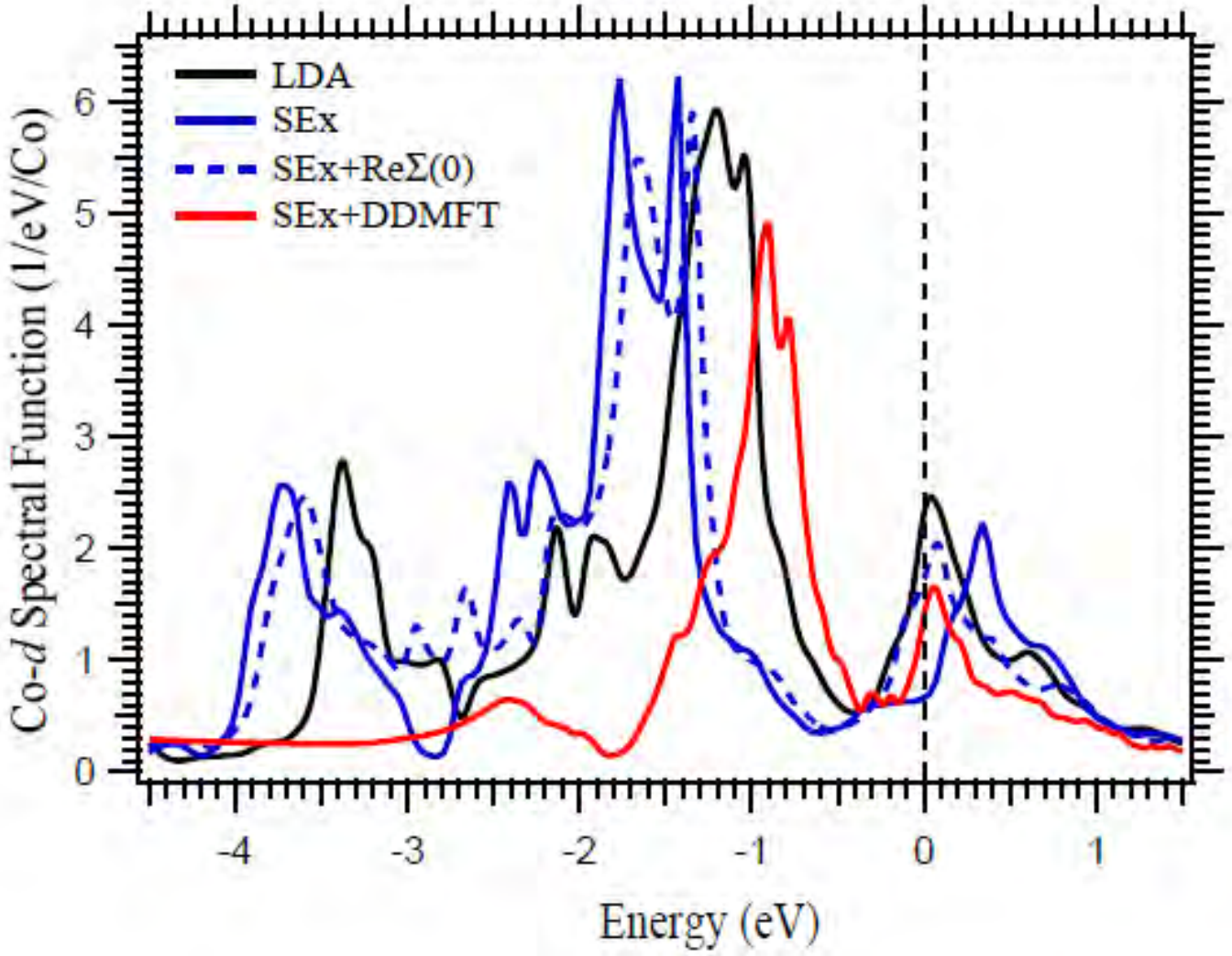
DFT+DMFT



Description of Fermi surface corrected by Screened Exchange+DMFT !

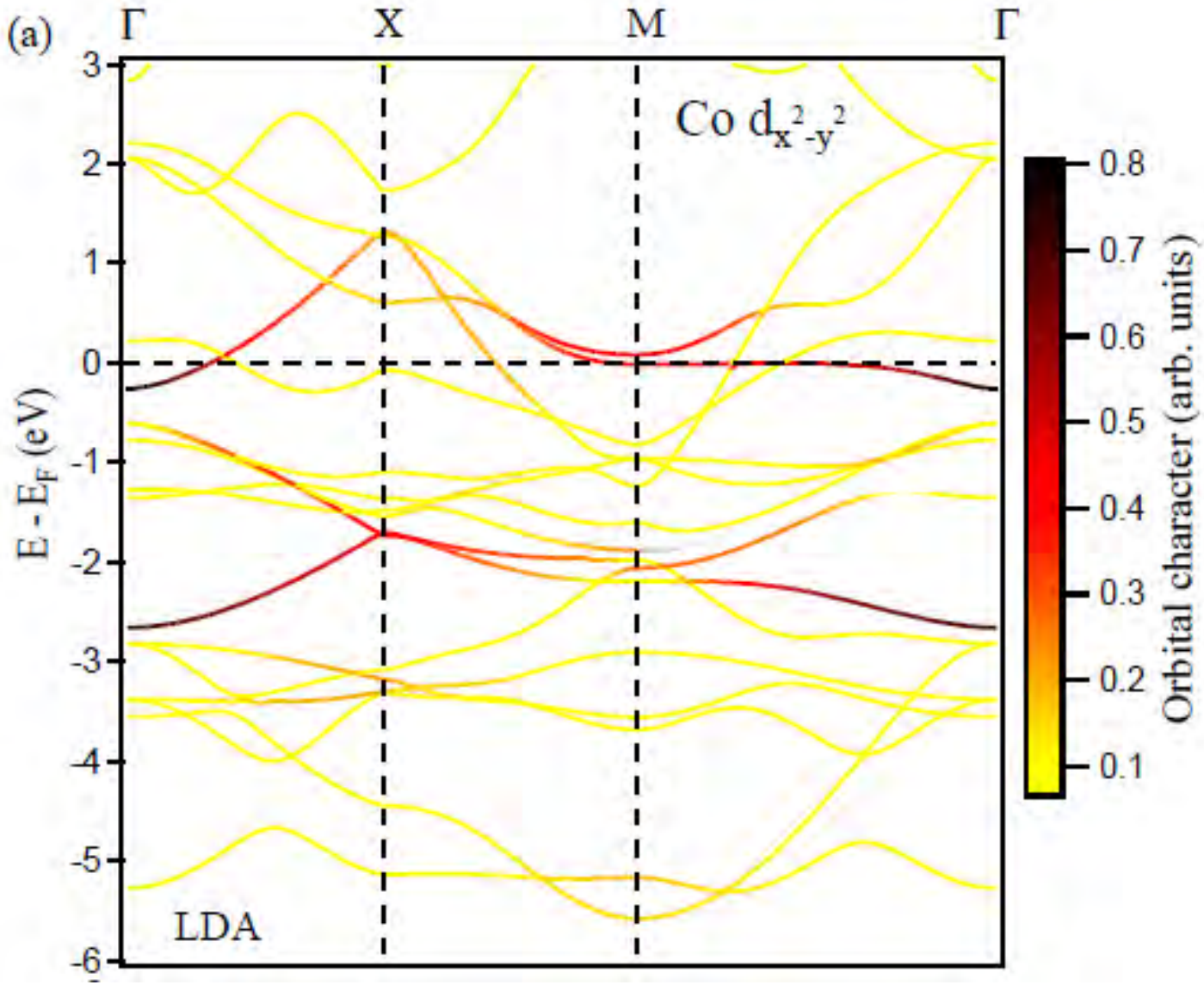
A. van Roekeghem et al., Phys. Rev. Lett. 2014

Momentum-integrated Co-3d spectral function



Solves yet another puzzle:
LDA DOS would suggest Stoner ferromagnetism (Sefat et al., PRB 2009), however: in nature no magnetic order.
[Note: CaCo2As2 is ferromagnetic]

Dx2-y2 – a very sensitive proxy …



Screened Exchange Dynamical Mean Field Theory …

- … a simplified version of GW+DMFT

Biermann, Aryasetiawan, Georges, PRL 2003

Sun and Kotliar, PRL 2004

(see also related "GD+SOPT+DMFT" scheme by Sun & Kotliar, PRL 2002)

Application to real materials:

SrVO3: Tomczak et al. , EPL 2012 and PRB 2014, for GW+DMFT

Fully self-consistent implementation for Sn/Si(111) : Hansmann et al., PRL 2013]

“GW+DMFT”

- A combination of Hedin’s GW approximation and DMFT

The Ψ[G,W] functional

The free energy of a solid can be expressed 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, Chitra et al. 2000]

Γ[G,W] = Hartree part + Ψ[G,W]

The GW+DMFT functional

- Γ[G,W] = Hartree part + Ψ[G,W]

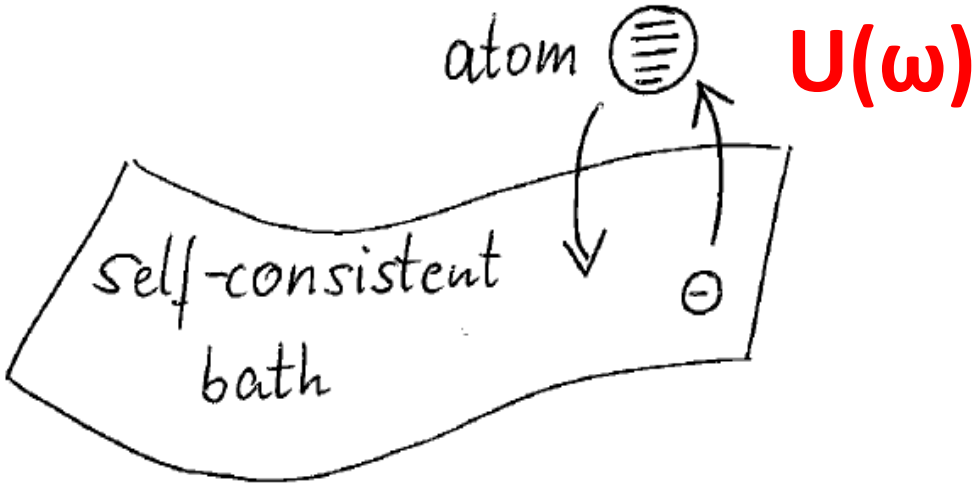
- $$\Psi \approx \Psi^{\mathrm{EDMFT}}[G_{ii}, W_{ii}] + \Psi^{GW}_{\mathrm{nonloc}}[G_{ij}, W_{ij}],$$
  $$\text{where } \Psi^{GW}_{\mathrm{nonloc}} = \Psi^{GW} - \Psi^{GW}_{\mathrm{loc}}.$$

Biermann, Aryasetiawan, Georges, PRL 2003, and arxiv 2004
Sun & Kotliar, PRL 2004
Ayral, Werner, Biermann, PRL 2012, PRB 2013
Hansmann, Ayral, Vaugier, Werner, Biermann, PRL 2013

Review: Biermann, J. Phys. Cond. Matt. (2014)

EDMFT

Calculate Gloc and Wloc from a dynamical impurity model (that is, an impurity model with bath and dynamical Hubbard interactions).



Determine bath (the dynamical mean field) and dynamical Hubbard U(ω) self-consistently

Smith and Si, 1996 and 2000. Chitra & Kotliar 2000

GW+DMFT Eqs.

Impurity model :

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

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

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

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

Update $\qquad\qquad$ Combine :

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

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

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

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

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

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

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

Motivation:

- Separation, at the GW level, of self-energy

into local dynamical and nonlocal static part:

$$\Sigma = GW = \Sigma_{loc}(\omega) + \Sigma_{nonlocal}(k)$$

(empirically found for pnictides in Tomczak, Schilfgaarde, Kotliar, PRL 2012;
for SrVO3, see Miyake et al, PRB 2012, Tomczak et al., PRB 2014)

=> GW+DMFT equivalent to DMFT on top of effective single-particle Hamiltonian $H=H_0+\Sigma_{nonlocal}(k)$

- Now: identify nonlocal part with screened exchange GW(0)

Screened Exchange Dynamical Mean Field Theory …

- … a simplified version of GW+DMFT

[Biermann, Aryasetiawan, Georges, PRL 2003]

[See also Tomczak et al. , EPL 2012 and PRB 2014, for GW+DMFT for SrVO3, and the recent self-consistent implementation for Sn/Si(111) : Hansmann et al., PRL 2013]

- … a dynamical non-perturbative generalization of Hedin's Coulomb-Hole-Screened-Exchange ("COHSEX") scheme

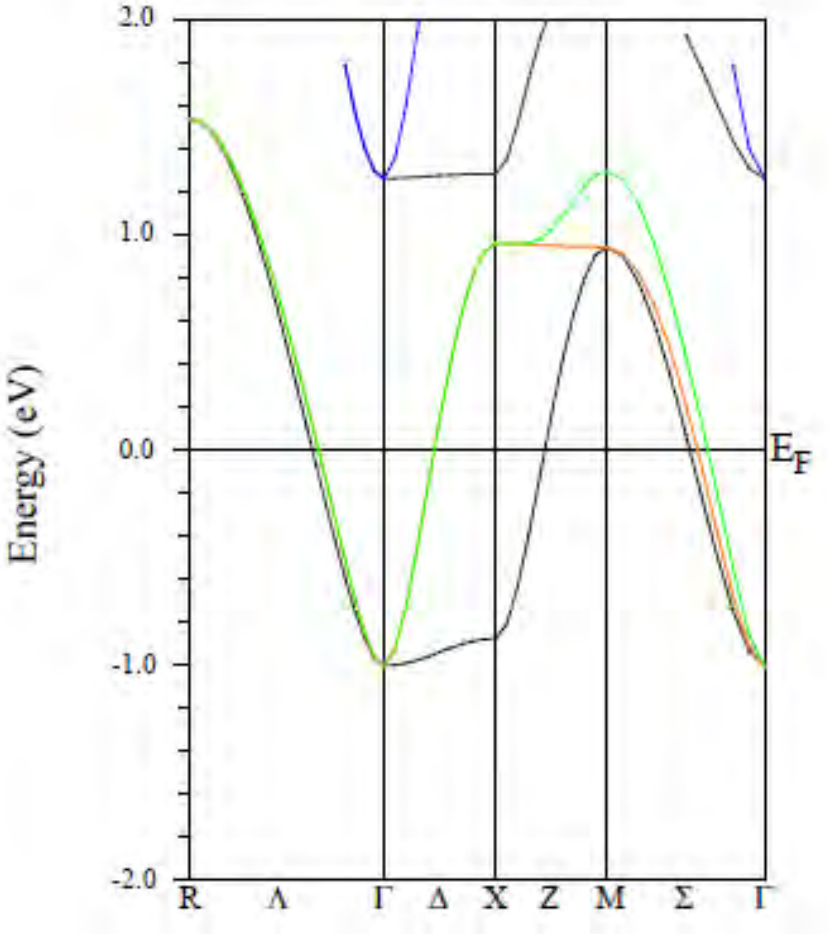
[Hedin, PRB (1965)]

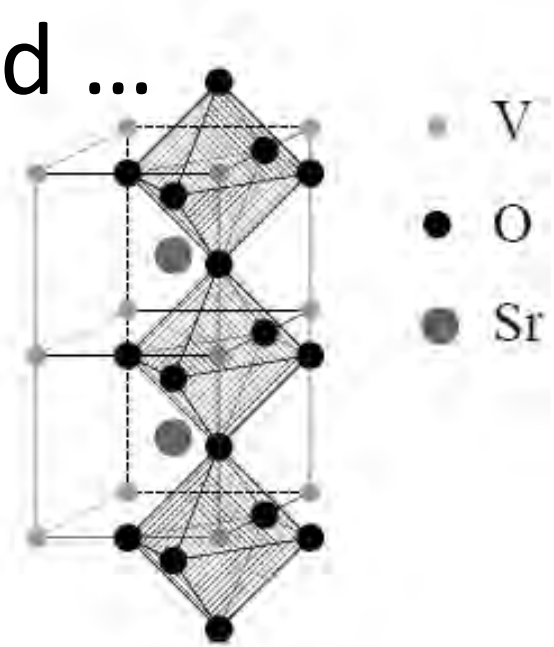
- … a combination of generalized Kohn-Sham schemes [Goerling and others] with "dynamical DMFT"(*)

(*) "Dynamical DMFT" = DMFT with frequency-dependent interactions

A simpler example: SrVO3

SrVO3: a drosophila compound …





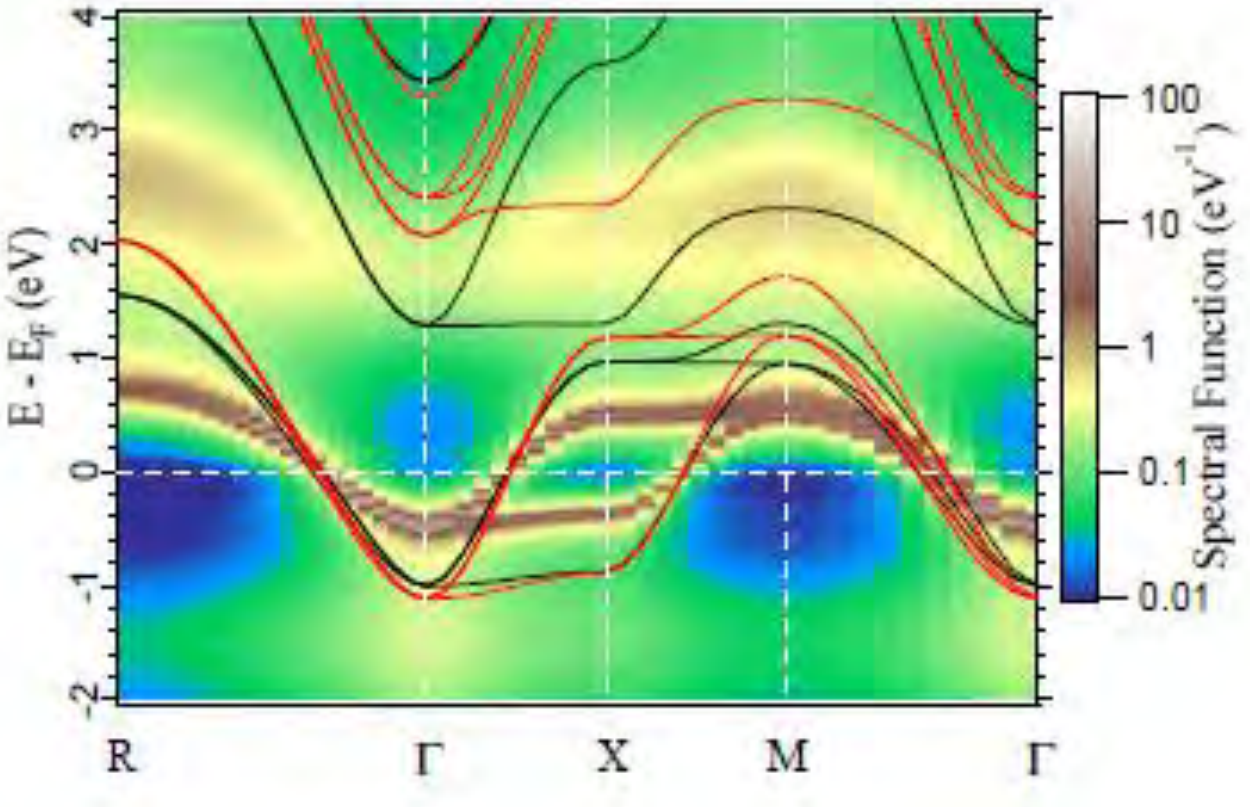
- Test compound for DFT+DMFT implementations (see e.g. Pavarini et al., PRL 2004 and various others …)
- GW+DMFT: Tomczak et al., EPL 2012, PRB 2014
- LDA+U(w)+DMFT: Casula et al., PRB 2012
- Various GW- or DMFT-inspired schemes: Gatti&Guzzo, PRB 2013, Sakuma PRB 2013, Taranto PRB 2013.

A simpler example: SrVO3

Hubbard band =>

QP bands =>

Hubbard band =>



Black: LDA

Red: Screened exchange

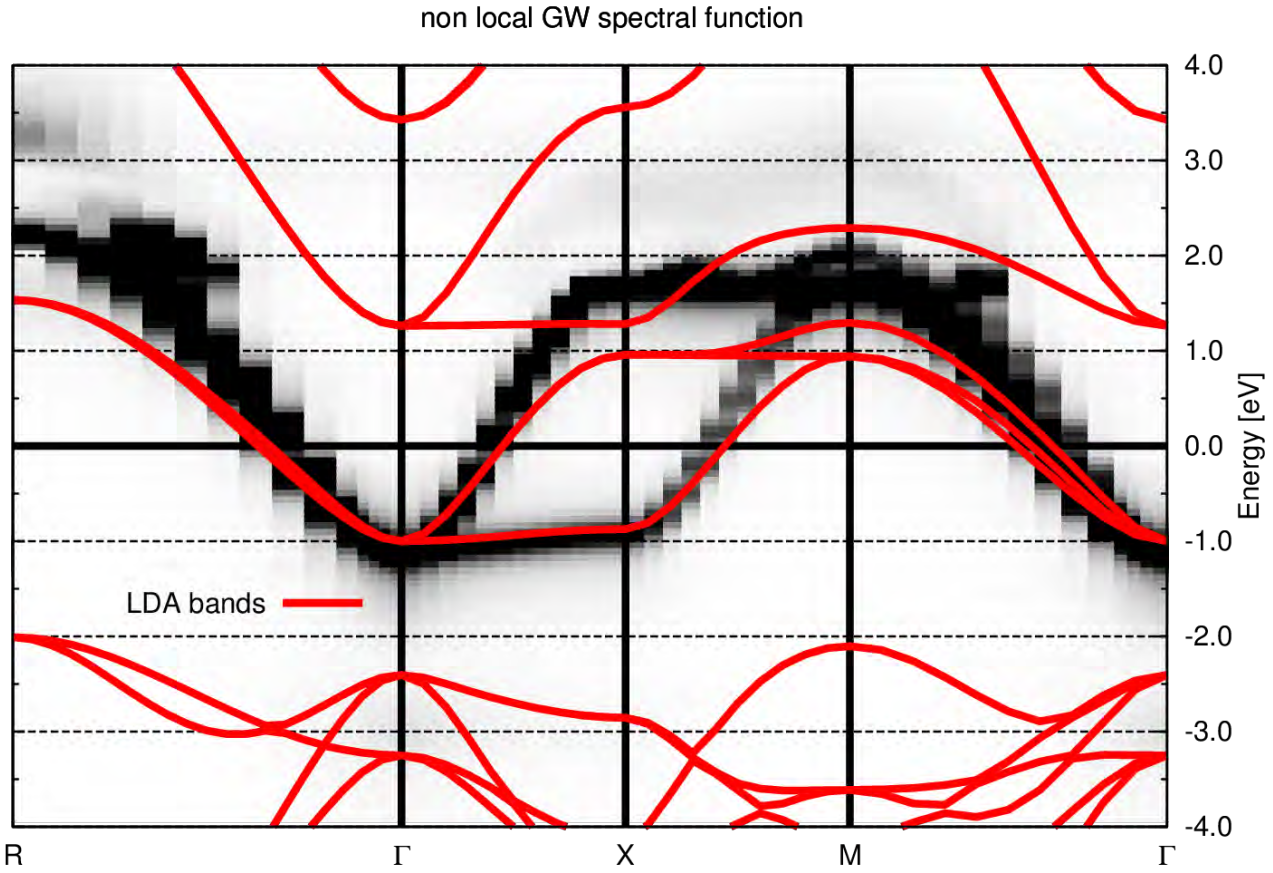
Color: Screened exchange dynamical mean field theory

Excellent agreement with ARPES!

See work by Fujimori's group

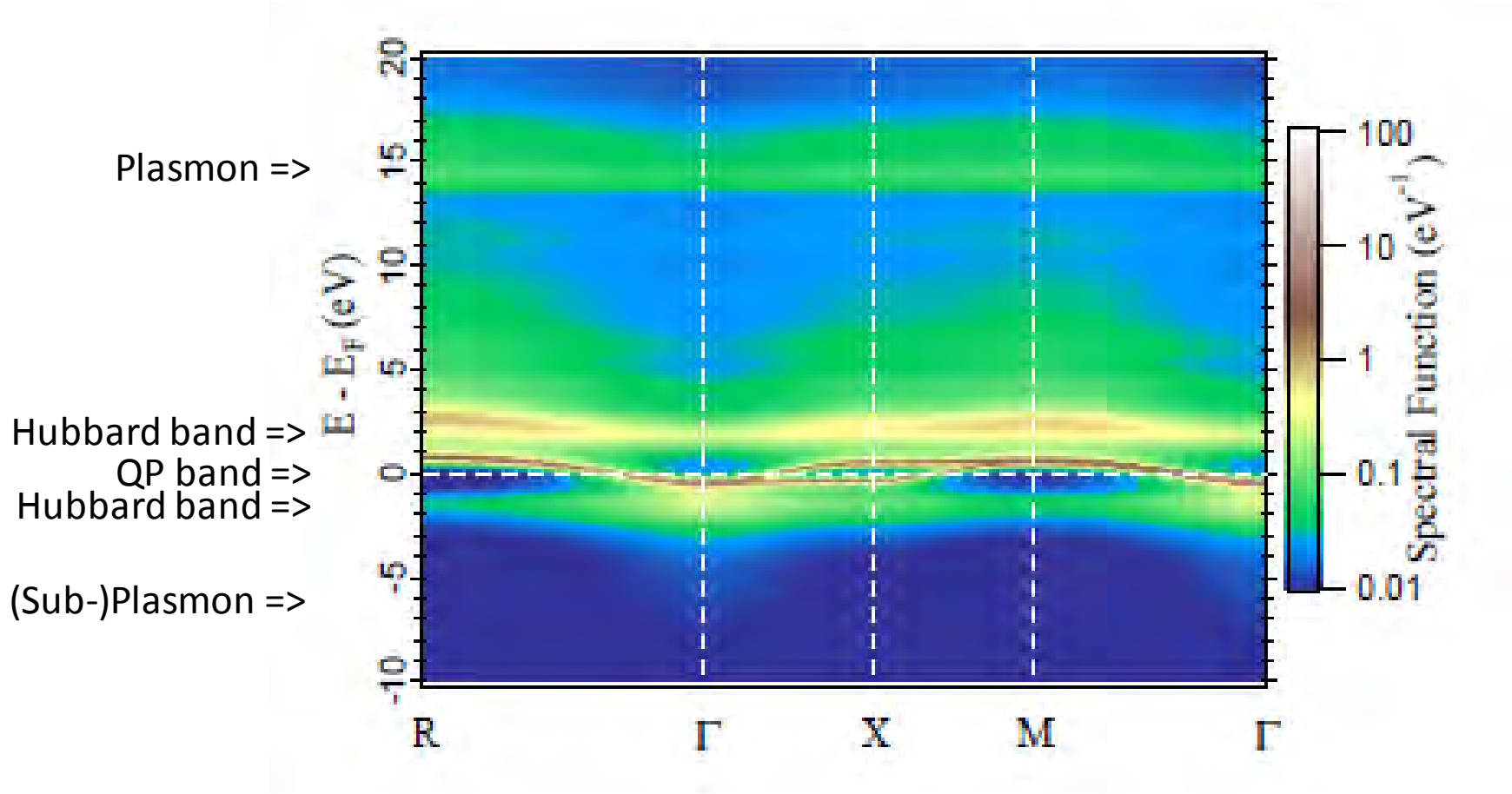
A. Van Roekeghem and S. Biermann, Europhysics Letters (2014)

Spectral function from “non-local GW”



From: Tomczak, Casula, Miyake, Biermann, PRB 2014

A simpler example: SrVO3

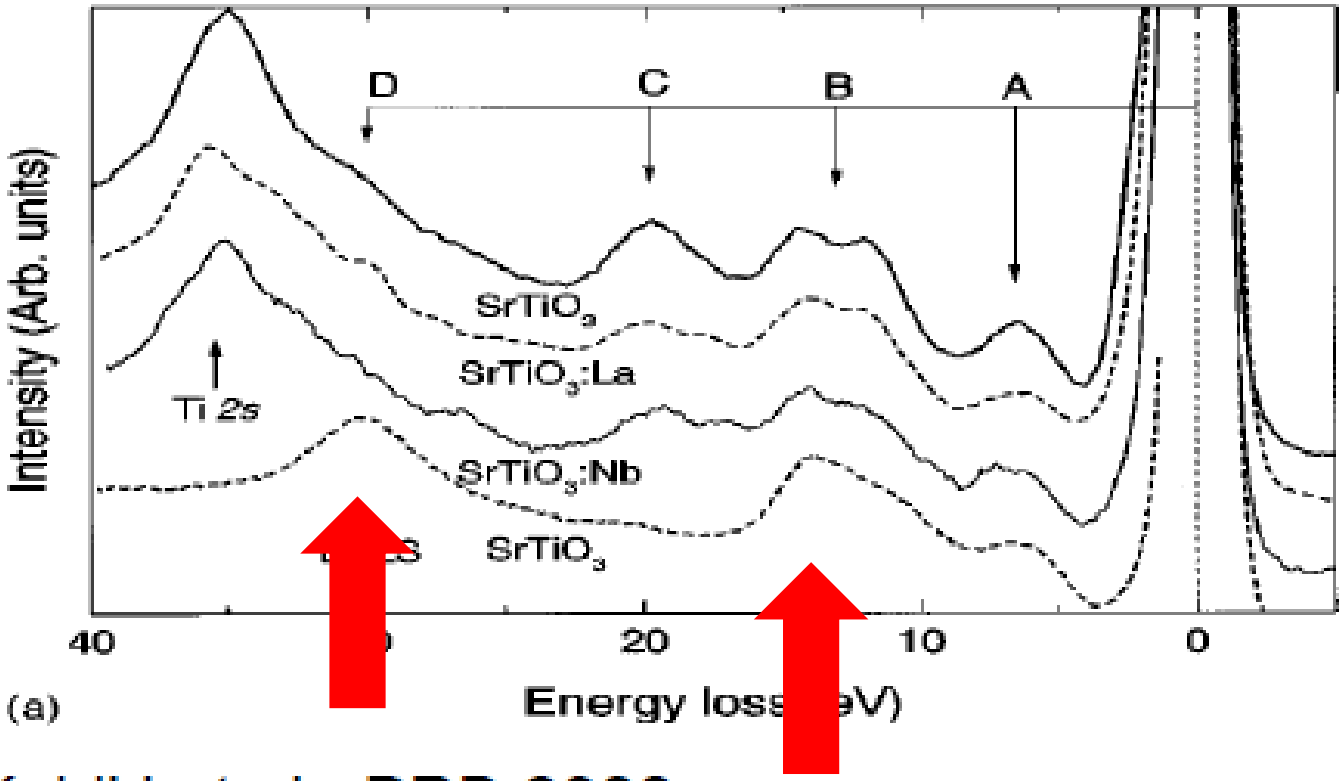


SrVO3 within Screened Exchange Dynamical Mean Field Theory

A. van Roekeghem and S. Biermann, Europhysics Letters (2014)

Consistent with full GW+DMFT calculations in Tomczak, Casula, Miyake, SB, PRB 2014

Plasmons seen in Electron Energy Loss Spectroscopy (EELS) !



Kohiki et al., PRB 2000

Side remark: why do DFT bands give a reasonable approximation to single-particle excitations of weakly correlated metals?

- Error cancellation between exchange and correlation ! (well-known for total energies. Here: for excitations …)
- Example: n-doped SrTiO3:

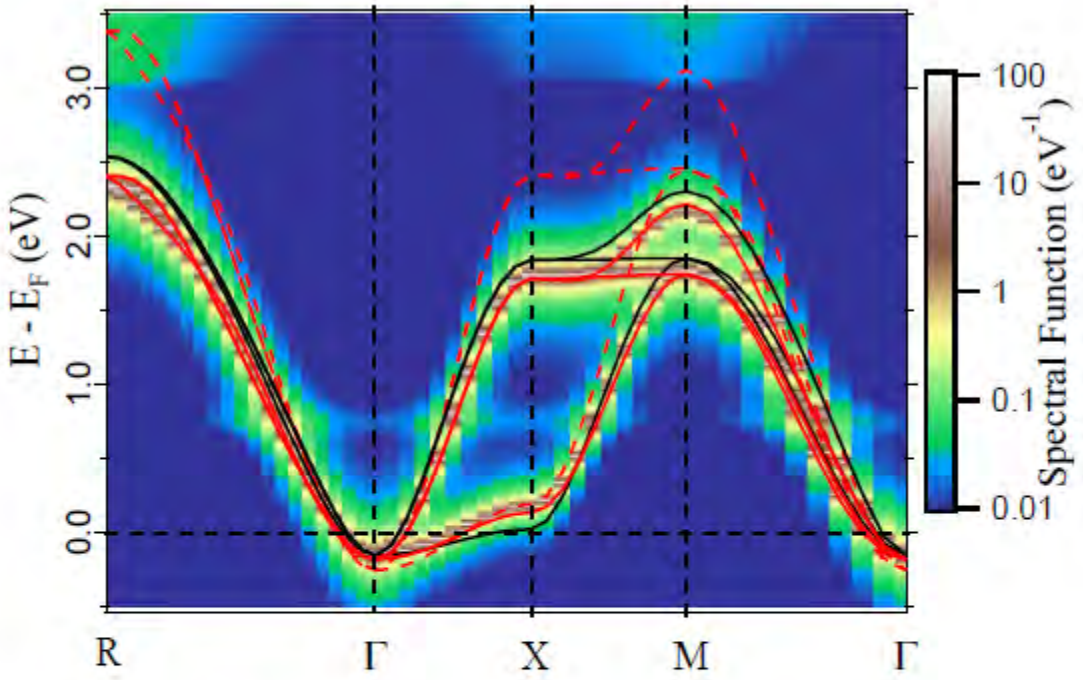


Fig. 4: Band structure of the t_{2g} states of $SrTiO_3$ within LDA (black lines), Screened Exchange (red dashes) and SEx renormalized by a plasmonic factor $Z_B = 0.7$ (red lines) superimposed on the SEx+DDMFT t_{2g} spectral function. The chemical potential corresponds to $n = 0.05$ electron doping per Ti atom, which gives a self-consistent Thomas-Fermi screening-length of $\lambda = 0.6\ a_0^{-1}$ according to the SEx density of states.

GW+DMFT for "real" systems?

- Ferromagnetic Nickel: static U, "$[\text{LDA+DMFT}]_{\text{local}}+\text{GW}_{\text{nonloc}}$" for Σ, self-consistent in DMFT part (inner loop) for fixed GW calculation

  (Biermann, Aryasetiawan, Georges, PRL 2003)

- SrVO3: as above, but based on quasi-particlized-GW (=> problem: GW_{loc} counted twice!)

  (Taranto et al., PRB 2013)

- SrVO3: dynamical U from cRPA, "$[\text{LDA+U(w)+DMFT}]_{\text{local}}+\text{GW}_{\text{nonloc}}$" for Σ as a one-shot combination without self-consistency

  (Sakuma et al., arXiv2013)

- **SrVO3: dynamical U from cRPA, true GW+DMFT, self-consistent in DMFT part (inner loop) for fixed GW calculation.**

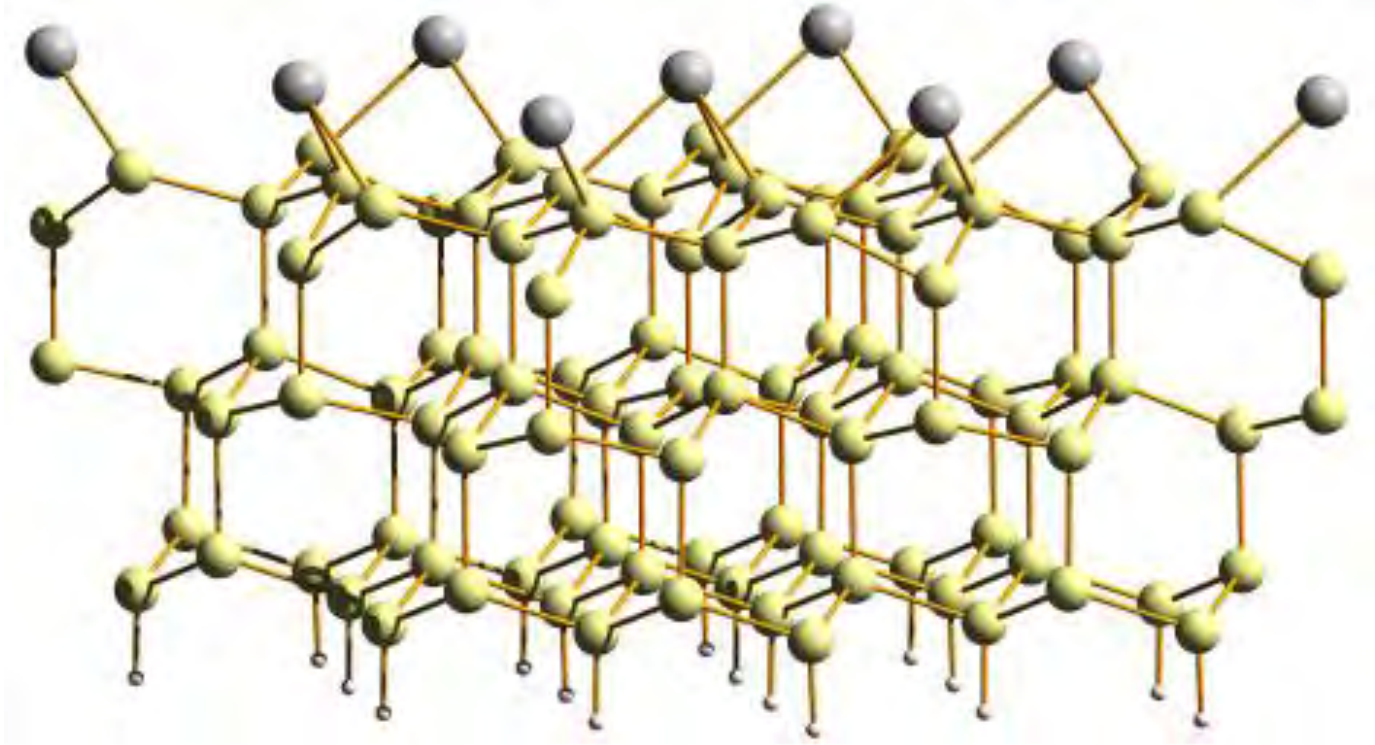
  (Tomczak et al., Europhys. Lett. 2012 and PRB 2014)

- **Systems of adatoms on surfaces: "Sn:Si(111)": full GW+DMFT (self-consistency at DMFT and GW level) within low-energy space**

  (Hansmann, Ayral, Vaugier, Werner, Biermann, Phys. Rev. Lett. 2013)

See also calculations for extended Hubbard model: Sun&Kotliar, PRL 2004, Karlsson JPCM 2007, Ayral, Biermann, Werner, PRL 2012 and PRB 2013

A realistic example: Sn/Si(111)

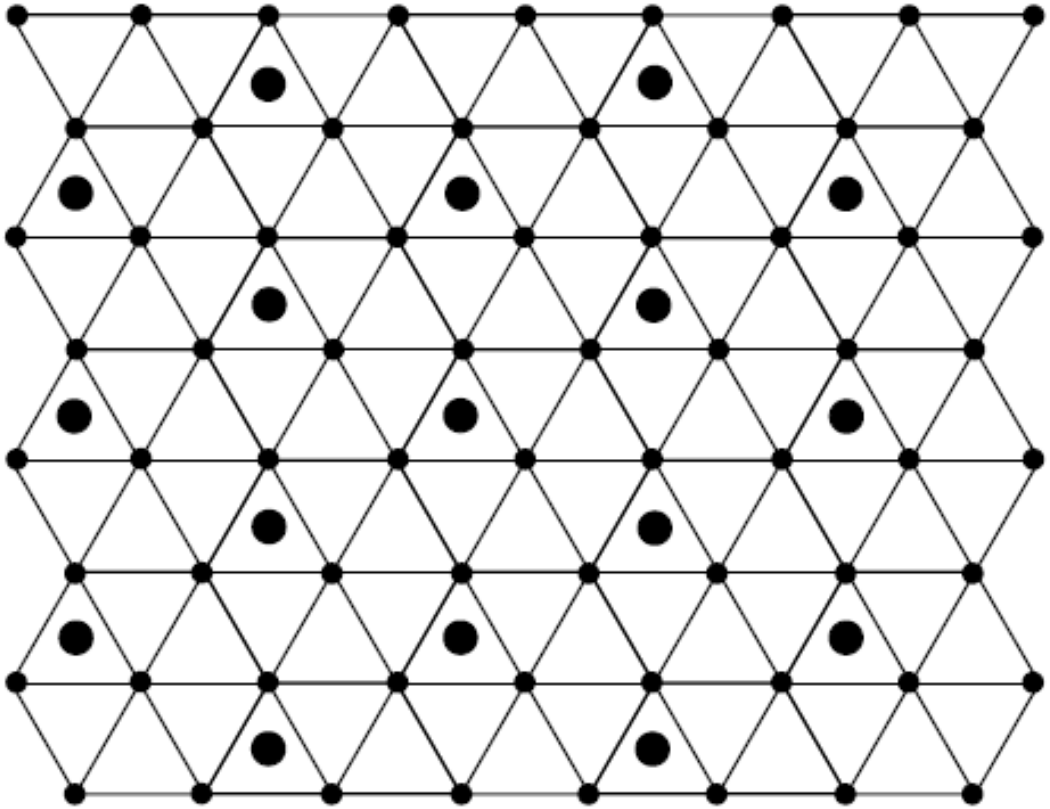


P. Hansmann

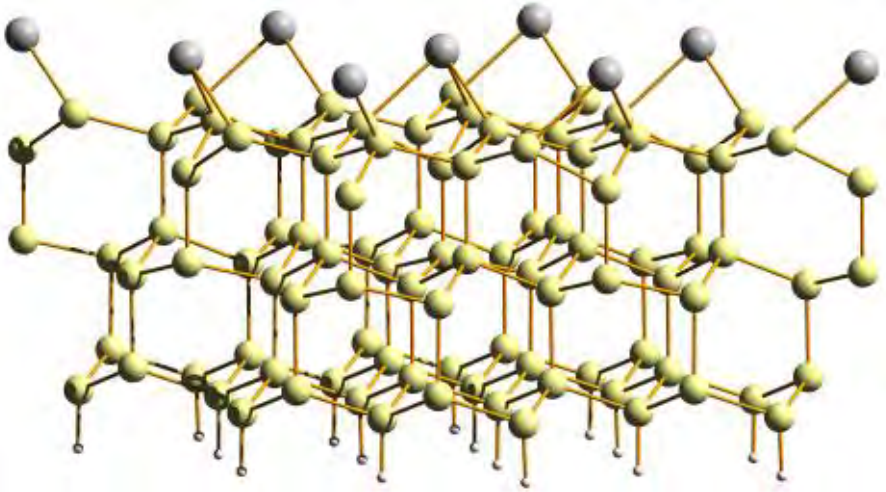
T. Ayral

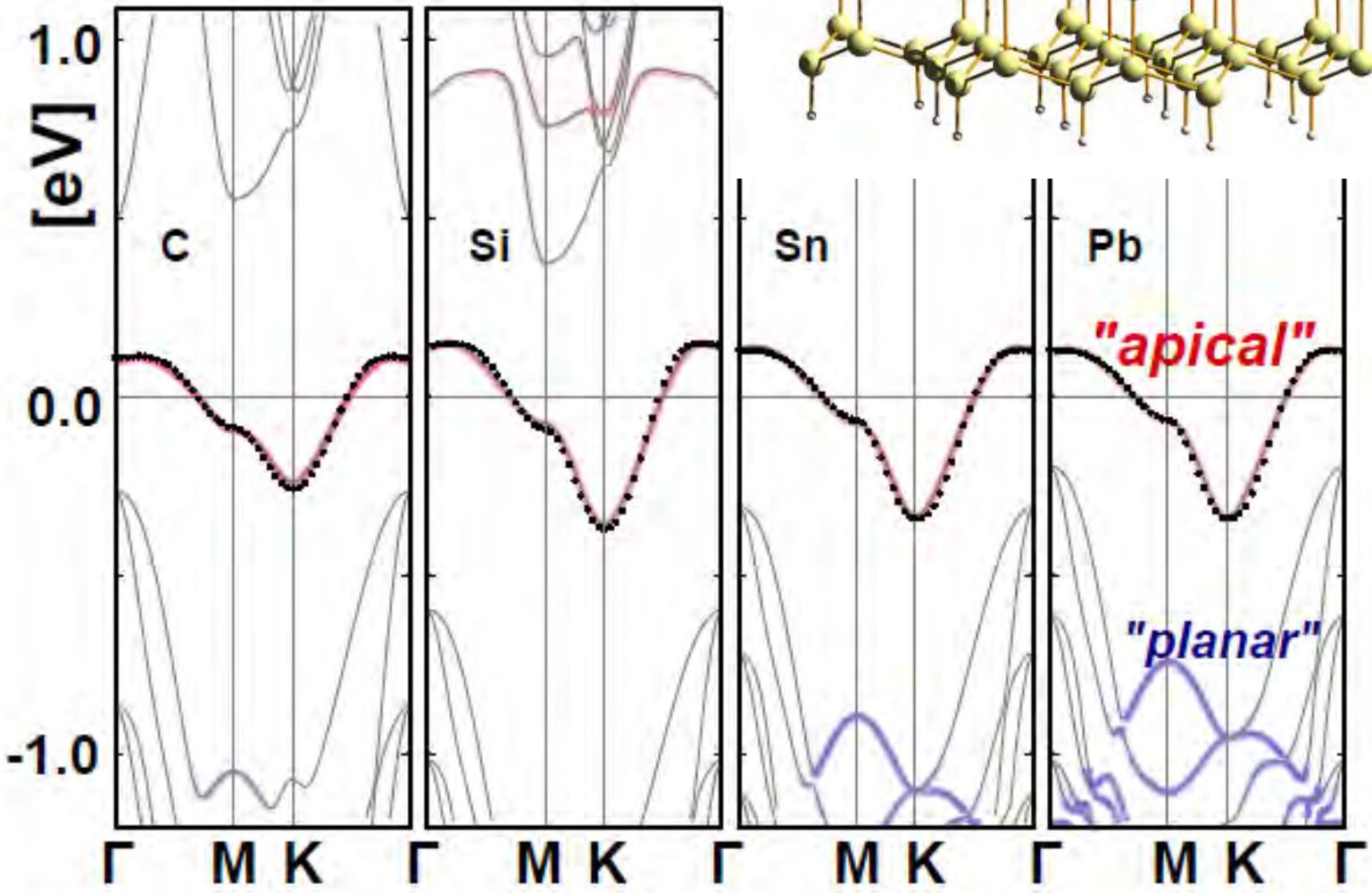
Monolayer of adatoms forms triangular lattice

2d triangular lattice by adatoms



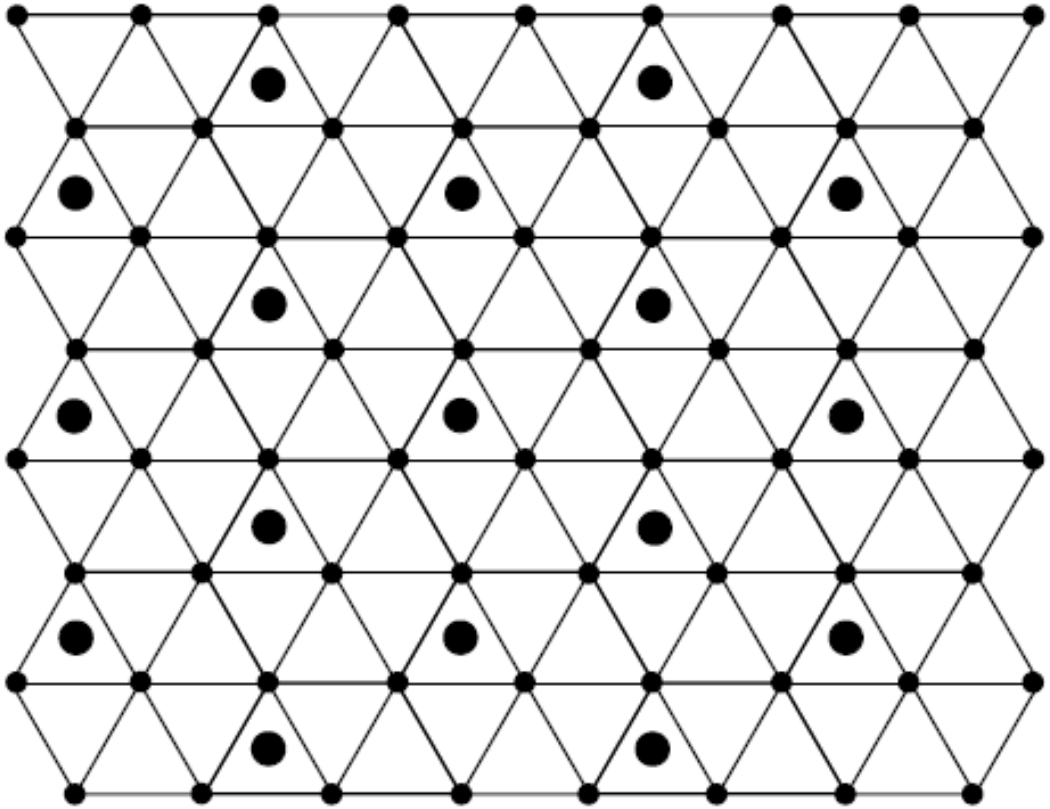
X/Si(111) with X=C, Si, Sn, Pb





P. Hansmann, T. Ayral, L. Vaugier, P. Werner, SB, JPCM 2013 and PRL 2013

Hubbard model on 2d triangular lattice formed by adatoms



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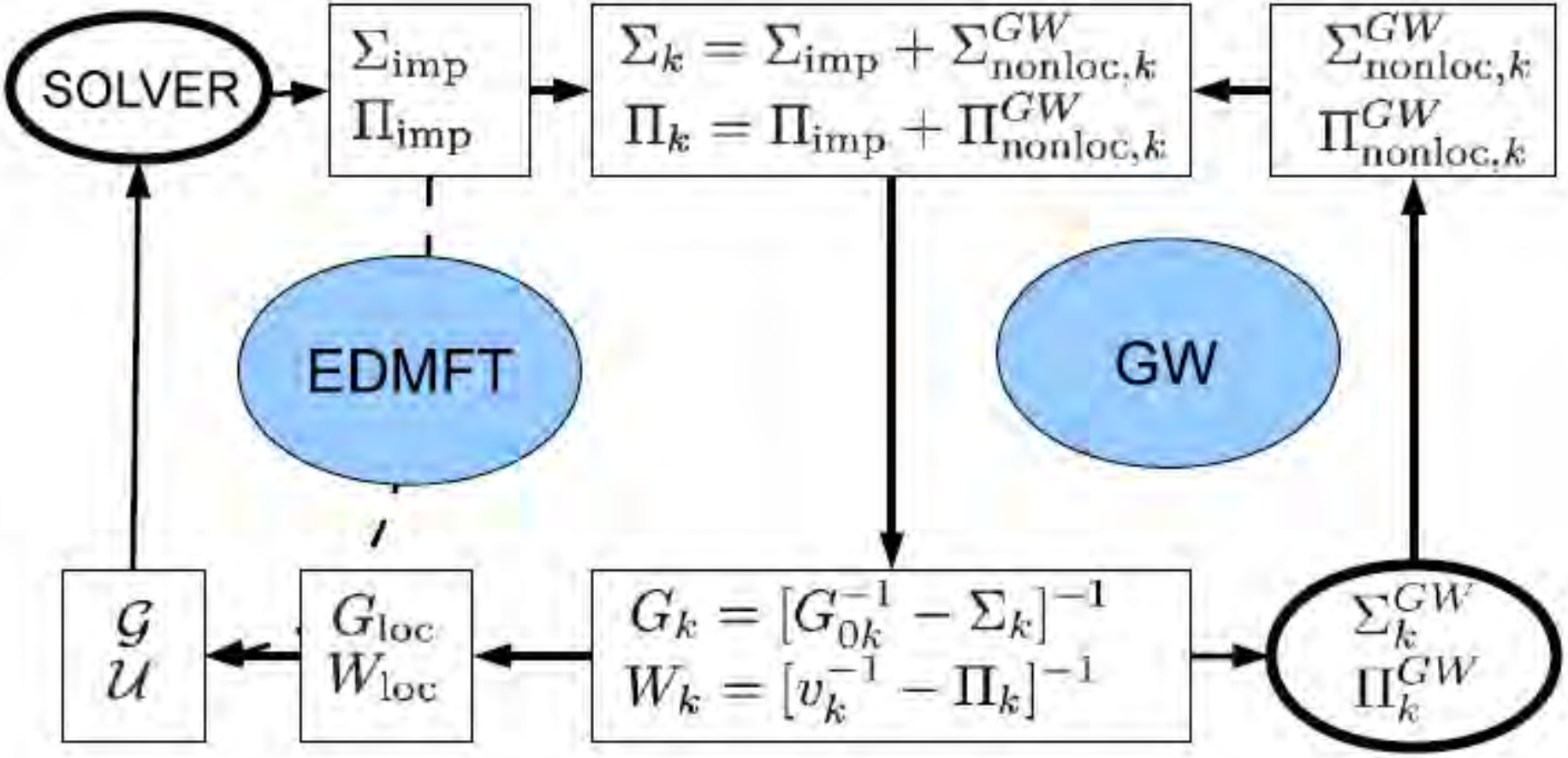
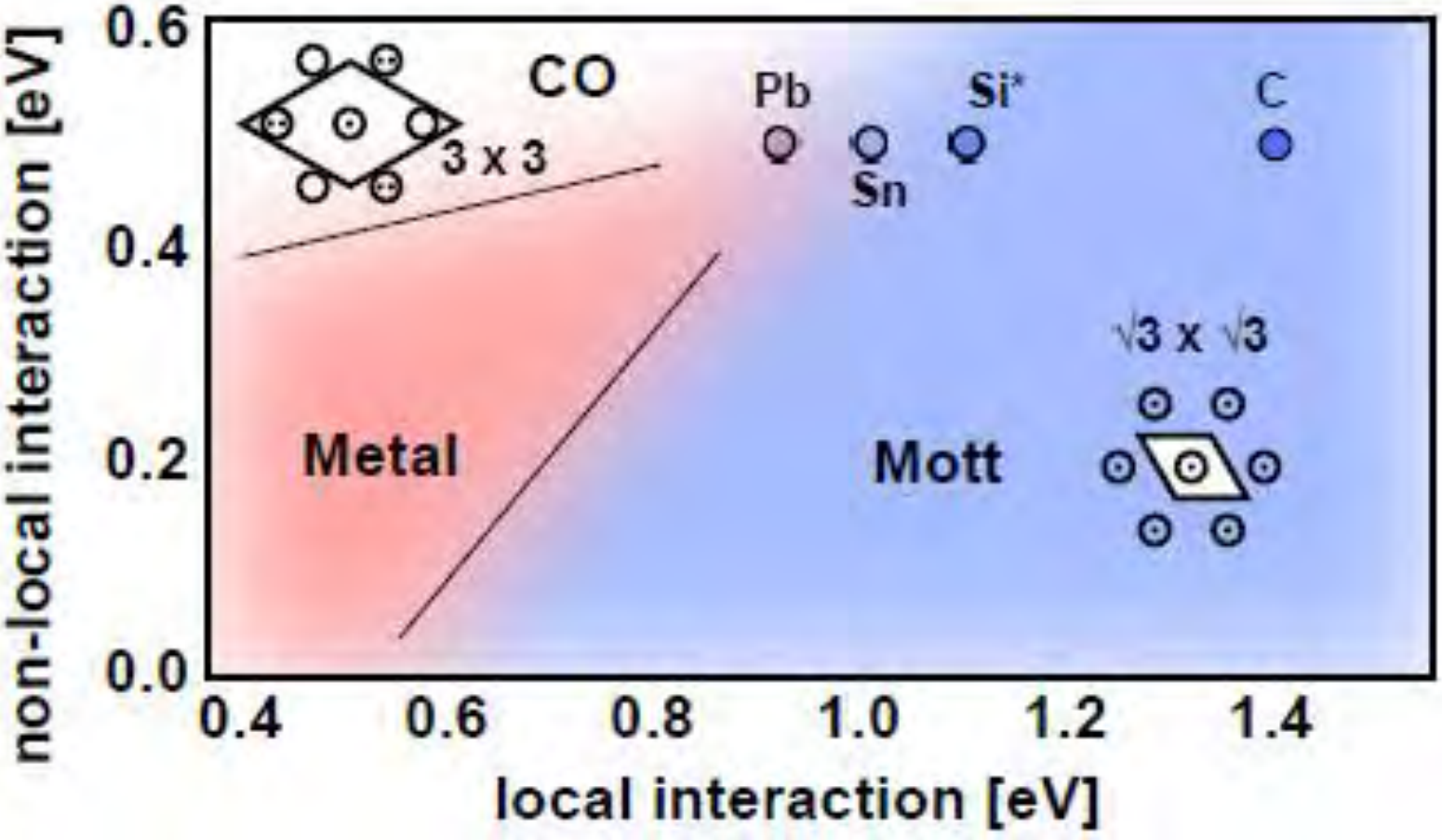
t''	0.5	5.0	10.0	10.0	[meV]
U_0	1.4	1.1	1.0	0.9	[eV]
U_1	0.5	0.5	0.5	0.5	[eV]
U_n			U_1/r_a		
V_0	6.0	4.7	4.4	4.3	[eV]
V_1	2.8	2.8	2.7	2.8	[eV]

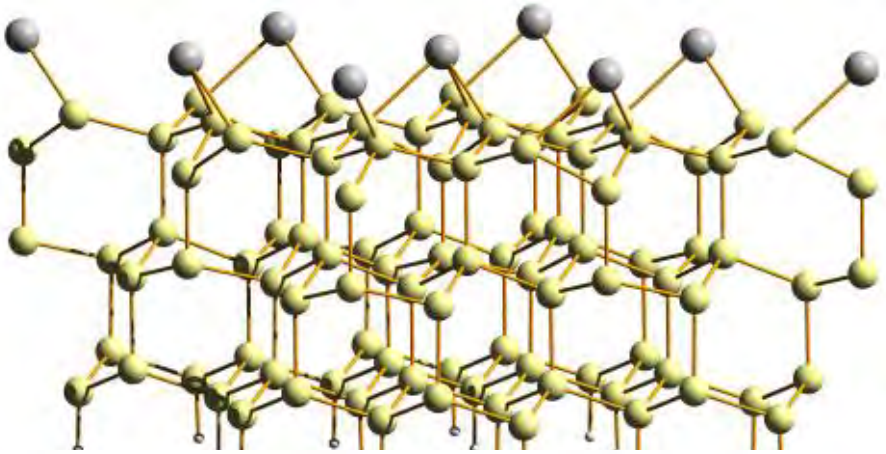
Fully self-consistent GW+DMFT:



Phase diagram

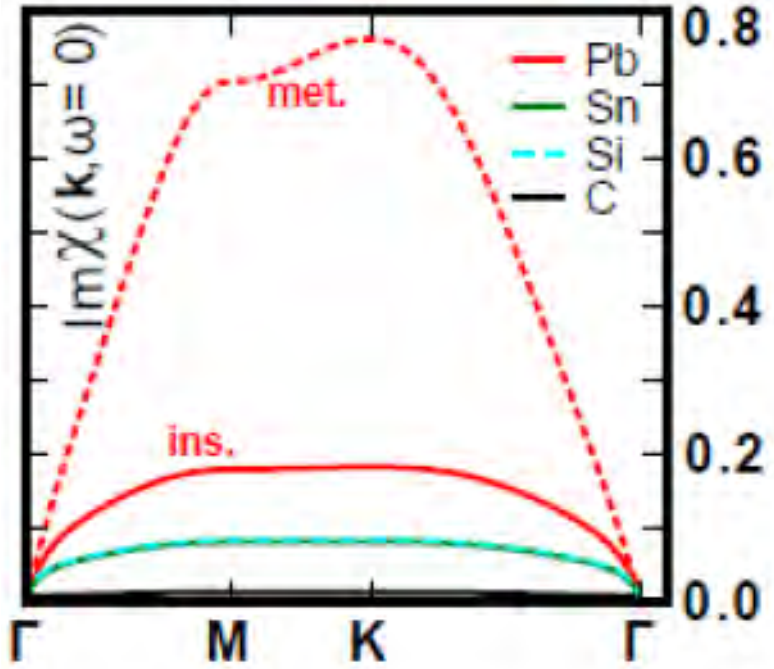


GW+DMFT for Sn/Si(111)



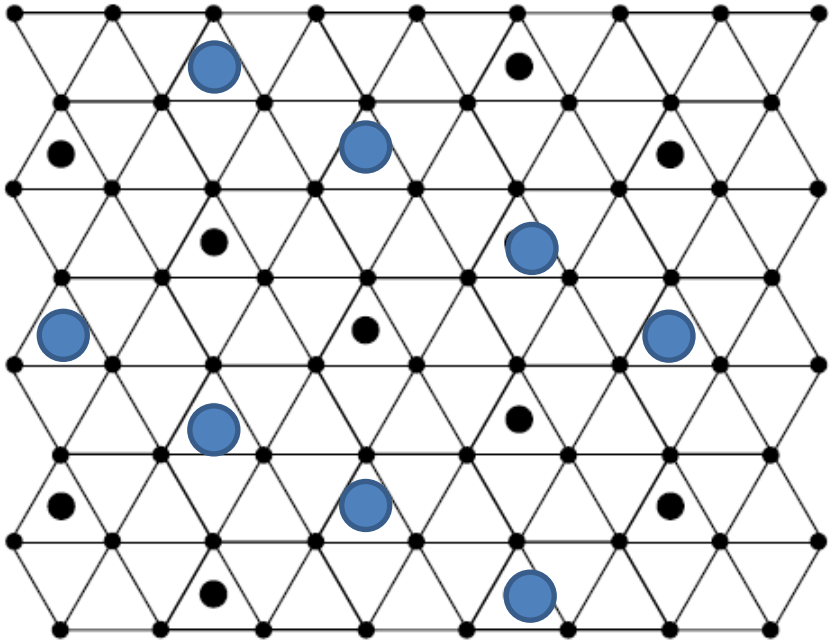
Charge-charge correlation function:

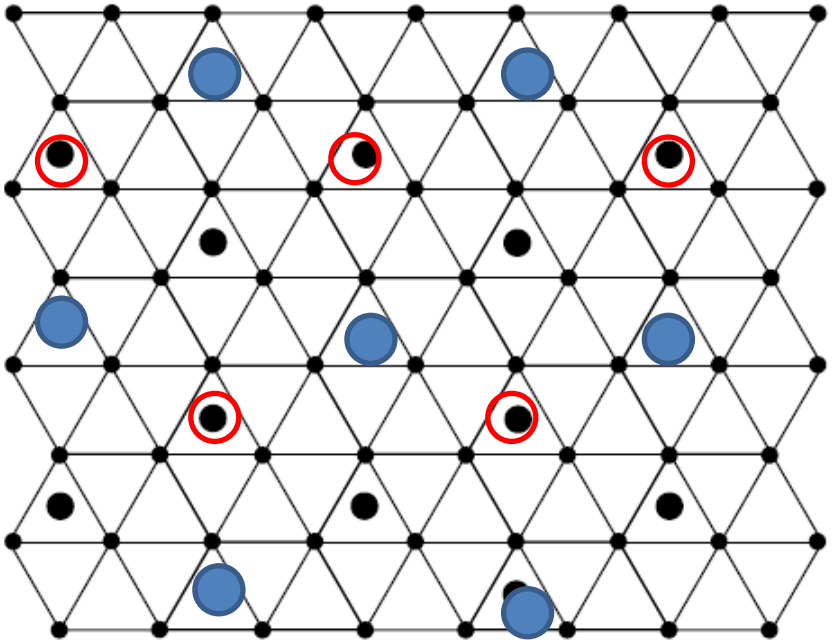
$$\mathrm{Im}\chi(\mathbf{k}, \omega = 0)$$



P. Hansmann, T. Ayral, L. Vaugier, P. Werner, SB, PRL 2013

2 charge order patterns





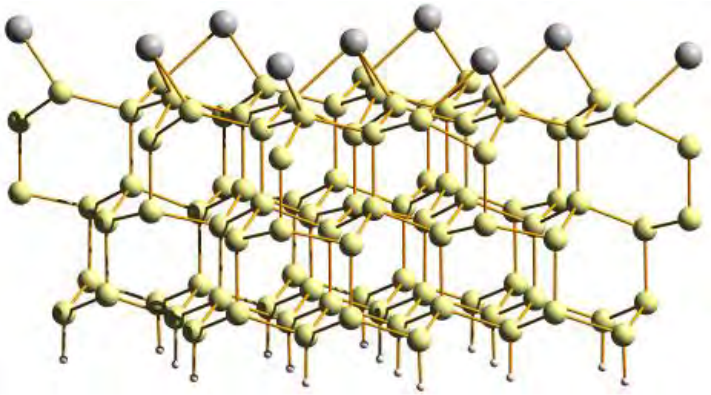
k=M

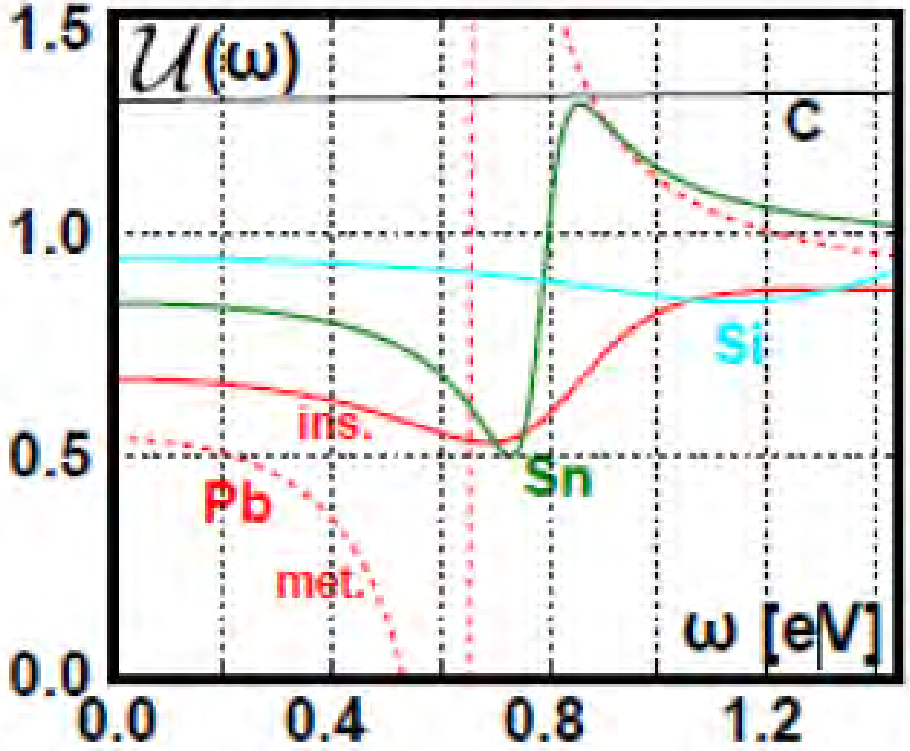
k=K

Doubly occupied site

singly occupied site

U(w) from GW+DMFT





P. Hansmann, T. Ayral, L. Vaugier, P. Werner, SB, PRL 2013

Extended Hubbard Model from LDA and cRPA ?

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$\mathcal{U}(\omega=0)$	1.3	0.94	0.84	0.67(ins.) 0.54(met.)	[eV] [eV]

Effective local interaction from GW+DMFT

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"U-V" is a lower bound !

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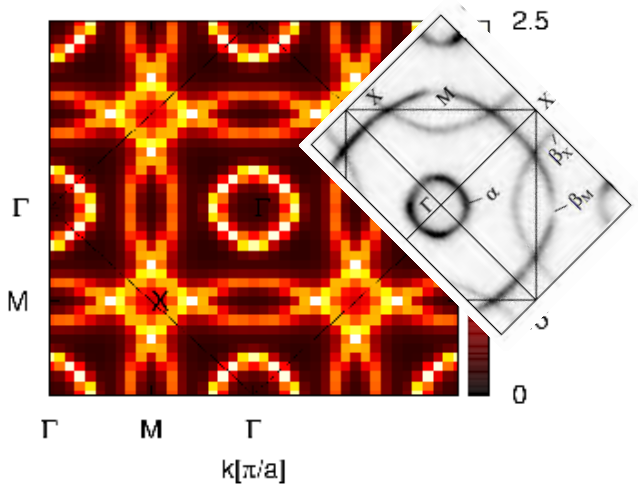
Summary …

Sr2RhO4 Fermi surface



Martins et al, Phys. Rev. Lett. (2011)

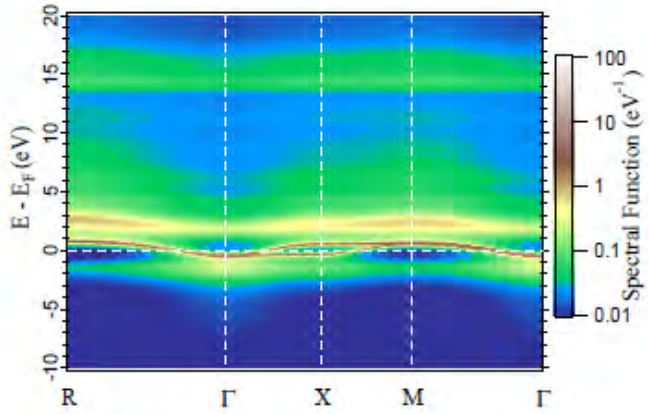
f-electron pigments: ceria

(cf. Rhodia's Neolor series)

Calculated colour of CeSF:

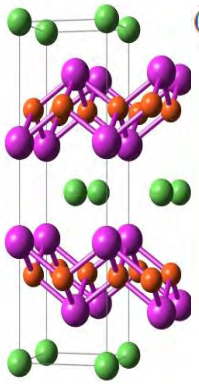
Tomczak et al., PNAS (2013)

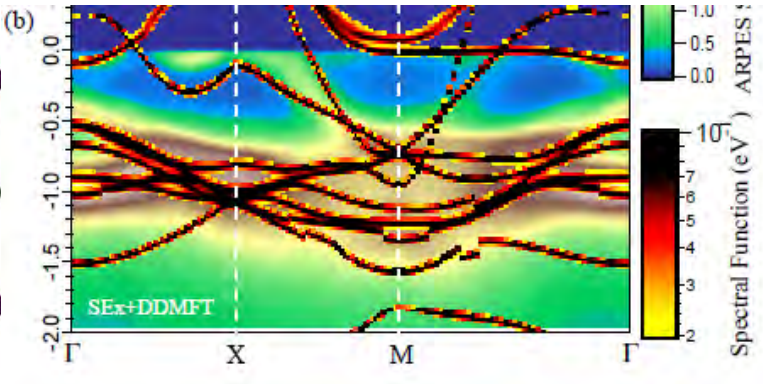
SrVO3 and SrTiO3



Van Roekeghem, SB, Europhys. Lett. (2014)

BaCo2As2





Van Roekeghem et al., PRL 2014