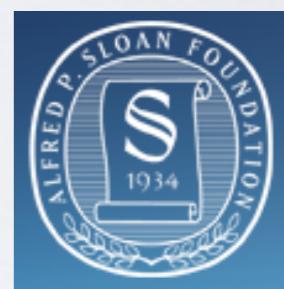


DFT+EMBEDDED DYNAMICAL MEAN FIELD THEORY FROM FUNCTIONAL PERSPECTIVE

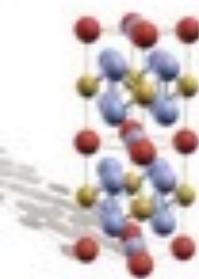
Kristjan Haule



Support:



Latest developments



1. Projectors and locality of correlations
2. *Exact double-counting of DFT+EDMFTF : PRL 115, 196403 (2015).*
3. *Stationary free energy functional (within Embedded DMFT approach) for structural optimization, PRL 115, 256402 (2015).*
4. Implementation of Forces within E-DMFT functional for optimization of internal structural parameter, arXiv:1602.02819.
5. Some details on the structure of the code.

Reminder: LWF and indirect approach



Basic variable is Green's function:

== dynamic analog of charge density

$$G(\mathbf{r}\tau, \mathbf{r}'\tau') = \langle T_\tau \psi^\dagger(\mathbf{r}'\tau') \psi(\mathbf{r}, \tau) \rangle \quad \rho(\mathbf{r}) = G(\mathbf{r}\tau, \mathbf{r}\tau)$$

Luttinger–Ward functional (1950):

$$\Gamma[\{G\}] = -\text{Tr}((G_0^{-1} - G^{-1})G) + \text{Tr} \log(-G) + \Phi[\{G\}]$$

material dependent term



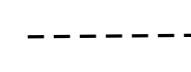
universal functional
independent of material
expressible by the perturbation theory

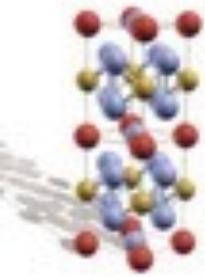
$\Phi[G]$ Is a sum of all connected two particle irreducible Feynman diagrams (skeleton diagrams).

$$\Phi[G] = 1/2 \text{---} \text{---} + 1/2 \text{---} \text{---} + 1/4 \text{---} \text{---} + \dots + \dots$$

The diagram shows the expansion of the Luttinger–Ward functional. It starts with a simple loop (1/2), followed by a loop with a dashed line (1/2), then a more complex loop with multiple lines (1/4), and so on. Dashed lines represent the potential $v_c(\mathbf{r} - \mathbf{r}')$.

legend:

 G
 $v_c(\mathbf{r} - \mathbf{r}') = \frac{1}{|\mathbf{r} - \mathbf{r}'|}$



Other approaches in LW language

Density Functional Theory:

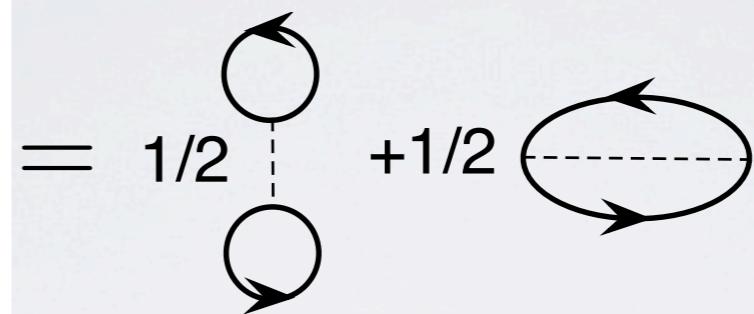
$$\Phi[\{G\}] \rightarrow E_H[\rho] + E_{XC}[\rho]$$

Exact DFT appears as
an approximation to the Green's function!

$E_{xc}[\{\rho\}]$ local to a point in 3D space in LDA

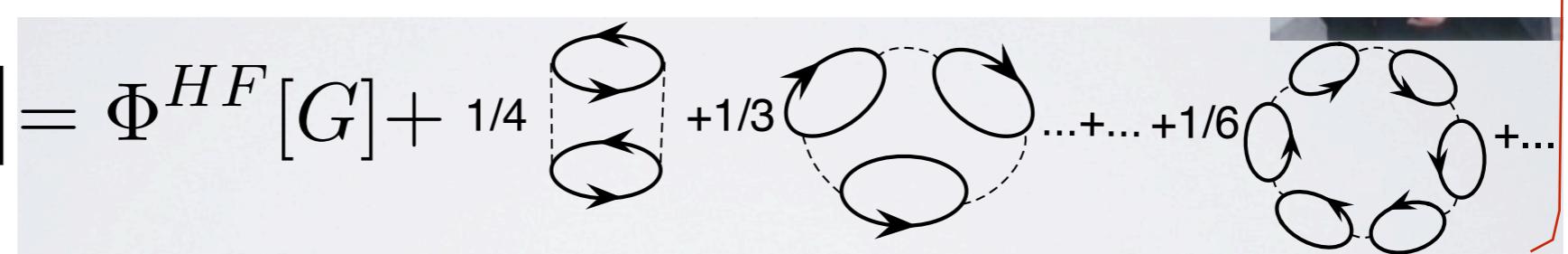
Hartree–Fock approximation:

$$\Phi[\{G\}] =$$



RPA&
GW:

$$\Phi[\{G\}] = \Phi^{HF}[G] +$$



Dynamical Mean Field
Theory:

$$\Phi[\{G_{ij}\}] \approx E_H[\{\rho\}] + \Phi[\{G_{ii}\}]$$

all local Feynman diagrams
(in fully dressed perturbation theory)

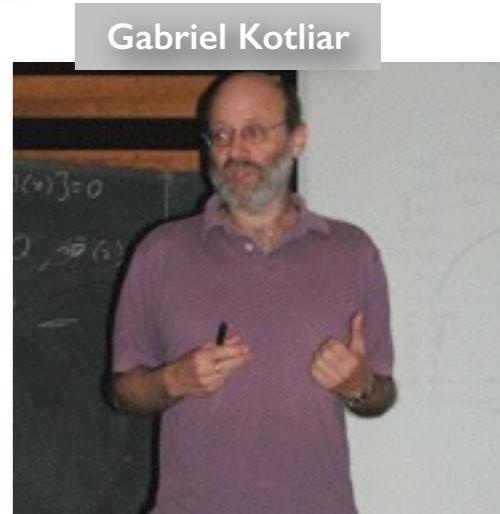
Truncation in the real space
of Feynman diagrams

Functional Point of view

DMFT for lattice models:

$$\Phi[\{G_{ij}\}] \rightarrow \sum_i \Phi[\{G_{ii}\}]$$

i is site or cluster



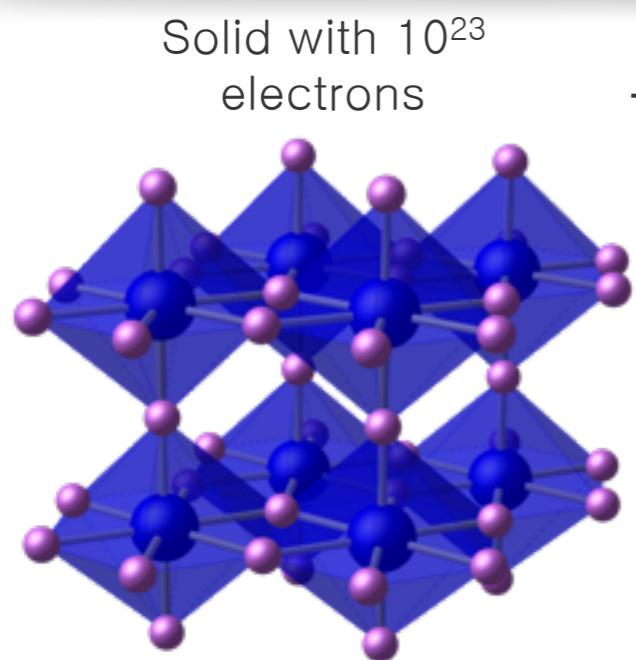
DMFT for continuous problems:

$$\Phi[\{G\}] \rightarrow \sum_{\mathbf{R}_i} \Phi[\{\hat{P}_{\mathbf{R}_i} G\}]$$

Need to define projector to site (or cluster): $\hat{P}_{\mathbf{R}_i}$

DMFT is projector dependent approximation

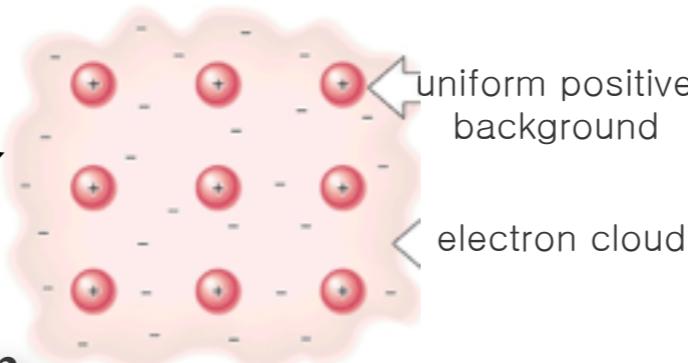
How is correlation potential determined?



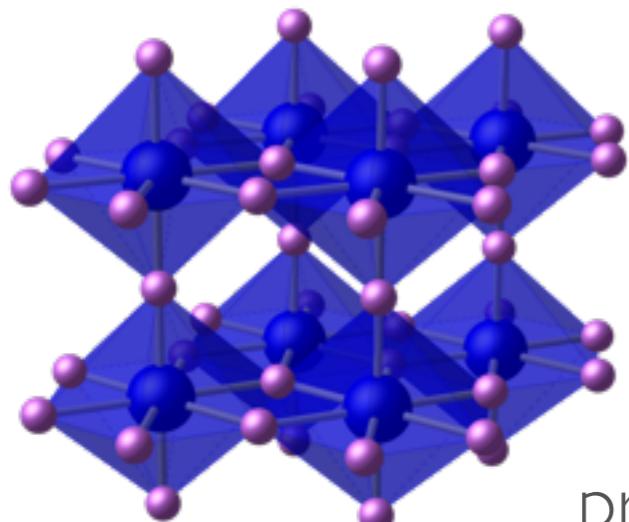
LDA

To determine e-e correlation potential,
each point in space
is mapped to

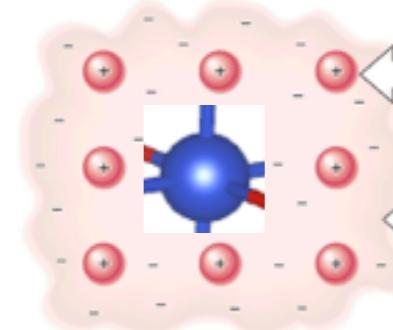
Electron gas problem



In DMFT we want to lift the restriction and compute all correlations local to a given site (not given point in space).



$$\hat{P}_{\mathbf{R}_i}$$



projector defines what is a “site” in DMFT,
typically an ion with open d or f shell.

The continuos DMFT problem

DMFT approximation: $\Phi[\{G\}] \rightarrow \sum_{\mathbf{R}_i} \Phi[\{\hat{P}_{\mathbf{R}_i} G\}]$

in continuum requires **discretization** of projector,

$$\hat{P}_{\mathbf{R}_i} \rightarrow P_{\mathbf{R}_i}(\alpha\beta) = \int d\mathbf{r} d\mathbf{r}' \mathcal{P}_{\mathbf{R}_i}(\alpha\beta; \mathbf{r}\mathbf{r}')$$

for example: $P_{\mathbf{R}_i}(\alpha\beta) = \int d\mathbf{r} d\mathbf{r}' \phi_\alpha(\mathbf{r} - \mathbf{R}_i) \phi_\beta^*(\mathbf{r}' - \mathbf{R}_i)$

where $\phi_\alpha(\mathbf{r} - \mathbf{R}_i) \equiv \langle \mathbf{r} | \phi_\alpha^i \rangle$ forms a basis on a given atom
so that:

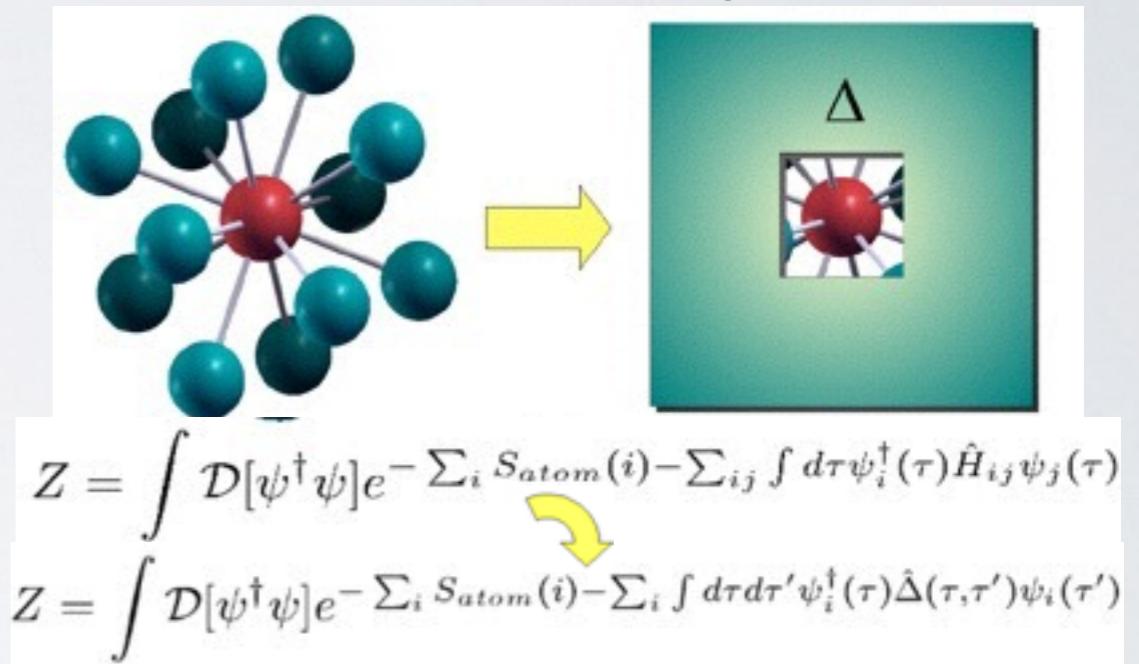
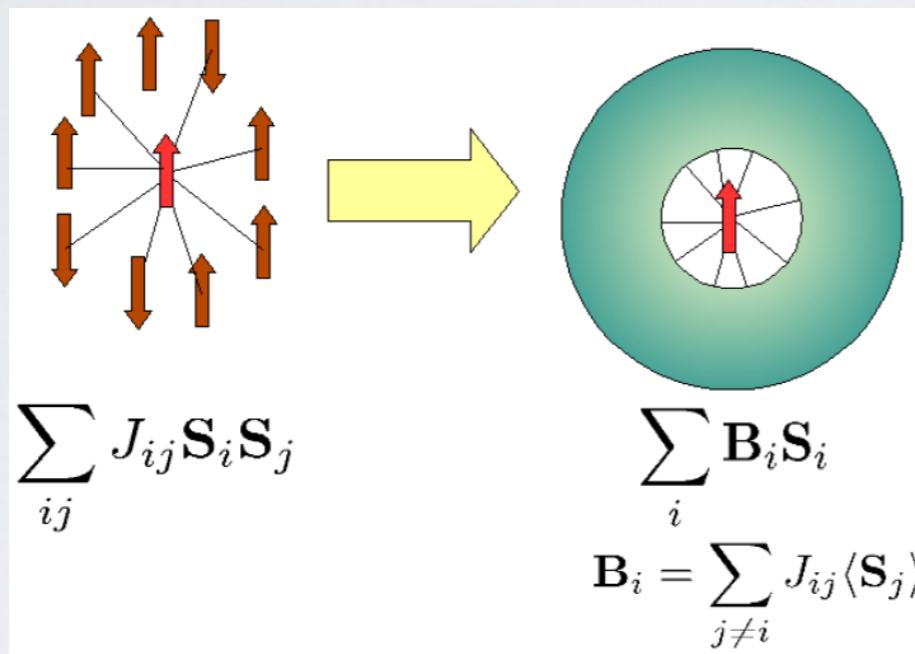
$$G_{local}^i(\mathbf{r}, \mathbf{r}') = \sum_{\alpha\beta} \langle \mathbf{r} | \phi_\alpha^i \rangle \langle \phi_\alpha^i | G | \phi_\beta^i \rangle \langle \phi_\beta^i | \mathbf{r}' \rangle$$


*quasi atomic orbitals
(locally complete set)*

α, β are orbital-spin indices

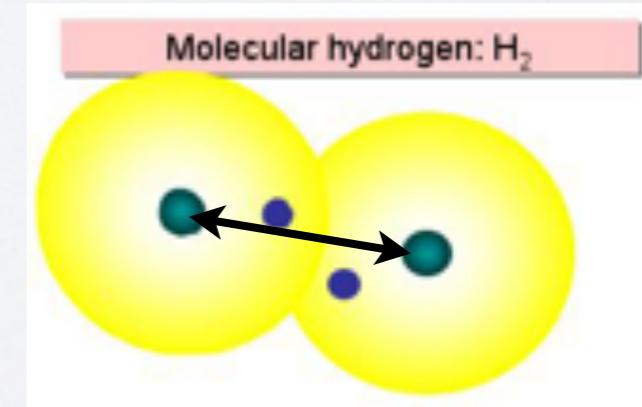
HOW LOCAL ARE CORRELATIONS?

Correlations are local in large d (large connectivity z) where DMFT is exact -- Weiss mean field theory



What about finite D? What about 0?

H_2 molecule:



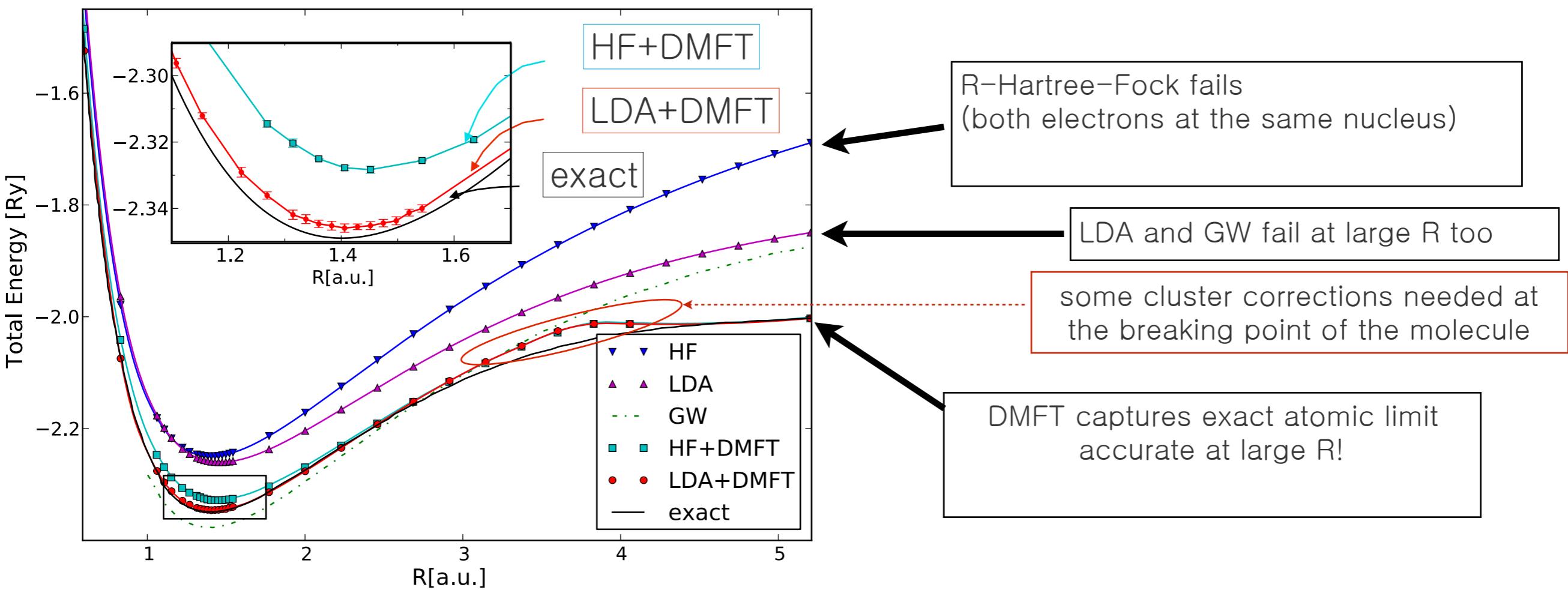
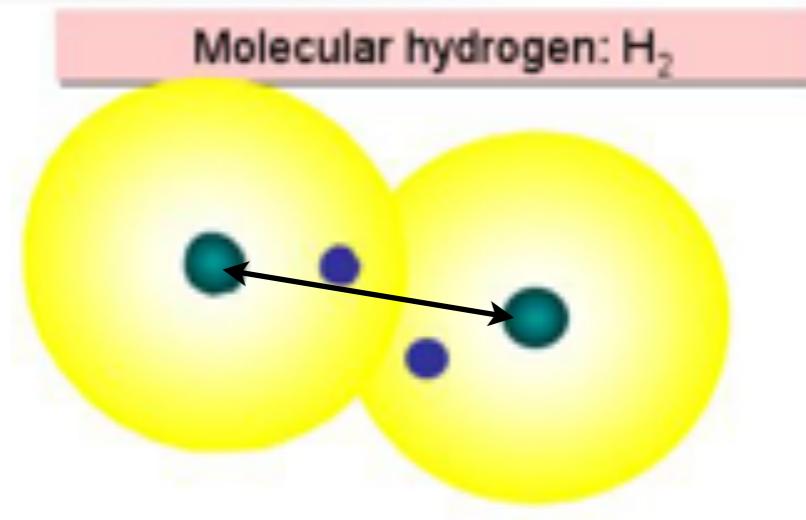
How local are correlations ?

0-D test of the single site DMFT.

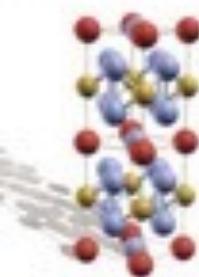
Archetypal problem of strong correlations:

DMFT exact in ∞D , or large connectivity Z

It is not expected to be good for low-D problems
(like H₂ molecule)



DFT+Embedded Dynamical Mean Field Theory



$$\Gamma[G] = \text{Tr} \log G - \text{Tr}((G_0^{-1} - G^{-1})G) + E_{Vc}^{H+XC}[\rho] + \Phi_{V_{DMFT}}^{DMFT}[G_{local}] - \Phi_{V_{DMFT}}^{H+XC}[\rho_{local}]$$

Green's function Hartree + XC functional sum of all “local” Feynman diagrams for correlated ions. double-counted interaction (we know exactly)

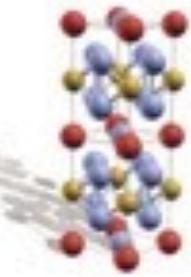
$\Gamma[G]$ Is stationary and gives free energy of the system.

$$\frac{\delta \Gamma[G]}{\delta G} = 0 \quad \text{because} \quad G^{-1} - G_0^{-1} + V_{H+XC}\delta(\mathbf{r} - \mathbf{r}')\delta(\tau - \tau') + \hat{P}\frac{\delta \Phi^{DMFT}[G_{local}]}{\delta G_{local}} - \hat{P}\frac{\delta \Phi^{DC}[\rho_{local}]}{\delta \rho_{local}}\delta(\mathbf{r} - \mathbf{r}')\delta(\tau - \tau') = 0$$

Stationarity : 1st order error in G leads to 2nd order error in free energy.

Note: Migdal-Galitskii formula gives non-stationary total energies in DFT+DMFT.

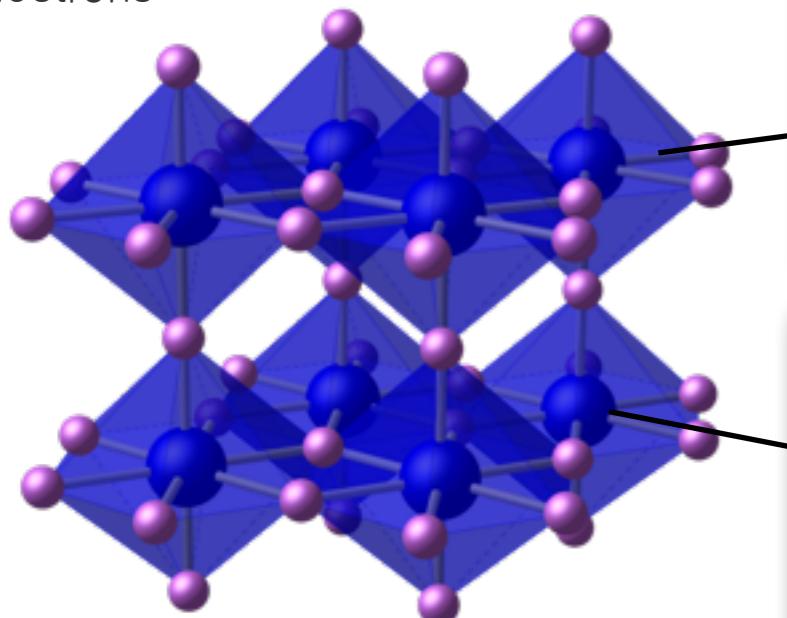
Embedded Dynamical Mean Field Theory Functional



$$\Gamma[G] = \text{Tr} \log G - \text{Tr}((G_0^{-1} - G^{-1})G) + E_{Vc}^{H+XC}[\rho] + \Phi_{V_{DMFT}}^{DMFT}[G_{local}] - \Phi_{V_{DMFT}}^{H+XC}[\rho_{local}]$$

We extremize a **DFT-DMFT** functional in real space: no need to build tight-binding model Hamiltonian (Wannier orbitals).

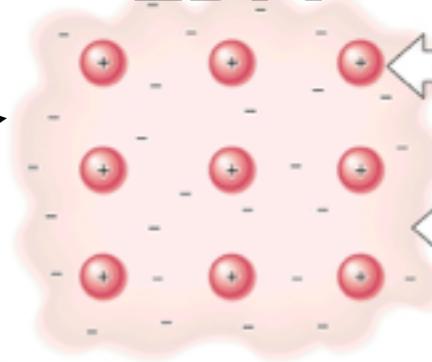
Solid with 10^{23} electrons



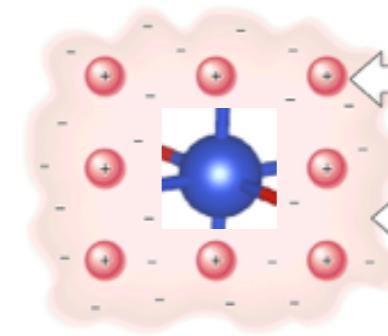
To determine e-e correlation potential, each point in space is mapped to the uniform electron gas problem.

To determine e-e correlation potential, each atom is mapped to auxiliary **quantum impurity** problem

LDA



E-DMFT



uniform positive background
+
electron cloud

Auxiliary problem is a non-interacting problem in self-consistent medium

electron cloud
+
interacting ion

Auxiliary problem is a “interacting atom” in a self-consistent medium/entanglement

Note: The trick of mapping is used only to determine the exchange-correlation potential, while the *kinetic energy* and *Hartree term* are always treated exactly.

Quantum impurity model solved by Monte Carlo

Embedded Dynamical Mean Field Theory Functional

Discretized problem can be handled in similar way as a lattice models.

Extremization:

$$\frac{\delta}{\delta G} \Gamma[\{G\}] = \frac{\delta}{\delta G} (\text{Tr} \log G - \text{Tr}((G_0^{-1} - G^{-1})G)) + \frac{\delta E_{V_c}^{H+XC}[\rho]}{\delta G} + \frac{\delta \sum_{\mathbf{R}_i} \Phi_{V_{DMFT}} [\{\int d\mathbf{r} d\mathbf{r}' \phi_\alpha(\mathbf{r} - \mathbf{R}_i) G(\mathbf{r}\mathbf{r}') \phi_\beta^*(\mathbf{r}' - \mathbf{R}_i)\}]}{\delta G} - \frac{\delta \sum_{\mathbf{R}_i} \Phi_{V_{DMFT}}^{H+XC} [\{\int d\mathbf{r} d\mathbf{r}' \phi_\alpha(\mathbf{r} - \mathbf{R}_i) \rho(\mathbf{r}\mathbf{r}') \phi_\beta^*(\mathbf{r}' - \mathbf{R}_i)\}]}{\delta G}$$

or

$$\begin{aligned} \frac{\delta}{\delta G} \Gamma[\{G\}] &= G^{-1} - G_0^{-1} + \frac{\delta E_{V_c}^{H+XC}[\rho]}{\delta \rho} \delta(\mathbf{r} - \mathbf{r}') \delta(\tau - \tau') && \left(\rho(\mathbf{r}) = \delta(\mathbf{r} - \mathbf{r}') \delta(\tau - \tau') G(\mathbf{r}\tau, \mathbf{r}'\tau') \right) \\ &+ \sum_{\alpha\beta} \frac{\delta \Phi_{V_{DMFT}} [\{G_{local}^i\}]}{\delta G_{local\beta\alpha}^i} \phi_\alpha(\mathbf{r} - \mathbf{R}_i) \phi_\beta^*(\mathbf{r}' - \mathbf{R}_i) \\ &- \sum_{\alpha\beta} \frac{\delta \Phi_{V_{DMFT}}^{H+XC} [\{\rho_{local}\}]}{\delta \rho_{local\beta\alpha}} \phi_\alpha(\mathbf{r} - \mathbf{R}_i) \delta(\tau - \tau') \phi_\beta^*(\mathbf{r}' - \mathbf{R}_i)] = 0 \end{aligned}$$

finally

$$G^{-1} = G_0^{-1} - V_{H+XC}(\mathbf{r}) \delta(\mathbf{r} - \mathbf{r}') \delta(\tau - \tau') - \langle \mathbf{r} | \phi_\alpha^i \rangle (\Sigma^{imp} - V^{DC})_{\alpha\beta} \langle \phi_\beta^i | \mathbf{r}' \rangle$$

where $\Sigma_{\alpha\beta}^{imp} = \frac{\delta \Phi_{V_{DMFT}} [\{G_{local}^i\}]}{\delta G_{local\beta\alpha}^i}$ and $V_{\alpha\beta}^{DC} = \frac{\delta \Phi_{V_{DMFT}}^{H+XC} [\{\rho_{local}\}]}{\delta \rho_{local\beta\alpha}} \delta(\tau - \tau')$

Embedded Dynamical Mean Field Theory Functional

$$G^{-1} = G_0^{-1} - \underbrace{V_{H+XC}(\mathbf{r})\delta(\mathbf{r} - \mathbf{r}')\delta(\tau - \tau')}_\text{DFT} - \underbrace{\langle \mathbf{r} | \phi_\alpha^i \rangle (\Sigma^{imp} - V^{DC})_{\alpha\beta} \langle \phi_\beta^i | \mathbf{r}' \rangle}_\text{quantum impurity S. embedded}$$

where $\Sigma_{\alpha\beta}^{imp} = \frac{\delta\Phi_{V_{DMFT}}[\{G_{local}^i\}]}{\delta G_{local\beta\alpha}^i}$ and $V_{\alpha\beta}^{DC} = \frac{\delta\Phi_{V_{DMFT}}^{H+XC}[\{\rho_{local}\}]}{\delta\rho_{local\beta\alpha}}\delta(\tau - \tau')$

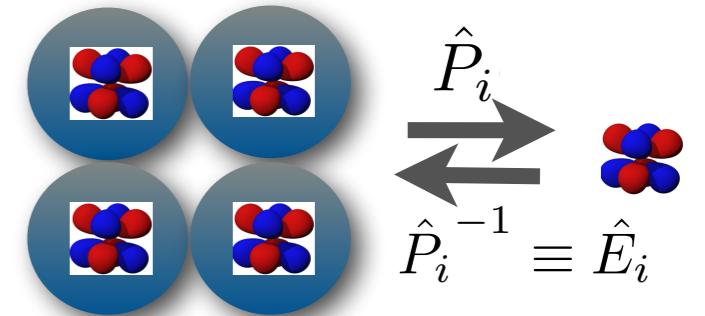
On each correlated site \mathbf{R}_i we have to solve a quantum impurity model with $\alpha\beta$ orbitals

$$\Sigma_{\alpha\beta}^{imp} = \frac{\delta\Phi_{V_{DMFT}}[\{G_{local}^i\}]}{\delta G_{local\beta\alpha}^i}$$

And **Embed** self-energies to continuum space by

$$\langle \mathbf{r} | \phi_\alpha^i \rangle \Sigma_{\alpha\beta}^{imp} \langle \phi_\beta^i | \mathbf{r}' \rangle$$

Notice that once the projector is defined, embedding is uniquely given by the same matrix elements of $\mathcal{P}_{\mathbf{R}_i}(\alpha\beta; \mathbf{rr}') = \phi_\alpha(\mathbf{r} - \mathbf{R}_i)\phi_\beta^*(\mathbf{r}' - \mathbf{R}_i)$



REQUIREMENT FOR STATIONARITY

Projector should not depend on the solution

Return to definition
of the projector:

$$G_{local, \mathbf{R}_i, \alpha\beta} = \int_{\mathbf{r}\mathbf{r}'} \mathcal{P}_{\mathbf{R}_i}(\alpha\beta; \mathbf{r}\mathbf{r}') G(\mathbf{r}\mathbf{r}')$$

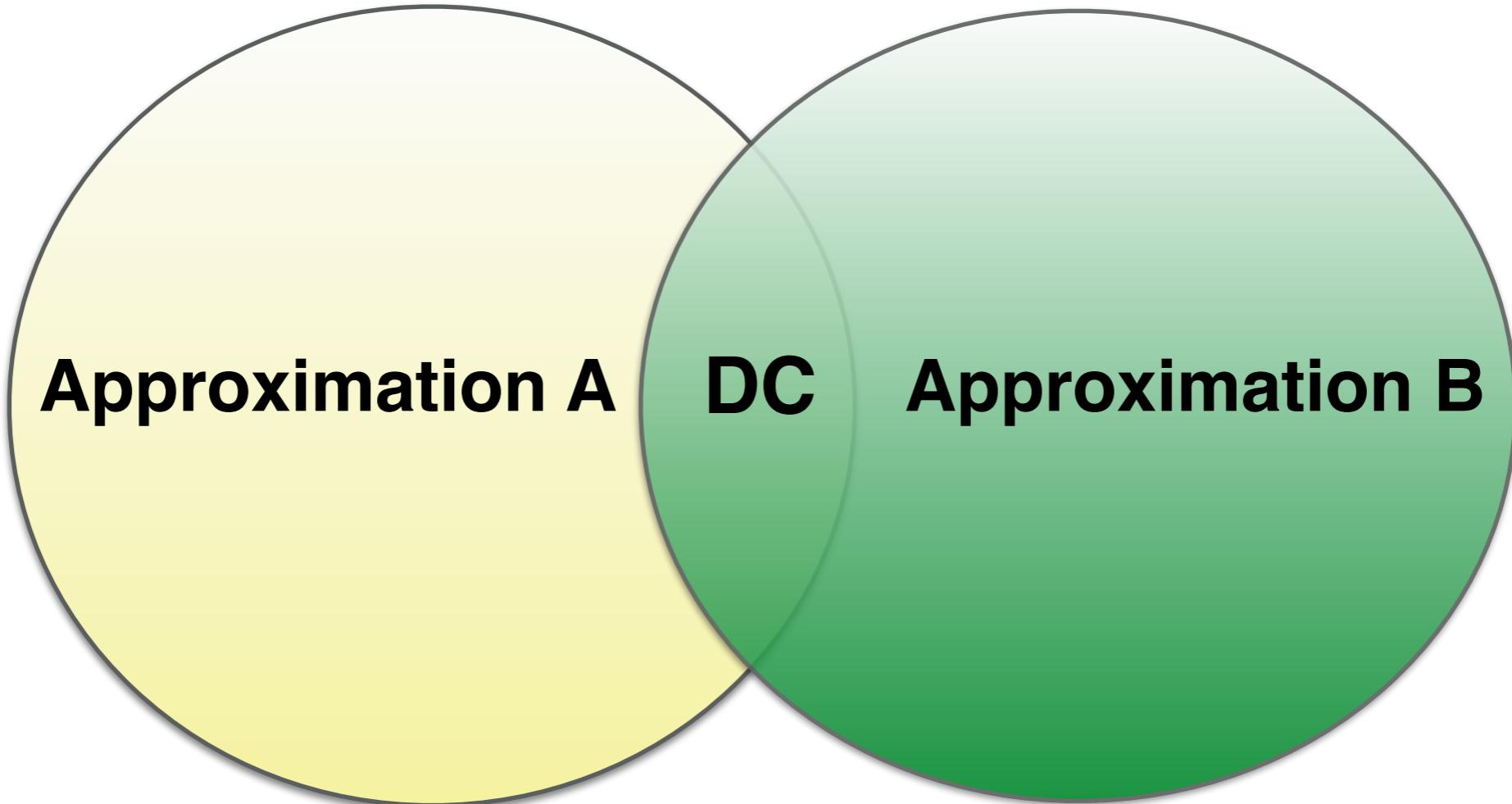
Return to saddle point Eq.:

$$\frac{\delta \Phi^{DMFT}[\{G_{local, \mathbf{R}_i}\}]}{\delta G(\mathbf{r}\mathbf{r}')} = \sum_{\alpha\beta} \frac{\delta G_{local, \mathbf{R}_i, \alpha\beta}}{\delta G(\mathbf{r}\mathbf{r}')} \frac{\delta \Phi[\{G_{local, \mathbf{R}_i}\}]}{\delta G_{local, \mathbf{R}_i, \alpha\beta}} = \sum_{\alpha\beta} \mathcal{P}_{\mathbf{R}_i}(\alpha\beta; \mathbf{r}\mathbf{r}') \frac{\delta \Phi[\{G_{local, \mathbf{R}_i, \alpha\beta}\}]}{\delta G_{local, \mathbf{R}_i, \alpha\beta}}$$

Here we implicitly assumed that $\frac{\delta P}{\delta G} = 0$ or $\frac{\delta \phi_\alpha(\mathbf{r} - \mathbf{R}_i)}{\delta \rho} = 0$
otherwise more complicated terms would appear...

Requirement: $\frac{\delta P}{\delta G} = 0$ is not satisfied with Wannier functions
because they essentially depend on the charge, and hence on G.

Double-Counting



Some part of exchange/correlations counted in both approximations.

Double-Counting

$$\Phi[\{G\}] \xrightarrow{\text{Exact functional approximated}} E_{V_c}^{H+XC}[\{\rho\}] + \sum_{\mathbf{R}_i \in corr} \Phi_{V_{DMFT}}[\{G_{local}^i\}] - \Phi_{V_{DMFT}}^{H+XC}[\{\rho_{local}^i\}]$$

↓ ↓ ↓

LDA functional Sum of all skeleton diagrams
local to correlated ions DC : intersection of DMFT
and LDA approximation

Hartree: $E_{V_C}^H[\{\rho\}] = \frac{1}{2} \int d\mathbf{r} d\mathbf{r}' V_C(|\mathbf{r} - \mathbf{r}'|) \rho(\mathbf{r}) \rho(\mathbf{r}')$

LDA-XC: $\Phi_{V_C}[\{G\}] \rightarrow E_{XC}^{LDA}[\{\rho\}] = \int d\mathbf{r} \rho(\mathbf{r}) \varepsilon_{V_C}^{XC}(\rho(\mathbf{r}))$

DMFT: $\Phi_{V_C}[\{G\}] \rightarrow \Phi_{V_{DMFT}}[\{G_{local}\}]$

?????

Φ_{DMFT} sums all Feyn. graphs (just like the exact Φ)
but uses only G_{local} and screened interaction
instead of full G and V_C

$$V_{DMFT}(\mathbf{r} - \mathbf{r}') = \frac{e^{-\lambda|\mathbf{r} - \mathbf{r}'|}}{|\mathbf{r} - \mathbf{r}'|}$$

example of screened Coulomb repulsion

$$\Phi[G_{local, \mathbf{R}_i}] = \frac{1}{2} + \frac{1}{2} i + \frac{1}{4} i^2 + \dots$$

Double-Counting of Hartree

Exact Hartree:

$$E_{V_C}^H[\rho] = \frac{1}{2} \int d\mathbf{r} d\mathbf{r}' V_C(|\mathbf{r} - \mathbf{r}'|) \rho(\mathbf{r}) \rho(\mathbf{r}')$$

LDA approximation

Exact Hartree Hartree term included

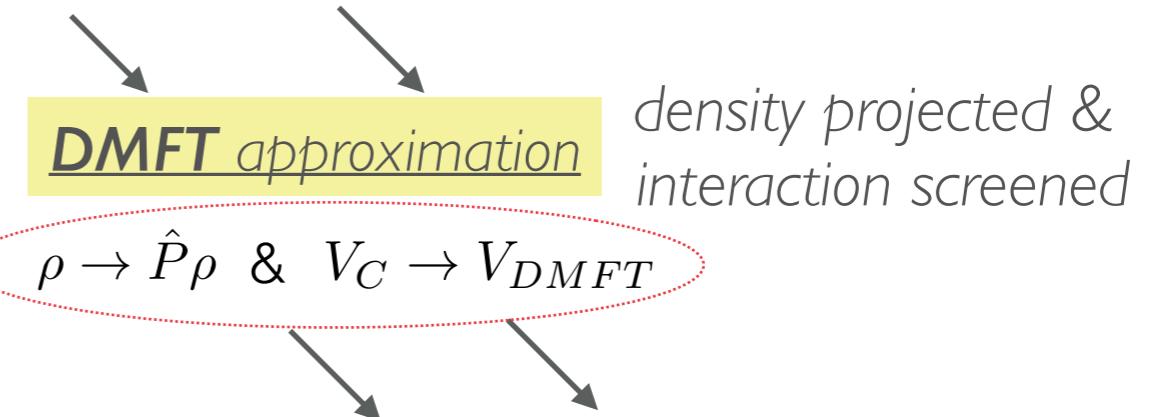
$$E_{V_C}^H[\rho] = \frac{1}{2} \int d\mathbf{r} d\mathbf{r}' V_C(|\mathbf{r} - \mathbf{r}'|) \rho(\mathbf{r}) \rho(\mathbf{r}')$$

$$E_{DMFT}^H[\rho] = \frac{1}{2} \int d\mathbf{r} d\mathbf{r}' (\hat{P}\rho(\mathbf{r}))(\hat{P}\rho(\mathbf{r}')) V_{DMFT}(\mathbf{r} - \mathbf{r}')$$

This approximation for Hartree term appears in Φ^{DMFT}

Double counting to subtract is the DMFT approximation for the Hartree term:

$$\Phi_{DMFT}^{DC, Hartree}[\{\rho\}] = \frac{1}{2} \int d\mathbf{r} d\mathbf{r}' (\hat{P}\rho(\mathbf{r}))(\hat{P}\rho(\mathbf{r}')) V_{DMFT}(\mathbf{r} - \mathbf{r}')$$



density projected &
interaction screened

Double-Counting of Exchange

Exact Exchange:

$$E^X[\rho] = -\frac{1}{2} \int d\mathbf{r} d\mathbf{r}' \rho(\mathbf{r}, \mathbf{r}') \rho(\mathbf{r}', \mathbf{r}) V_C(|\mathbf{r} - \mathbf{r}'|)$$

LDA approximation:

exchange of electron gas,
matching electron density

$$E_F = (2\pi^2 \rho)^{2/3} / (2m) \text{ and}$$

$$\rho_\sigma^0(\mathbf{r}, \mathbf{r}') = \int \frac{d^3 k}{(2\pi)^3} e^{i\mathbf{k}(\mathbf{r}-\mathbf{r}')} f\left(\frac{k^2}{2m} - E_F\right)$$

$$E_{LDA}^X[\rho] = -\frac{1}{2} \int d\mathbf{r} d\mathbf{r}' \rho^0(\mathbf{r}, \mathbf{r}') \rho^0(\mathbf{r}', \mathbf{r}) V_C(|\mathbf{r} - \mathbf{r}'|)$$

$$E_{LDA}^X[\rho] = -\frac{0.9163 \text{ Ry}}{\left(\frac{3}{4\pi} \rho\right)^{1/3}}$$

$$E_{V_{DMFT}}^X[\{\rho\}] = -\frac{1}{2} \int d\mathbf{r} d\mathbf{r}' \left(\sum_{mm'} \langle \mathbf{r} | \phi_m^i \rangle \langle \phi_m^i | \rho | \phi_{m'}^i \rangle \langle \phi_{m'}^i | \mathbf{r}' \rangle \right) \left(\sum_{m''m'''} \langle \mathbf{r}' | \phi_{m''}^i \rangle \langle \phi_{m''}^i | \rho | \phi_{m'''}^i \rangle \langle \phi_{m'''}^i | \mathbf{r} \rangle \right) V_{DMFT}(\mathbf{r} - \mathbf{r}')$$

$$= -\frac{1}{2} \sum_{m, m', m'', m'''} \langle \phi_m^i | \rho | \phi_{m'}^i \rangle \langle \phi_{m''}^i | \rho | \phi_{m'''}^i \rangle \int d\mathbf{r} d\mathbf{r}' \phi_{m'''}^{i*}(\mathbf{r}) \phi_{m'}^{i*}(\mathbf{r}') V_{DMFT}(\mathbf{r} - \mathbf{r}') \phi_{m''}^i(\mathbf{r}') \phi_m^i(\mathbf{r})$$

$$= -\frac{1}{2} \sum_{m, m', m'', m'''} \rho_{mm'}^i \rho_{m''m'''}^i \langle \phi_{m'''}^i | V_{DMFT} | \phi_{m''}^i \phi_m^i \rangle$$

DMFT approximation

$$\rho \rightarrow \hat{P}\rho \text{ & } V_C \rightarrow V_{DMFT}$$

density projected &
interaction screened

Double-Counting of Exchange

Exact Exchange:

$$E^X[\rho] = -\frac{1}{2} \int d\mathbf{r} d\mathbf{r}' \rho(\mathbf{r}, \mathbf{r}') \rho(\mathbf{r}', \mathbf{r}) V_C(|\mathbf{r} - \mathbf{r}'|)$$

LDA approximation:

exchange of electron gas,
matching electron density

$$E_F = (2\pi^2 \rho)^{2/3} / (2m) \text{ and}$$

$$\rho_\sigma^0(\mathbf{r}, \mathbf{r}') = \int \frac{d^3 k}{(2\pi)^3} e^{i\mathbf{k}(\mathbf{r}-\mathbf{r}')} f\left(\frac{k^2}{2m} - E_F\right)$$

$$E_{LDA}^X[\rho] = -\frac{1}{2} \int d\mathbf{r} d\mathbf{r}' \rho^0(\mathbf{r}, \mathbf{r}') \rho^0(\mathbf{r}', \mathbf{r}) V_C(|\mathbf{r} - \mathbf{r}'|)$$

DMFT approximation

$$\rho \rightarrow \hat{P}\rho \quad \& \quad V_C \rightarrow V_{DMFT}$$

$$E_{V_{DMFT}}^X[\rho] = -\frac{1}{2} \int d\mathbf{r} d\mathbf{r}' (\hat{P}\rho(\mathbf{r}, \mathbf{r}')) (\hat{P}\rho(\mathbf{r}', \mathbf{r})) V_{DMFT}(|\mathbf{r} - \mathbf{r}'|)$$

density projected &
interaction screened

Result is: $\Phi^{DC,X} = -\frac{1}{2} \int d\mathbf{r} d\mathbf{r}' \rho^0(\mathbf{r}, \mathbf{r}') \rho^0(\mathbf{r}', \mathbf{r}) V_{DMFT}(\mathbf{r} - \mathbf{r}')$

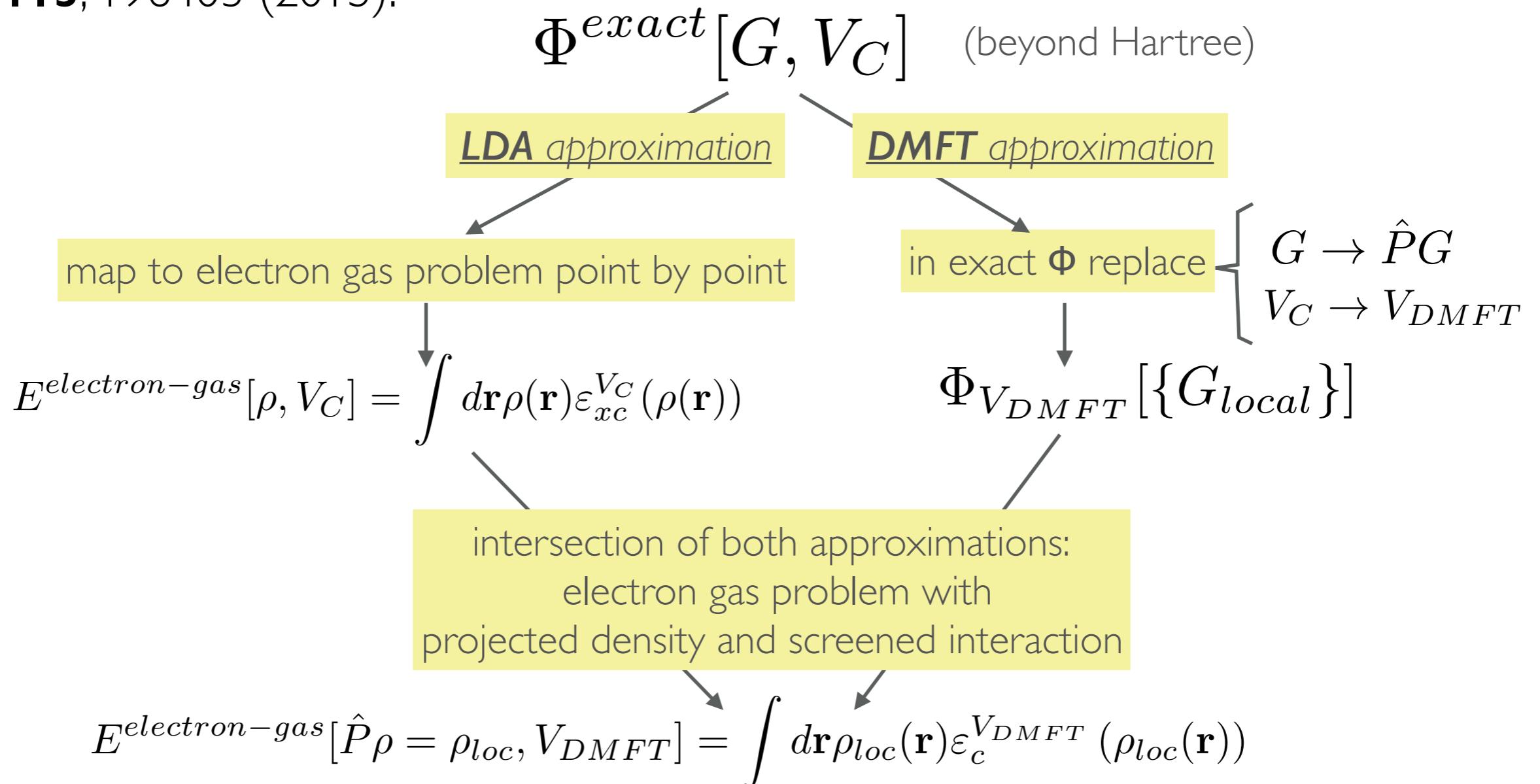
$$\rho^0(\mathbf{r}, \mathbf{r}') = \int \frac{d^3 k}{(2\pi)^3} e^{i\mathbf{k}(\mathbf{r}-\mathbf{r}')} f\left(\frac{k^2}{2m} - E_F\right) \quad E_F = \left(2\pi^2 (\hat{P}\rho)^{2/3}\right) / (2m)$$

Intersection of both approximations: apply **both approximations** to the functional

- 1) Interaction is screened in DC term
- 2) Use projected density in DC term
- 3) Replace exact expression by electron gas expression

Double-Counting of Correlations

KH, PRL **115**, 196403 (2015).



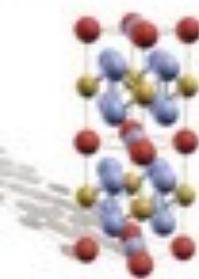
Double counting:

$$\Phi^{DC}[\rho_{local}] = \frac{1}{2} \int d\mathbf{r} d\mathbf{r}' \rho_{local}(\mathbf{r}) V_{DMFT}(\mathbf{r} - \mathbf{r}') \rho_{local}(\mathbf{r}') +$$

$$+ \int d\mathbf{r} \rho_{local}(\mathbf{r}) \epsilon_{xc}^{V_{DMFT}} [\rho_{local}(\mathbf{r})]$$

electron gas interacting with screened Coulomb interaction

Stationary Free Energy Functional



$$\delta\Gamma[G]/\delta G = 0$$

For numeric stability, the stationary DFT+DMFT functional is needed but the implementation is challenging.

$$\Gamma[G] = \text{Tr} \log G - \text{Tr}[(G_0^{-1} - G^{-1})G] + E^H[\rho] + E^{xc}[\rho] + \Phi^{\text{DMFT}}[\hat{P}G] - \Phi^{\text{DC}}[\hat{P}\rho] + E_{\text{nuc-nuc}}$$

↑
Can be computed from frequency dependent band structure $\varepsilon_{\mathbf{k}\omega_n,i}$

↑
Very hard to compute

Idea : Use the free energy F_{imp} of the auxiliary impurity problem:

$$F_{imp} = \text{Tr} \log G_{imp} - \text{Tr}(\Sigma_{imp} G_{imp}) + \Phi[G_{imp}] \quad \text{and} \quad \Phi[G_{imp}] == \Phi[\hat{P}G]$$

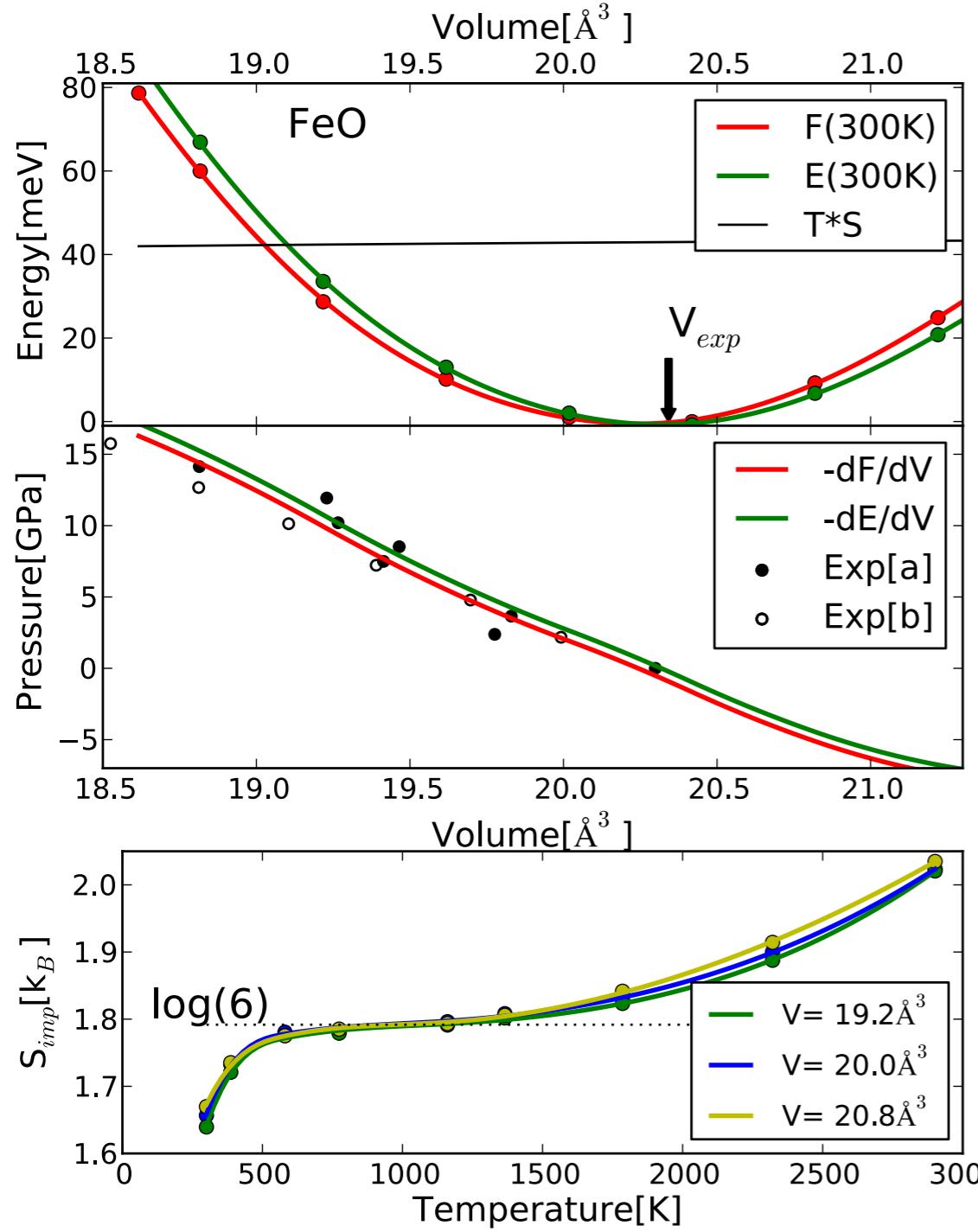
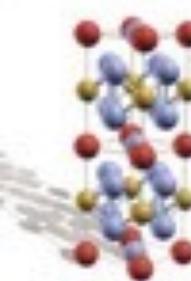
$$F_{solid} = F_{imp} + \text{Tr} \log G - \text{Tr} \log G_{imp} + E^H + E^{XC} + E_{nuc-nuc} - \Phi^{DC}[\{\hat{P}\rho\}]$$

For the impurity problem we can compute with CTQMC very precisely all necessary quantities

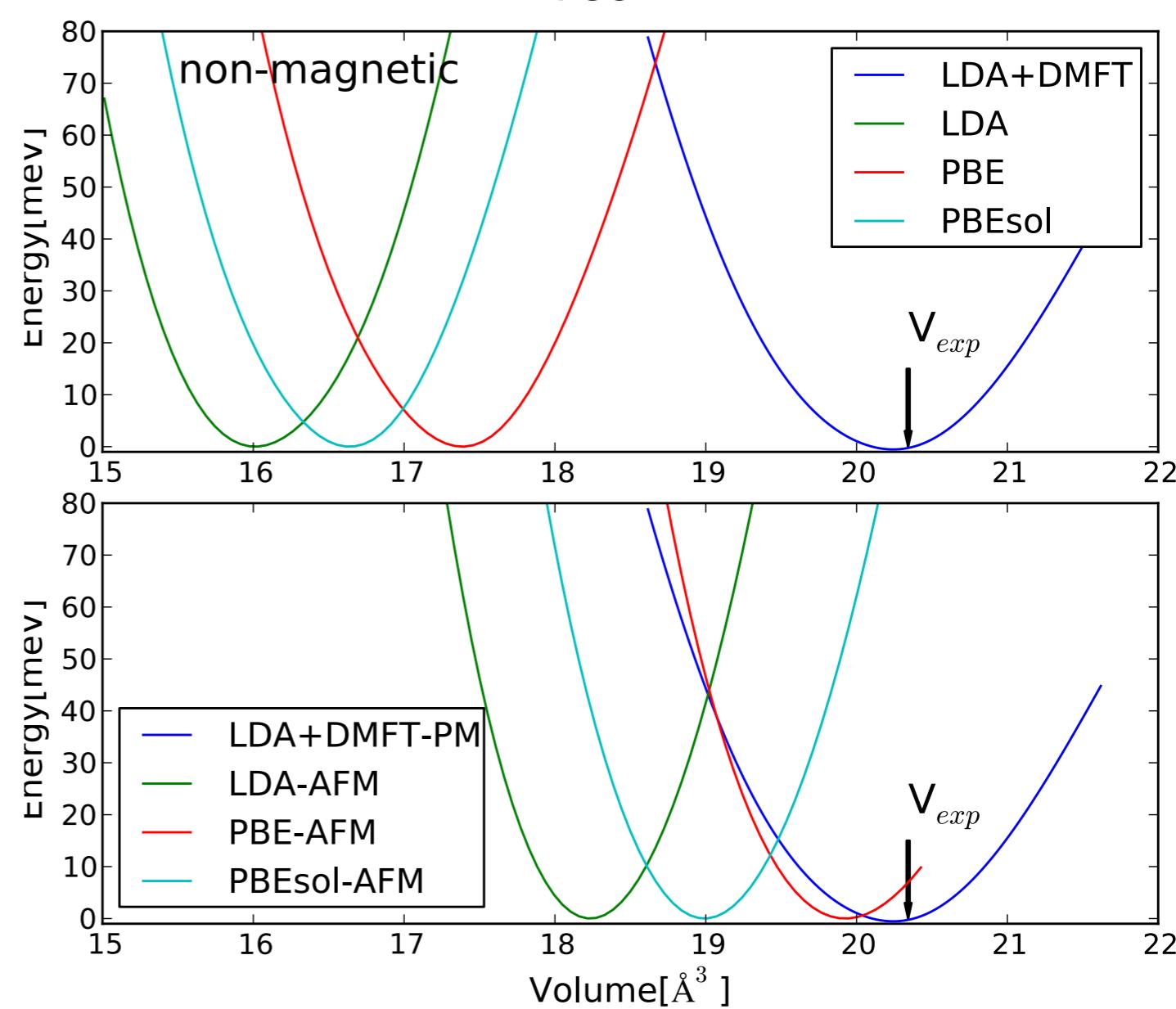
$$F_{imp} = \text{Tr}((\Delta + \varepsilon_{imp} - \omega_n \frac{d\Delta}{d\omega_n})G_{imp}) + E_{imp}^{\text{potential}} - T S_{imp}$$

$$S_{imp}(T) = S_{imp}(T_>) - \frac{E_{imp}(T_>)}{T_>} + \frac{E_{imp}(T)}{T} - \int_{1/T_>}^{1/T} E_{imp}(1/\beta) d\beta$$

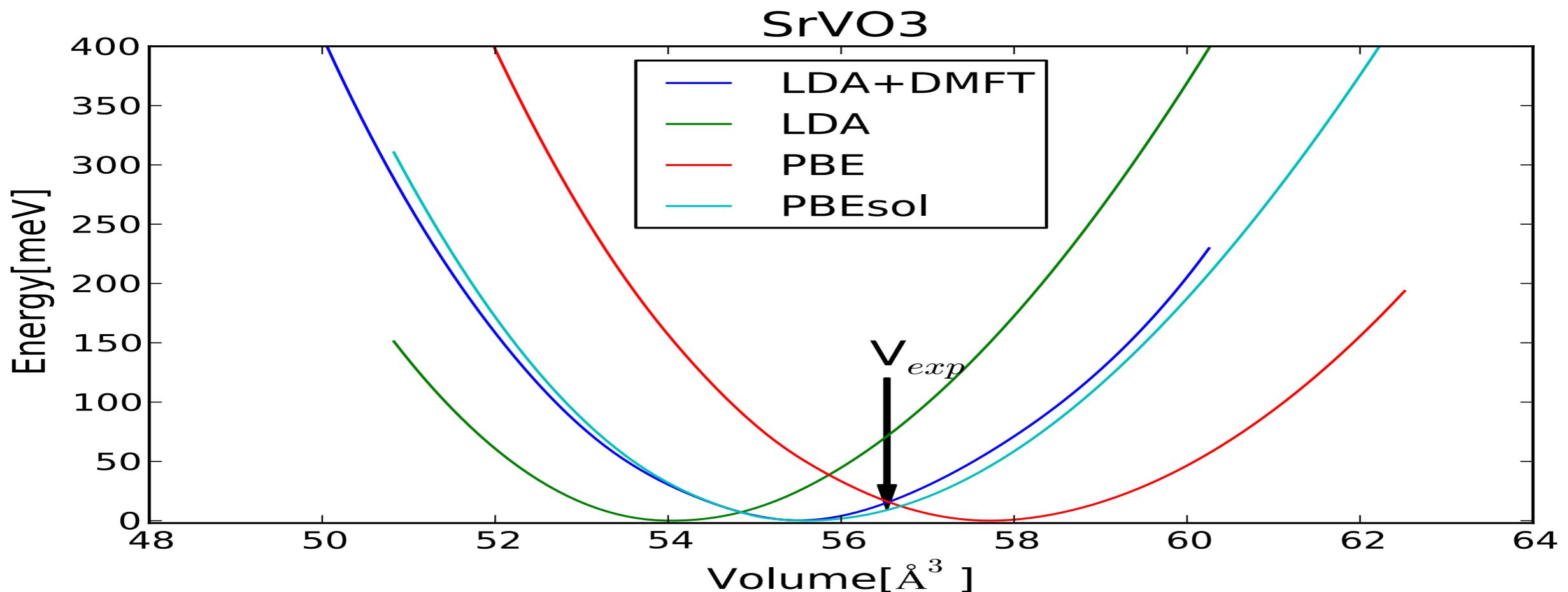
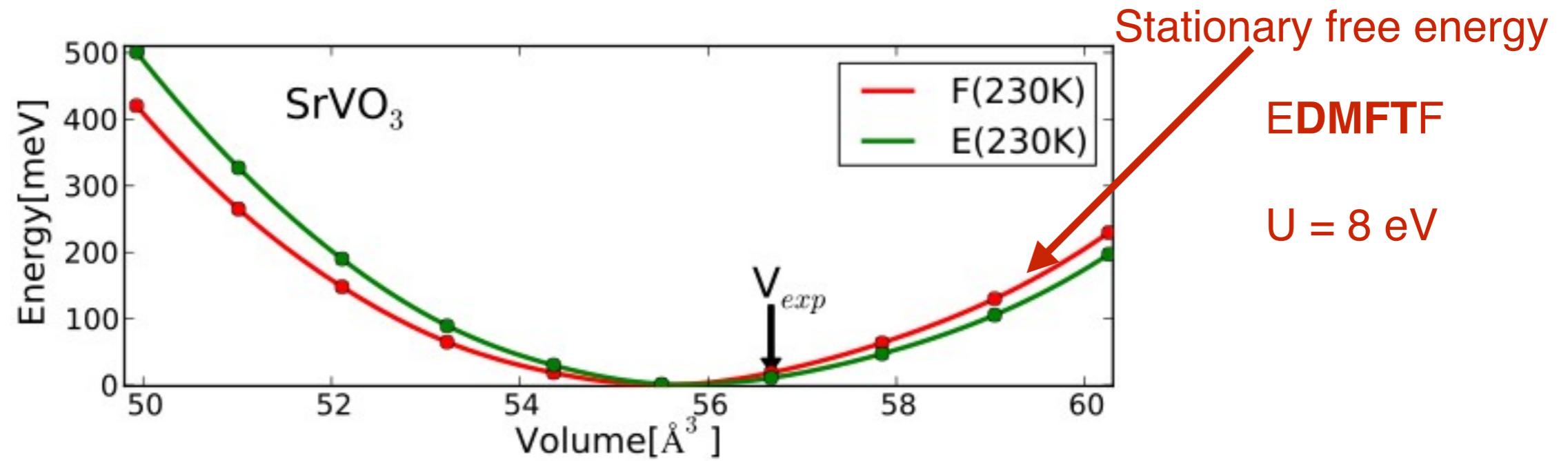
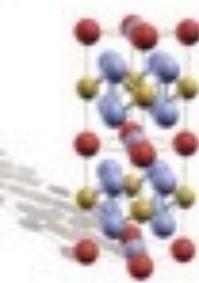
paramagnetic Mott insulator FeO



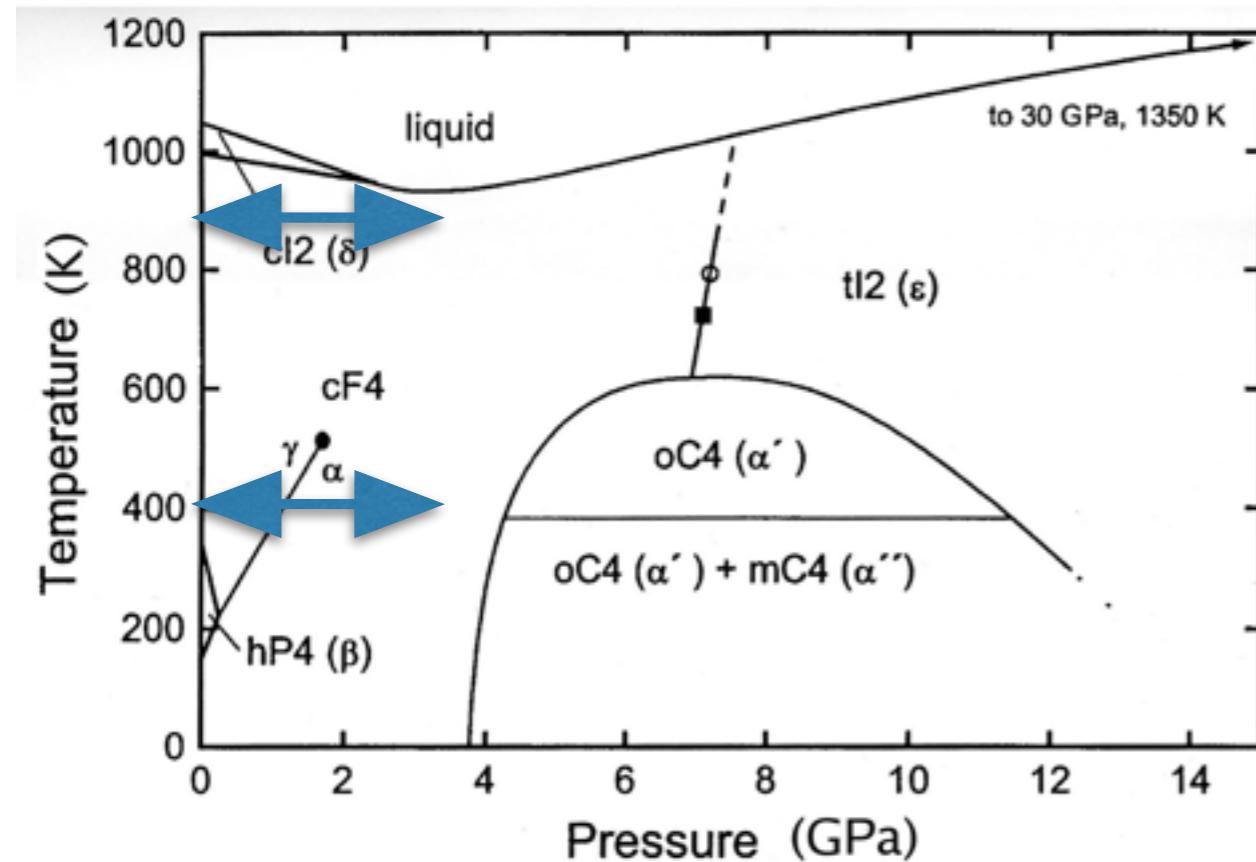
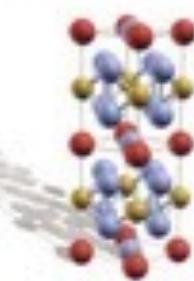
comparison with other functionals



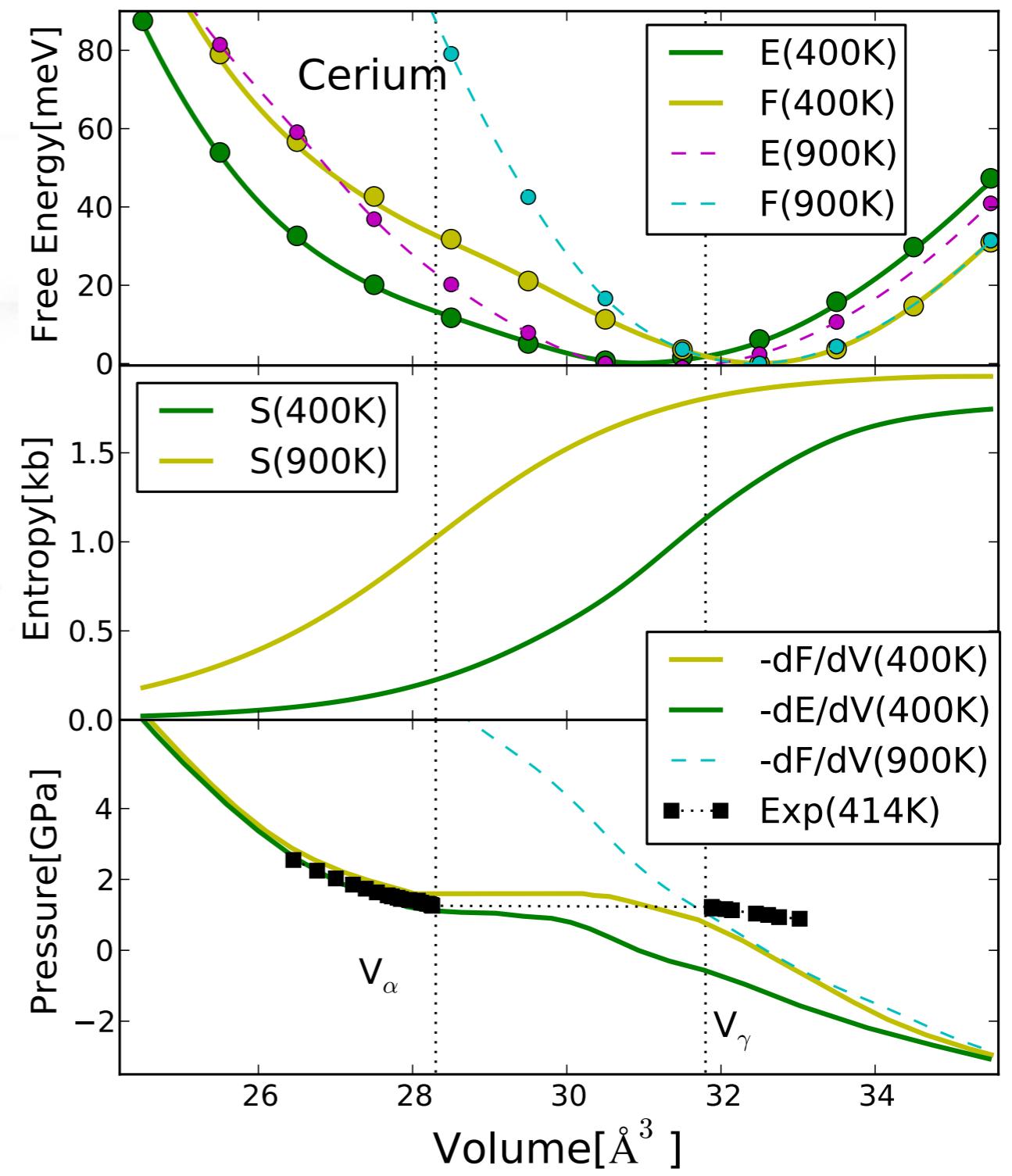
Example SrVO₃



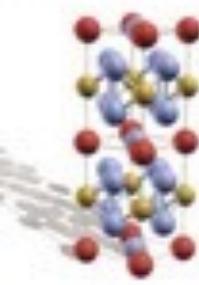
Isostructural transition in elemental Cerium



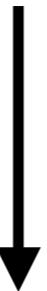
First order (entropy driven) transition



Embedded Dynamical Mean Field Theory Functional



Stationary **Embedded DMFT** functional extremized in real space.

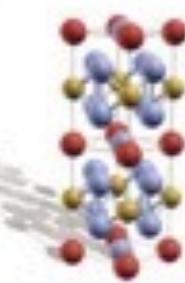


Free energy functional can be **analytically differentiated** to give forces on all atoms.



Can predict complex crystal structures

Force on all atoms from derivative of the functional



$$\frac{\delta \Gamma[G]}{\delta \mathbf{R}_\mu} = \frac{\delta G}{\delta \mathbf{R}_\mu} \left(\frac{\partial \Gamma[G]}{\partial G} \right)_{R_\mu} + \left(\frac{\partial \Gamma[G]}{\partial \mathbf{R}_\mu} \right)_G$$

vanishes

$$\begin{aligned} \frac{\delta \Gamma[\{G\}]}{\delta \mathbf{R}_\mu} &= \frac{\partial}{\partial \mathbf{R}_\mu} \left(\text{Tr} \log(G) - \text{Tr}((G_0^{-1} - G^{-1})G) + \Phi[\{G\}] + E_{nuc-nuc} \right)_G \\ &= \frac{\partial}{\partial \mathbf{R}_\mu} \left(-\text{Tr} \left([i\omega + \mu + \nabla^2 - V_{nuc}(\mathbf{r})] \delta(\mathbf{r} - \mathbf{r}') G \right) + E_{nuc-nuc} \right) \\ &= \text{Tr} \left(\rho \frac{\partial}{\partial \mathbf{R}_\mu} V_{nuc} \right) + \frac{\partial}{\partial \mathbf{R}_\mu} E_{nuc} \end{aligned}$$



$$\mathbf{F}^{HF} = -\text{Tr} \left(\rho \frac{\partial V_{nuc}}{\partial \mathbf{R}_\mu} \right) - \frac{\partial E_{nuc}}{\partial \mathbf{R}_\mu}$$

The Hellman-Feynman force

Force on all atoms from derivative of the functional

But the LAPW basis set, and
the DMFT projector, are not → “**Pulay forces**” appear
fixed in space, but rather
move with the atom.

We need to differentiate the implemented
expression for the free energy.

Free energy expression again

Recall:

$$\Gamma[\{G\}] = \text{Tr} \log G - \text{Tr}((G_0^{-1} - G^{-1})G) + E_{V_C}^{H+XC}[\rho] + \sum_{\mathbf{R}_i \in corr} \Phi_{V_{DMFT}}^{DMFT}[G_{loc}^i] - \Phi_{V_{DMFT}}^{DC}[\rho_{loc}^i]$$

at the DMFT solution the Dyson Eq. is satisfied

$$G^{-1} = G_0^{-1} - V_{H+XC}(\mathbf{r})\delta(\mathbf{r} - \mathbf{r}')\delta(\tau - \tau') - \langle \mathbf{r} | \phi_\alpha^i \rangle (\Sigma^{imp} - V^{DC})_{\alpha\beta} \langle \phi_\beta^i | \mathbf{r}' \rangle$$

hence the free can be computed by

$$F = \text{Tr} \log(G) - \text{Tr}(V_{H+XC})\rho + E_{V_C}^{H+XC}[\rho] + \sum_{\mathbf{R}_i} \left\{ -\text{Tr}((\Sigma^{imp} - V^{DC})G_{loc}^i) + \Phi_{V_{DMFT}}^{DMFT}[G_{loc}^i] - \Phi_{V_{DMFT}}^{DC}[\rho_{loc}^i] \right\}$$

nuclear-nuclear energy is added;
canonical ensemble needs $+ \mu N$

Free energy expression implementation

To implement $\text{Tr} \log G$ we compute generalized Kohn-Sham orbitals:

$$\langle \psi_{j\mathbf{k}\omega_n} | \left(T + V_{nuc} + V_{H+XC} + \sum_{mm', \mathbf{R}_\mu} |\phi_m^\mu\rangle \langle \phi_m^\mu| \Sigma_{i\omega_n} - V_{DC} |\phi_{m'}^\mu\rangle \langle \phi_{m'}^\mu| \right) | \psi_{i\mathbf{k}\omega_n} \rangle = \delta_{ij} \varepsilon_{\mathbf{k}\omega_n, i}$$

so that $\langle \psi_{j\mathbf{k}\omega_n} | G | \psi_{i\mathbf{k}\omega_n} \rangle = \frac{\delta_{ij}}{i\omega_n + \mu - \varepsilon_{\mathbf{k}\omega_n, i}}$, i.e., G is diagonalized

then

$$\text{Tr} \log(-G) = -\text{Tr} \log(-i\omega_n - \mu + \varepsilon_{\mathbf{k}\omega_n})$$

and

$$\begin{aligned} F = & -\text{Tr} \log(-i\omega_n - \mu + \varepsilon_{\mathbf{k}\omega_n}) - \text{Tr}(V_{H+XC})\rho + E^{H+XC}[\rho] + E_{nuc-nuc} + \mu N \\ & + \sum_{\mathbf{R}_i} \left\{ -\text{Tr}((\Sigma - V_{DC})G_{loc}^i) + \Phi^{DMFT}[G_{loc}^i] - \Phi^{DC}[\rho_{loc}^i] \right\} \end{aligned}$$

Derivative of the free energy

The free energy :

$$F = \underbrace{-\text{Tr} \log(-i\omega_n - \mu + \varepsilon_{\mathbf{k}\omega_n})}_{+ \sum_{\mathbf{R}_i} \left\{ \underbrace{-\text{Tr}((\Sigma - V_{DC})G_{loc}^i)}_{-\text{Tr}(\rho \frac{\delta V_{H+XC}}{\delta \mathbf{R}_\mu})} + \Phi^{DMFT}[G_{loc}^i] - \Phi^{DC}[\rho_{loc}^i] \right\}} + \underbrace{E^{H+XC}[\rho]}_{-\text{Tr}(G_{loc} \frac{\delta \Sigma - \delta V_{DC}}{\delta \mathbf{R}_\mu})} + \underbrace{E_{nuc-nuc}}_{-\text{Tr}(G_{loc} \frac{\delta \Sigma + \delta V_{DC}}{\delta \mathbf{R}_\mu})} + \underbrace{\mu N}_{\frac{\delta \mu}{\delta \mathbf{R}_\mu}}$$

$$\frac{\delta F}{\delta \mathbf{R}_\mu} = \text{Tr} \left(\frac{1}{i\omega + \mu - \varepsilon_{\mathbf{k}\omega_n}} \frac{\delta(\varepsilon_{\mathbf{k}\omega_n} - \mu)}{\delta \mathbf{R}_\mu} \right) - \text{Tr}(\rho \frac{\delta V_{H+XC}}{\delta \mathbf{R}_\mu}) + \frac{\delta E_{nuc-nuc}}{\delta \mathbf{R}_\mu} + N \frac{\delta \mu}{\delta \mathbf{R}_\mu}$$

$$\frac{\delta F}{\delta \mathbf{R}_\mu} = \text{Tr} \left(\frac{1}{i\omega + \mu - \varepsilon_{\mathbf{k}\omega_n}} \frac{\delta(\varepsilon_{\mathbf{k}\omega_n})}{\delta \mathbf{R}_\mu} \right) - \text{Tr}(\rho \frac{\delta(V_{KS})}{\delta \mathbf{R}_\mu}) - \text{Tr}(G_{loc} \frac{\delta \Sigma + \delta V_{DC}}{\delta \mathbf{R}_\mu})$$

Recall: $F^{HF} = -\text{Tr}(\rho \frac{\partial V_{nuc}}{\partial \mathbf{R}_\mu}) - \frac{\partial E_{nuc}}{\partial \mathbf{R}_\mu}$

Derivative of the free energy

$$\mathbf{F}_\mu^{Poly} = -\text{Tr} \left(\frac{1}{i\omega_n + \mu - \varepsilon_{\mathbf{k}\omega_n}} \frac{\delta \varepsilon_{\mathbf{k}\omega_n}}{\delta \mathbf{R}_\mu} \right) + \text{Tr} \left(\rho \frac{\delta V_{KS}}{\delta \mathbf{R}_\mu} \right) + \text{Tr} \left(G_{loc} \frac{\delta \Sigma - \delta V_{DC}}{\delta \mathbf{R}_\mu} \right)$$

$\delta\Sigma(\omega)$ very hard to compute.

appears in two terms.

But: Functional is stationary, and $\delta\Sigma(\omega)$ cancel out.

Derivative of the free energy

To prove that $\delta(\Sigma - V_{DC})$ cancels, we recall eigenvalue Eq.

$$\langle \psi_{i\mathbf{k}\omega_n} | \left(T + V_{nuc} + V_{H+XC} + \sum_{mm', \mathbf{R}_\mu} |\phi_m^\mu\rangle \langle \phi_m^\mu| \Sigma_{i\omega_n} - V_{DC} |\phi_{m'}^\mu\rangle \langle \phi_{m'}^i| \right) - \varepsilon_{\mathbf{k}\omega_n, i} |\psi_{i\mathbf{k}\omega_n}\rangle = 0$$

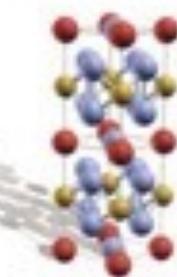
which is satisfied for each atomic position \mathbf{R}_μ hence

$$\langle \psi_{i\mathbf{k}\omega_n} | \left(\delta(T + V_{nuc} + V_{H+XC}) + \sum_{mm', \mathbf{R}_\mu} \delta(|\phi_m^\mu\rangle \langle \phi_m^\mu| \Sigma_{i\omega_n} - V_{DC} |\phi_{m'}^\mu\rangle \langle \phi_{m'}^i|) \right) - \delta\varepsilon_{\mathbf{k}\omega_n, i} |\psi_{i\mathbf{k}\omega_n}\rangle = 0$$

therefore $\delta\varepsilon_{\mathbf{k}\omega_n, i} = \sum_{\mathbf{R}_\mu, mm'} \langle \psi_{i\mathbf{k}\omega_n} | \phi_m^\mu \rangle \langle \phi_m^\mu | \delta(\Sigma - V_{DC}) | \phi_{m'}^\mu \rangle \langle \phi_{m'}^\mu | \psi_{i\mathbf{k}\omega_n} \rangle + \dots$
+derivative of the projector+DFT terms

hence

$$\begin{aligned} \text{Tr}\left(\frac{\delta\varepsilon_{\mathbf{k}\omega_n}}{i\omega + \mu - \varepsilon_{\mathbf{k}\omega_n}}\right) &= \text{Tr}(|\psi_{i\mathbf{k}\omega_n}\rangle \frac{1}{i\omega + \mu - \varepsilon_{\mathbf{k}\omega_n}} \langle \psi_{i\mathbf{k}\omega_n}| \sum_{\mathbf{R}_\mu, mm'} |\phi_m^\mu\rangle \langle \phi_m^\mu| \delta(\Sigma - V_{DC}) |\phi_{m'}^\mu\rangle \langle \phi_{m'}^\mu|) + \dots \\ &= \text{Tr}(G \sum_{\mathbf{R}_\mu, mm'} |\phi_m^\mu\rangle \langle \phi_m^\mu| \delta(\Sigma - V_{DC}) |\phi_{m'}^\mu\rangle \langle \phi_{m'}^\mu|) + \dots \\ \mathbf{F}_\mu^{Poly} &= -\text{Tr}\left(\frac{1}{i\omega_n + \mu - \varepsilon_{\mathbf{k}\omega_n}} \frac{\delta\varepsilon_{\mathbf{k}\omega_n}}{d\mathbf{R}_\mu}\right) + \text{Tr}\left(\rho \frac{\delta V_{KS}}{\delta \mathbf{R}_\mu}\right) + \text{Tr}\left(G_{loc} \frac{\delta\Sigma - \delta V_{DC}}{\delta \mathbf{R}_\mu}\right) \\ &= \text{Tr}(G_{loc} \delta(\Sigma - V_{DC})) + \dots \end{aligned}$$



Final results for forces in a mixed basis set

Pulay force in mixed basis:

DFT-like terms

$$\mathbf{F}_\mu^{Pulay} = -\text{Tr} \left(\tilde{\rho} A^{0\dagger} \frac{\delta H^0}{\delta \mathbf{R}_\mu} A^0 - (\widetilde{\rho\varepsilon}) A^{0\dagger} \frac{\delta O}{\delta \mathbf{R}_\mu} A^0 \right) + \text{Tr} \left(\rho \frac{\delta V_{KS}}{\delta \mathbf{R}_\mu} \right)$$

$$-\frac{1}{\beta} \sum_{i\omega_n} \sum_{\mathbf{KK}', m'm} \bar{G}_{\mathbf{KK}'} (\Sigma - V_{DC})_{m'm} \frac{\delta (\langle \chi_{\mathbf{K}'} | \phi_{m'} \rangle \langle \phi_m | \chi_{\mathbf{K}} \rangle)}{\delta \mathbf{R}_\mu}$$

derivative of the DMFT projector, because
the DMF basis moves with the atom

depends on the DMFT density matrices

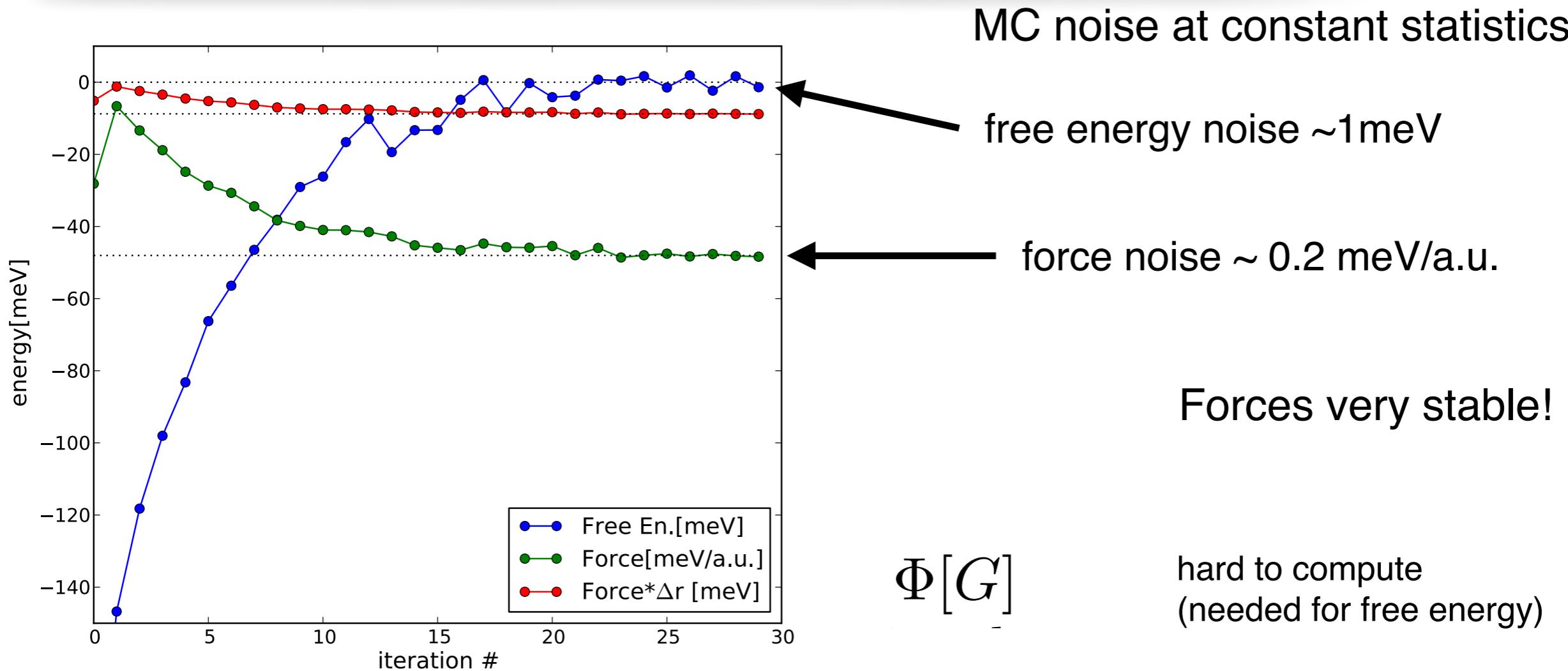
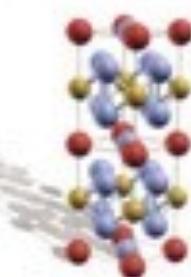
$$\tilde{\rho} \equiv \frac{1}{\beta} \sum_{i\omega_n} B_{\omega_n}^R \frac{1}{i\omega_n + \mu - \varepsilon_{\mathbf{k}\omega_n}} B_{\omega_n}^L$$

$$(\widetilde{\rho\varepsilon}) \equiv \frac{1}{\beta} \sum_{i\omega_n} B_{\omega_n}^R \frac{\varepsilon_{\mathbf{k}\omega_n}}{i\omega_n + \mu - \varepsilon_{\mathbf{k}\omega_n}} B_{\omega_n}^L$$

Success: Forces do not depend on $\Phi[G]$ or $\delta\Sigma/\delta G = \delta^2\Phi/\delta G^2$

which are hard to compute.

Forces more stable than free energies

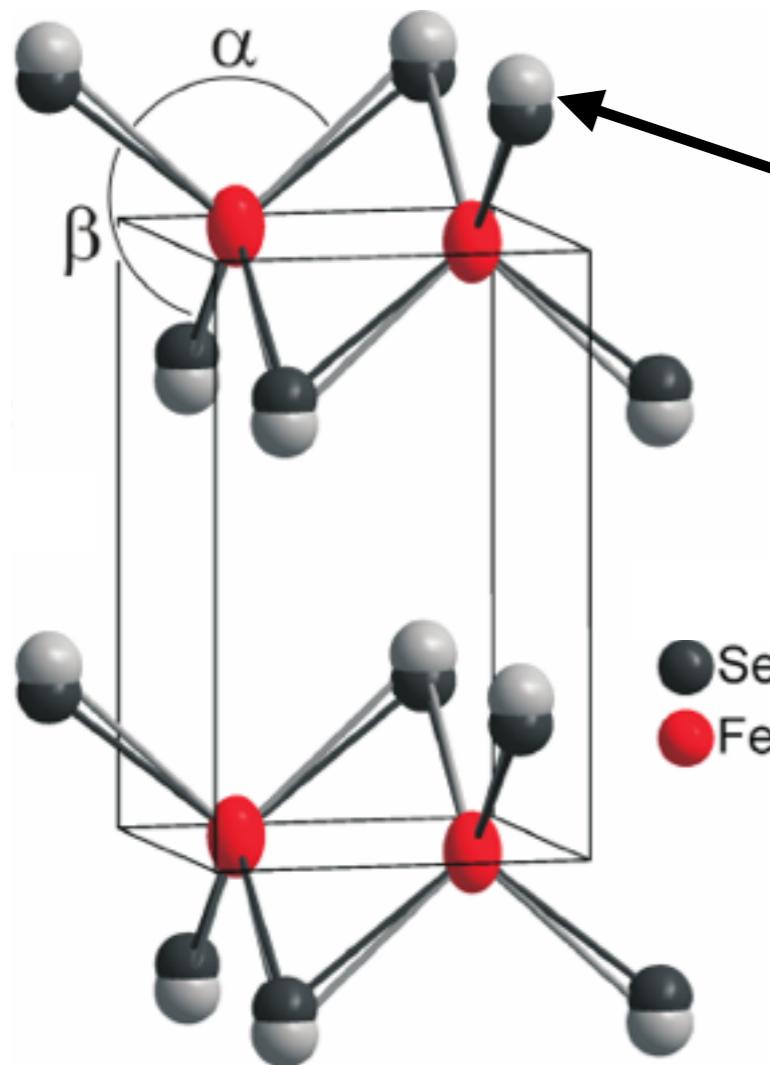
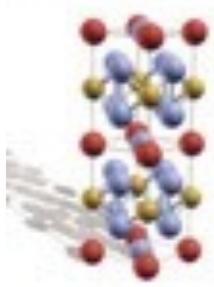


$$\Sigma = \delta\Phi[G]/\delta G$$

easy to compute
only this is needed for the force

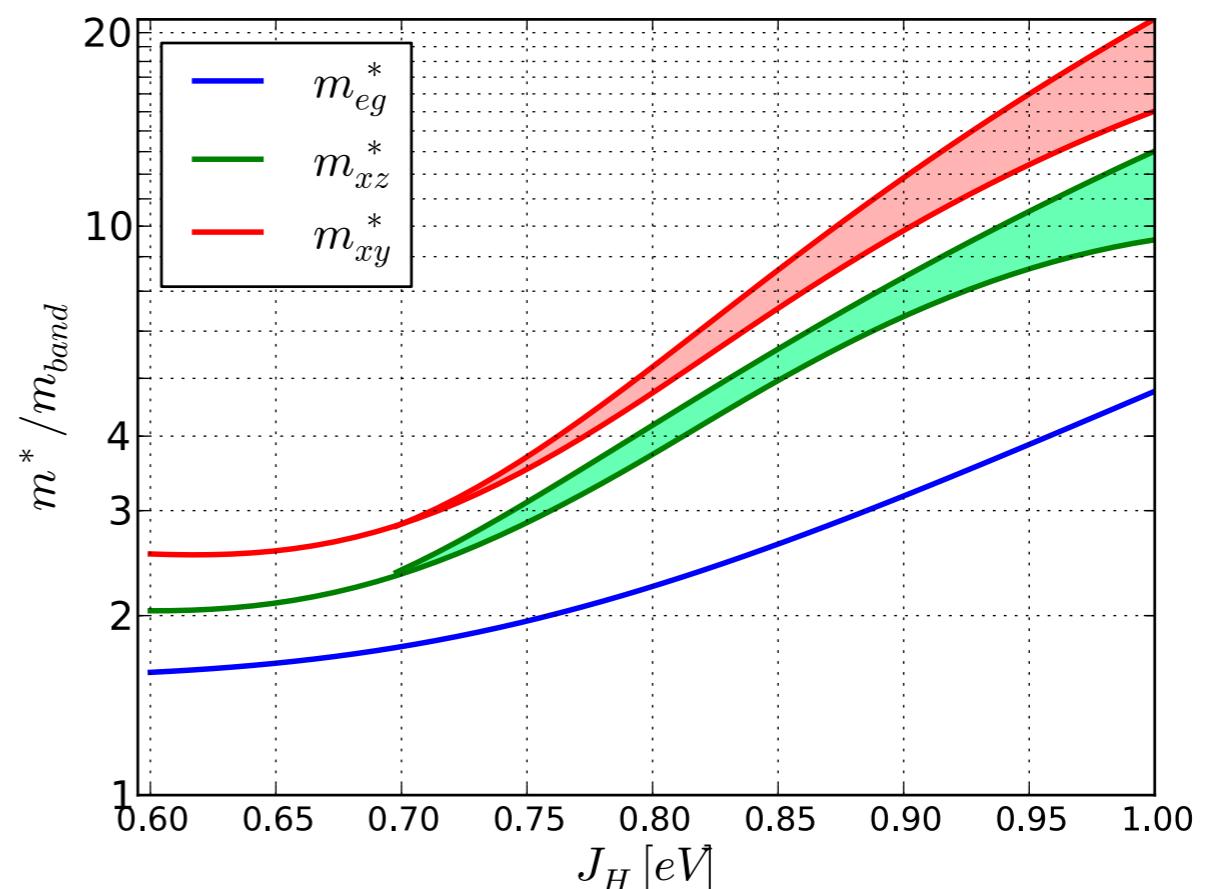
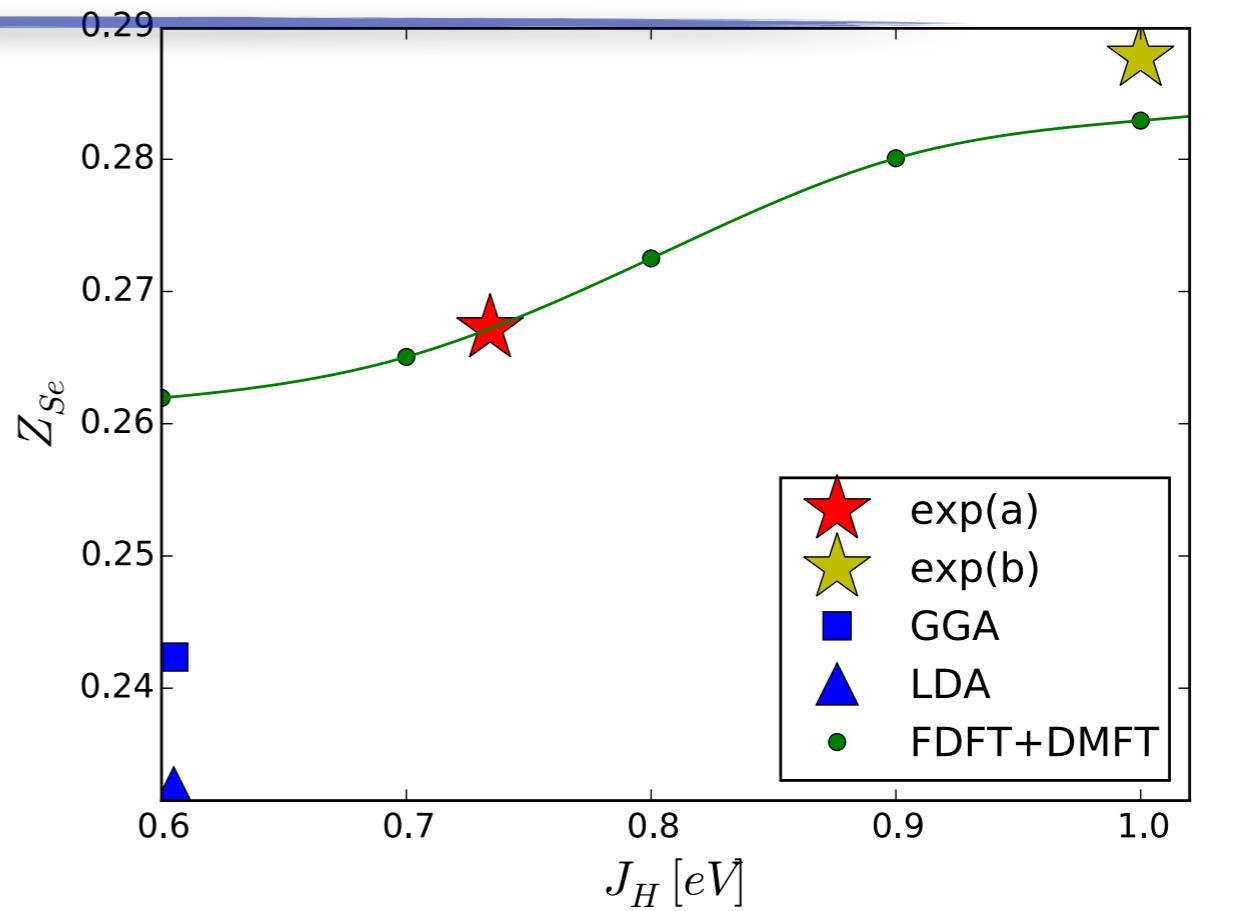
$\delta^2 \Phi[G]/\delta G^2$ hard to compute
(needed for dynamical matrix)

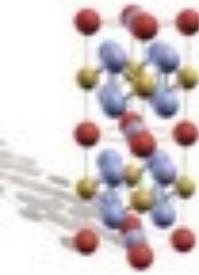
Optimizing FeSe structure - Hunds metal



exp(a): T. M. McQueen, ... R.J.Cava, PRB 79, 014522 (2009).

exp(b): R. S. Kumar, ... C. Chen, The Journal of Physical Chemistry B 114, 12597 (2010).





Electronic structure package: EDMFTF

Download: <http://hauleweb.rutgers.edu/tutorials>

Some tutorials:

DMFT_W2K Tutorials and Installation Instructions

- [Installation](#)
- [Overview](#)
- [Tutorial on single band Hubbard model](#)
- [Tutorial 1 on SrVO₃](#)
- [Tutorial 2 on LaVO₃](#)
- [Tutorial 3 on elemental Cerium](#)
- [Tutorial 4 on Sr₂IrO₄](#)

- Projection & Embedding instead of downloading in the full potential (APW+lo,LAPW) basis.
- Continuous time quantum Monte Carlo, OCA, NCA...
- Stationary implementation of free energy
- Forces on all atoms



Database:

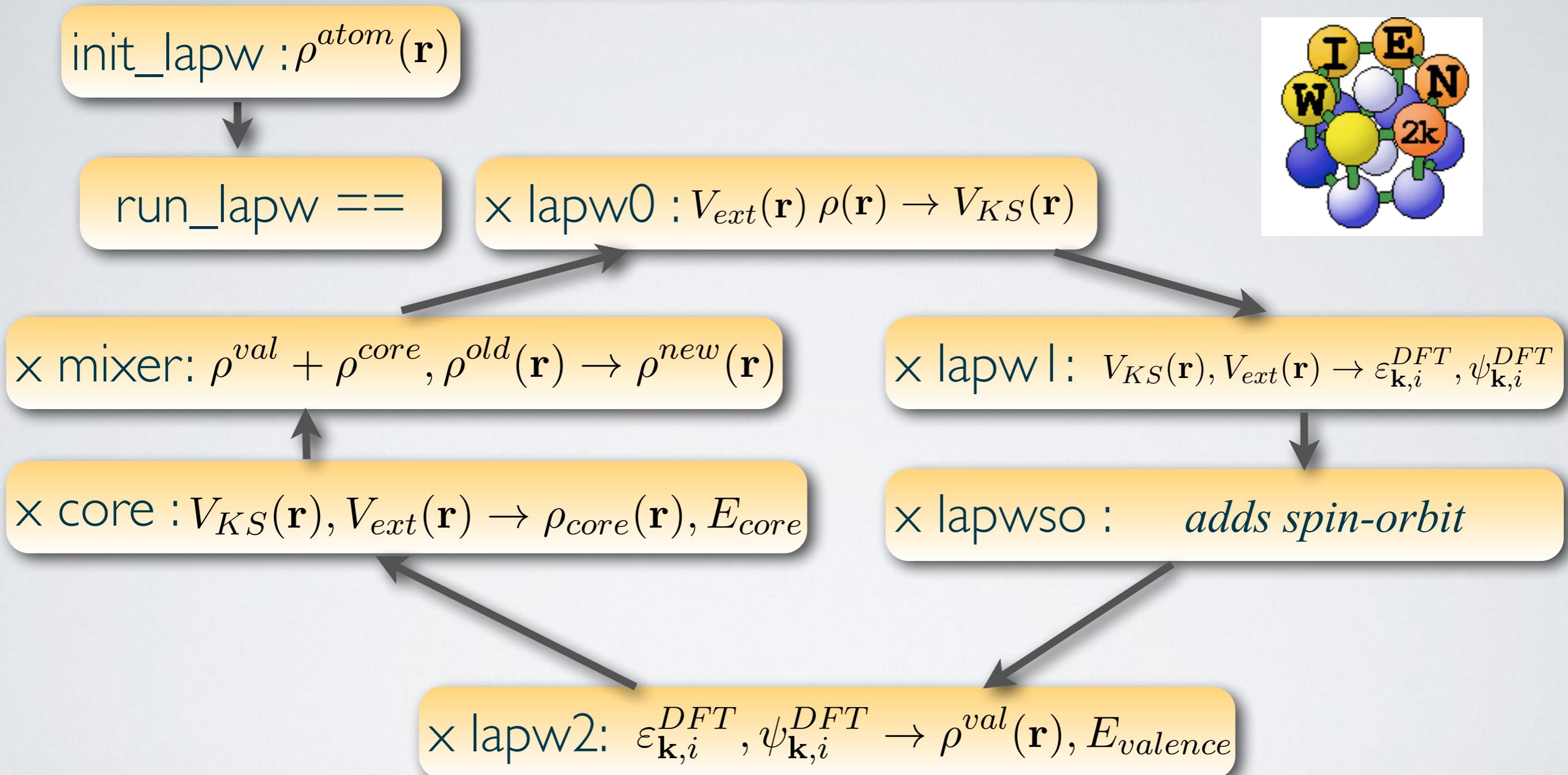
<http://hauleweb.rutgers.edu/>

Download the DMFT-Wien2K source code

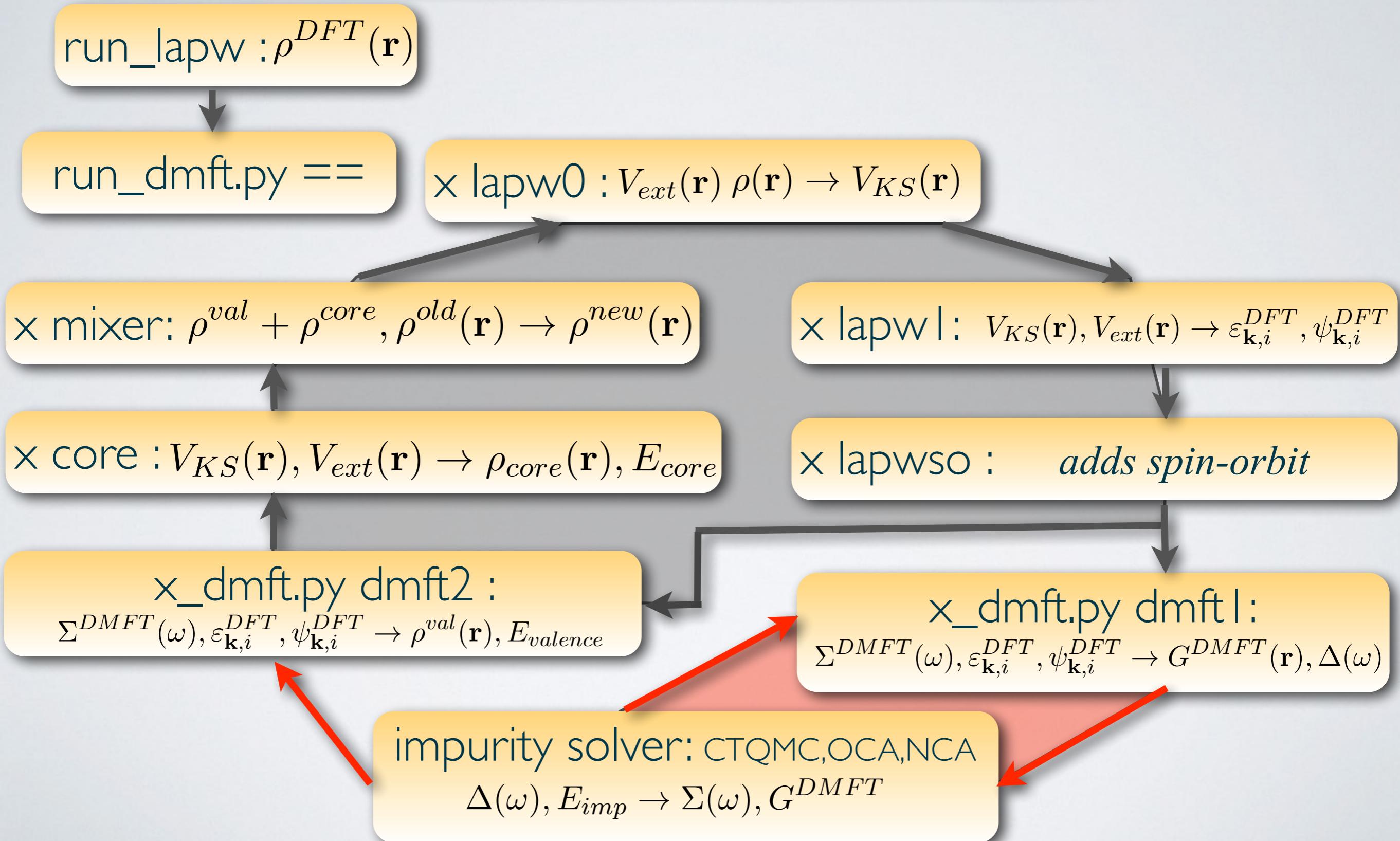
[dmft_w2k.tgz \(version 2012\)](#)

[dmft_w2k.tgz \(version 2015\)](#)

DFT PART



DFT+DMFT COMBINED



x_dmft.py dmft |:
 $\Sigma^{DMFT}(\omega), \varepsilon_{\mathbf{k},i}^{DFT}, \psi_{\mathbf{k},i}^{DFT} \rightarrow G^{DMFT}(\mathbf{r}), \Delta(\omega)$

input

$\Sigma(\omega), \varepsilon_{\mathbf{k},i}^{DFT}, \psi_{\mathbf{k},i}^{DFT}(\mathbf{r}) \longrightarrow G_{local}(\omega), \Delta(\omega), E_{imp}, n_{local}$

output

1) Construct projector: $P(\mathbf{r}\mathbf{r}', \mathbf{R}_\mu, mm') = \langle \mathbf{r} | \phi_m^\mu \rangle \langle \phi_{m'}^\mu | \mathbf{r}' \rangle$

where $\langle \mathbf{r} | \phi_m^\mu \rangle = u_l(|\mathbf{r} - \mathbf{R}_\mu|) Y_{lm}(\widehat{\mathbf{r} - \mathbf{R}_\mu})$

2) Embed self-energy: $\bar{\Sigma}_{ij}(\mathbf{k}, \omega) = \sum_{\mathbf{R}_\mu} \langle \psi_{\mathbf{k},i}^{DFT} | \phi_m^\mu \rangle (\Sigma_{mm'}^\mu(\omega) - V_{DC}^\mu) \langle \phi_{m'}^\mu | \psi_{\mathbf{k},j}^{DFT} \rangle$

3) Calculate local Green's function, hybridization, imp. levels:

$$G_{local\ mm'}^\mu = \sum_{\mathbf{k},ij} \langle \phi_m^\mu | \psi_{\mathbf{k},i}^{DFT} \rangle (\omega + \mu - \varepsilon_{\mathbf{k}} - \bar{\Sigma}(\mathbf{k}, \omega))_{ij}^{-1} \langle \psi_{\mathbf{k},j}^{DFT} | \phi_{m'}^\mu \rangle = \left(\frac{1}{\omega - E_{imp}^\mu - \Sigma^\mu(\omega) - \Delta^\mu(\omega)} \right)_{mm'}$$

symmetrization over all group operations is performed

x_dmft.py dmft2 :

$$\Sigma^{DMFT}(\omega), \varepsilon_{\mathbf{k},i}^{DFT}, \psi_{\mathbf{k},i}^{DFT} \rightarrow \rho_{val}^{DMFT}(\mathbf{r}), E_{valence}$$

input

$$\Sigma(\omega), \varepsilon_{\mathbf{k},i}^{DFT}, \psi_{\mathbf{k},i}^{DFT}(\mathbf{r}) \longrightarrow \rho_{val}^{DMFT}(\mathbf{r}), E_{valence}, F_{valence}, \mathbf{F}^{\mathbf{R}_\mu}$$

output

- 1) Construct projector: $P(\mathbf{r}\mathbf{r}', \mathbf{R}_\mu, mm') = \langle \mathbf{r} | \phi_m^\mu \rangle \langle \phi_{m'}^\mu | \mathbf{r}' \rangle$
where $\langle \mathbf{r} | \phi_m^\mu \rangle = u_l(|\mathbf{r} - \mathbf{R}_\mu|) Y_{lm}(\widehat{\mathbf{r} - \mathbf{R}_\mu})$
- 2) Embed self-energy: $\bar{\Sigma}(\mathbf{r}, \mathbf{r}') = \sum_{\mathbf{R}_\mu} \langle \mathbf{r} | \phi_m^\mu \rangle (\Sigma_{mm'}^\mu(i\omega) - V_{DC}^\mu) \langle \phi_{m'}^\mu | \mathbf{r}' \rangle$
- 3) Solve the Dyson Eq.: $(-\nabla^2 + V_{KS} + \bar{\Sigma}) |\psi_{\mathbf{k},i\omega_n,i}\rangle = |\psi_{\mathbf{k},i\omega_n,i}\rangle \varepsilon_{\mathbf{k},i\omega_n,i}^{DMFT}$
or $(\varepsilon_{\mathbf{k},i_1}^{DFT} \delta_{i_1, i_2} + \langle \psi_{\mathbf{k},i_1}^{DFT} | \bar{\Sigma} | \psi_{\mathbf{k},i_2}^{DFT} \rangle) \langle \psi_{\mathbf{k},i_2}^{DFT} | \psi_{\mathbf{k},i\omega,i} \rangle = \langle \psi_{\mathbf{k},i_1}^{DFT} | \psi_{\mathbf{k},i\omega_n,i} \rangle \varepsilon_{\mathbf{k},i\omega_n,i}^{DMFT}$
- 4) Determine the chemical potential: $N_{val} = T \sum_{i\omega_n, \mathbf{k}, i} \frac{1}{i\omega + \mu - \varepsilon_{\mathbf{k},i\omega_n,i}}$
- 5) Calculate DMFT electronic charge in space:

$$\rho_{val}^{DMFT}(\mathbf{r}) = \sum_{\mathbf{k}, ij} \psi_{\mathbf{k},i}^{DFT}(\mathbf{r}) T \sum_{i\omega_n} [(i\omega + \mu - \varepsilon_{\mathbf{k}}^{DFT} - \bar{\Sigma}_{\mathbf{k}}(\omega))^{-1}]_{ij} \psi_{\mathbf{k},j}^{DFT*}(\mathbf{r})$$
- 6) Calculate DMFT free energy and forces on all atoms
symmetrization over group operations not performed

<http://summer2016.ccs.usherbrooke.ca/dmft/>

Initialize the DMFT calculation

```
$> ssh -X stud[..]@summer2016.ccs.usherbrooke.edu  
$> qsub -I -X  
$> module load edmftf  
$> export OMP_NUM_THREADS=2  
$> cd MnO  
$> init_dmft.py
```

start interactive session

load the module

don't use too many cores!

this sets up DMFT projector

To answer the questions, look at:

<http://hauleweb.rutgers.edu/tutorials/>

click: [Tutorial 1 on MnO](#)

Continue... initialize the DMFT calculation

```
$> mkdir ..../DMFT_MnO; cd ..../DMFT_MnO      fresh start in new dir  
$> dmft_copy.py ..../MnO                      copy necessary files here  
$> x kgen -f MnO                                increase number of k-points  
          2000  
$> cp $RESULT/MnO/params.dat .                  get params file  
$> szero.py -e 38.22 -T 0.025853               create blank Sigma (T=1/beta=1/38.68)  
$> cp $RESULT/submit2.sh .                      obtain submission script  
$> exit                                         stop interactive session  
$> cd DMFT_MnO                                 return to the current dir  
$> qsub submit2.sh                               submit to the queue
```

Monitor the job

```
$> less dmft_info.out                                check the master log file  
$> less ':log'                                     check execution log  
$> plot -u1:3,1:5 -x:10 MnO.dlt1                  plot hybridization function  
$> plot -x:20 -g -u1:3,1:5 imp.0/Gf.out.??.1    plot the DMFT output G  
$> less info.iterate                               see current energy/mu/Vdc/...  
$> plot -g -u1:9,1:10 info.iterate                plot lattice & impurity occupancy  
$> grep ':CHARGE' MnO.dayfile                   how well is charge converged
```

it might take too much time to converge...

After some time you should kill your job, and continue with postprocessing

To kill your job, type

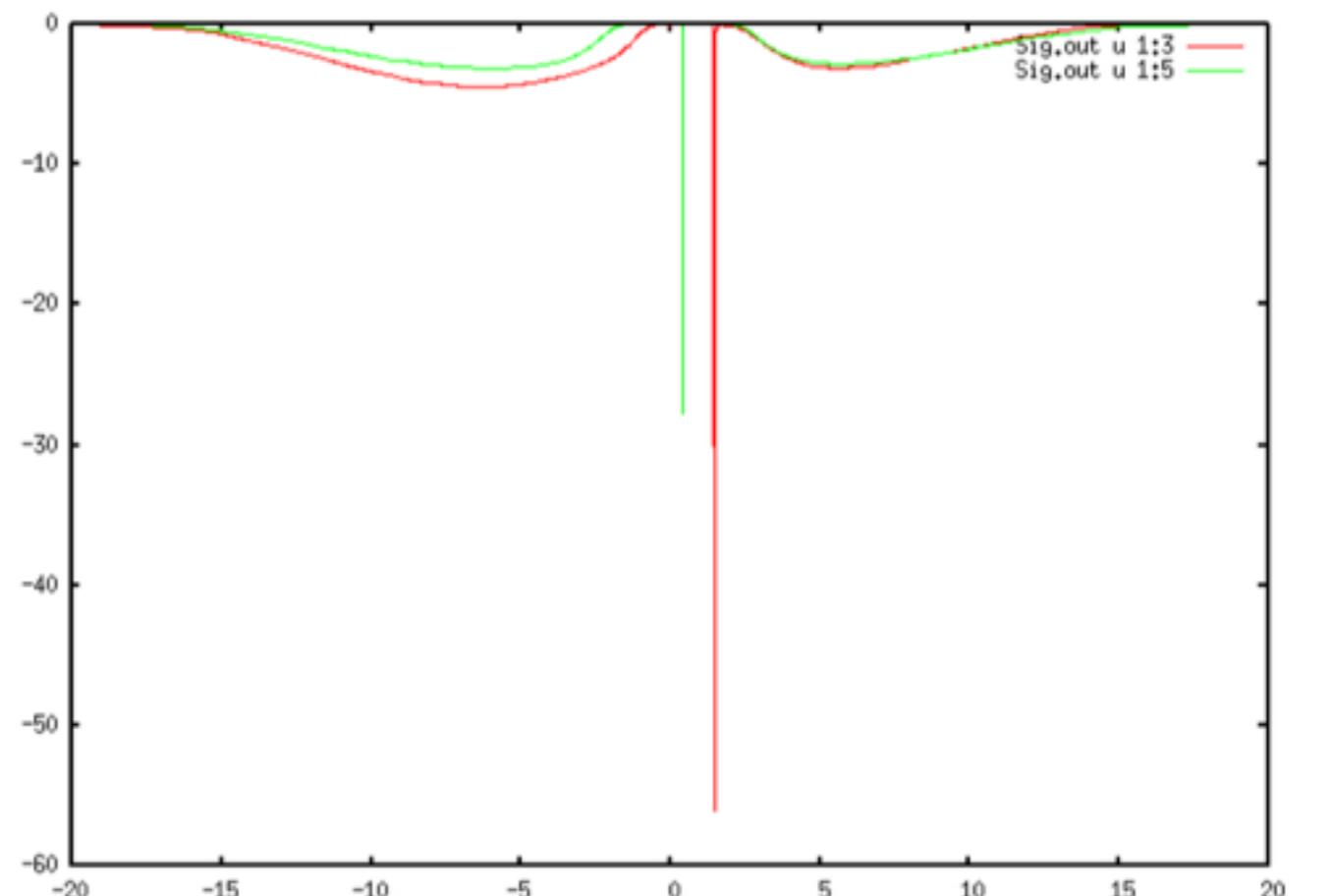
```
$> qstat  
$> qdel <Job ID>
```

find your job ID

Postprocessing maxent

```
$> mkdir maxent; cd maxent                                new directory  
$> saverage.py $RESULT/MnO/sig.inp.1?.1                  average over a few MC steps  
$> cp $RESULT/MnO/maxent/maxent_params.dat .             parameters for maxent  
$> qsub -l -X                                         interactive session  
$> module load edmftf  
$> cd DMFT_MnO/maxent                                    go back to the new dir  
$> maxent_run.py sig.inpx                               run maxent  
$> plot -u1:3,1:5 Sig.out                                plot Sigma on real axis
```

you should get:



Postprocessing DOS

```
$> mkdir .../onreal; cd .../onreal  
$> dmft_copy.py $RESULT/MnO  
$> cp ..../maxent/Sig.out sig.ip
```

new directory

copy converged DMFT outputs

replace $\Sigma(\text{iom})$ with $\Sigma(\text{om})$

edit the second line of **MnO.indmfl** file and change the flag **matsubara** to 0

```
0 0.025 0.025 200 -3.000000 1.000000 # matsubara,..
```

```
$> x lapw0 -f MnO  
$> x lapw1 -f MnO  
$> x_dmft.py dmft1  
$> plot -x-10:10 -uall MnO.cdos  
$> plot -x-10:10 -u1:3,1:5 MnO.gc1
```

recompute KS potential

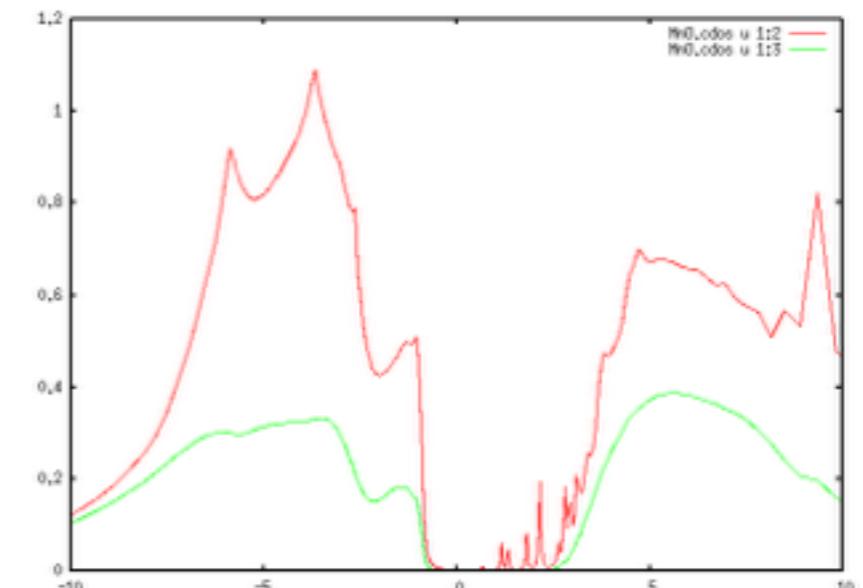
recompute KS eigensystem

compute DOS and G on real axis

plots partial DOS

plots local G(ω)

you should get:



Post-processing band structure

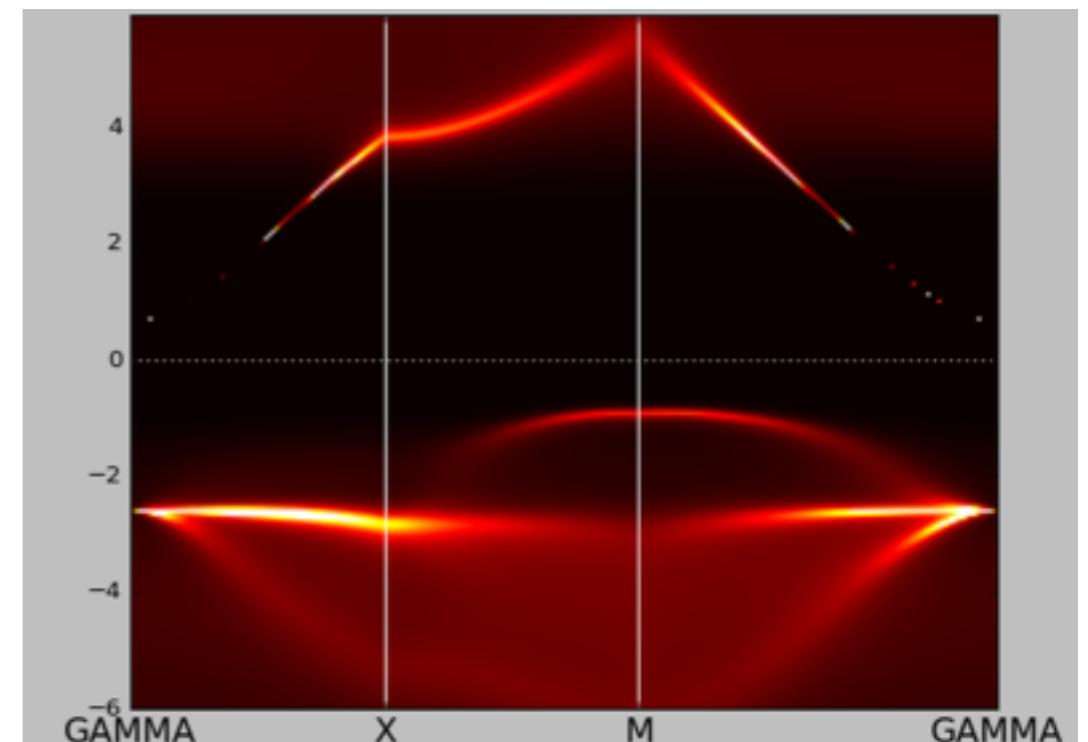
```
$> cp $RESULT/MnO/onreal/MnO.klist_band .           get k-path  
$> x lapw1 -f MnO -band                           KS eigvals on k-path
```

edit the second line of **MnO.indmfl** file and change **omega_min**,
omega_max to -6 6

```
0 0.025 0.025 200 -6.000000 6.000000 # matsubara,..
```

```
$> x_dmft.py dmftp                                compute dmft eigvals  
$> cp $RESULT/MnO/EF.dat .                         get final EF  
$> wakplot.py 0.02                                plot spectral function
```

you should get:



FeSe

Repeat all above steps for FeSe reading the tutorial at:

<http://hauleweb.rutgers.edu/tutorials/>

click: [Tutorial 2 on FeSe](#)

Thank you!