Charge Self-Consistency

Fully self-consistent “DFT+many-body” methods

Elias Assmann

Institute for Solid State Physics, TU Wien

Ab initio DΓA Workshop,
Vorderstoder 2013-09-02

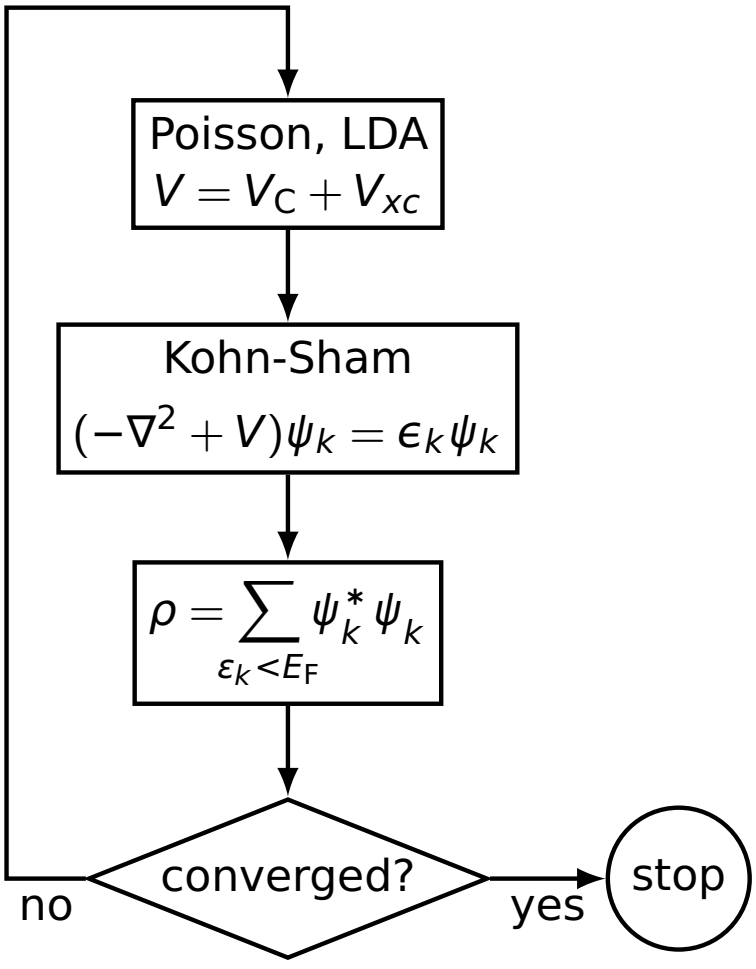
What's the Big Idea?

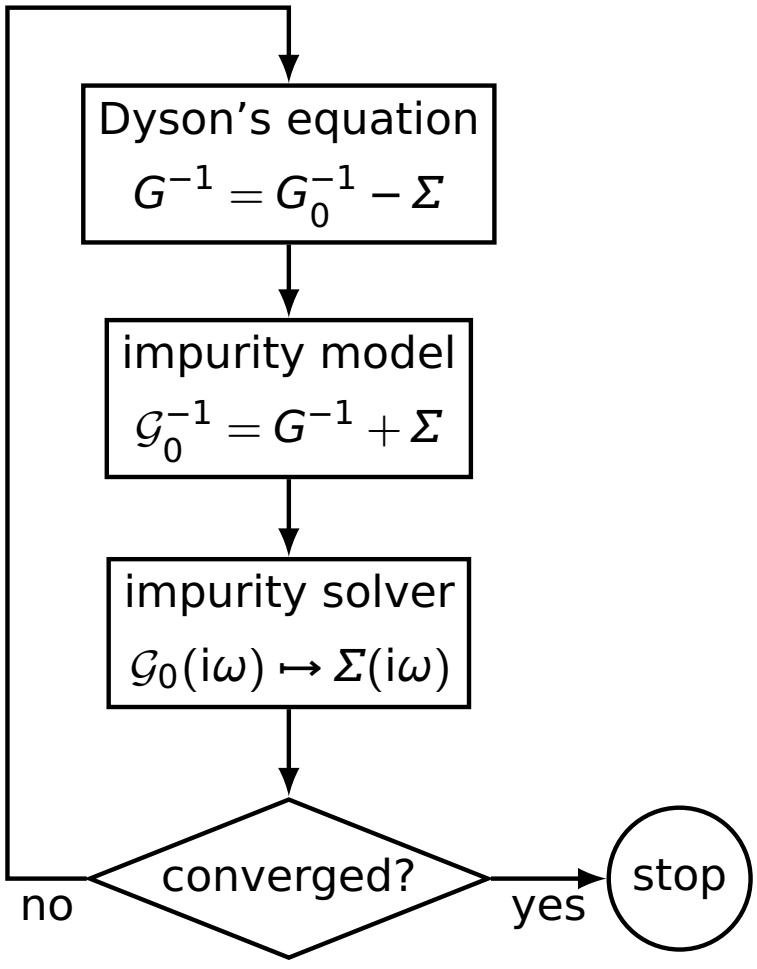
- self-consistent LDA calculation ($\rho(\boldsymbol{r})$) as basis for DMFT
- DMFT may change occupations $\langle \hat{n}_i \rangle$

$\rightsquigarrow$ changed density ($\tilde{\rho}(\boldsymbol{r})$)

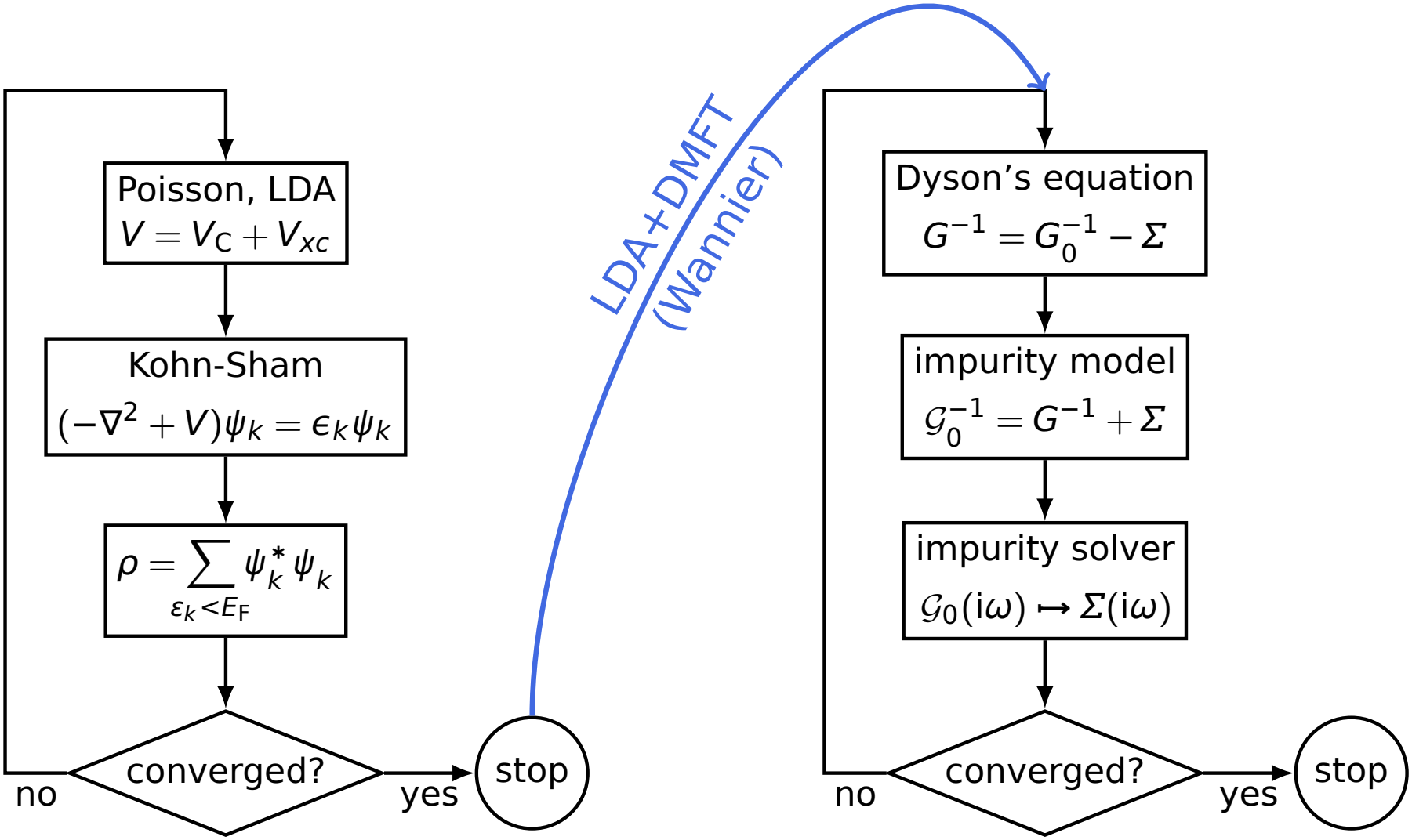
$\Rightarrow$ $V_{\text{eff}}[\rho]$, $\tilde{\rho}(\boldsymbol{r})$ not LDA-self-consistent

A Tale of Two Cycles

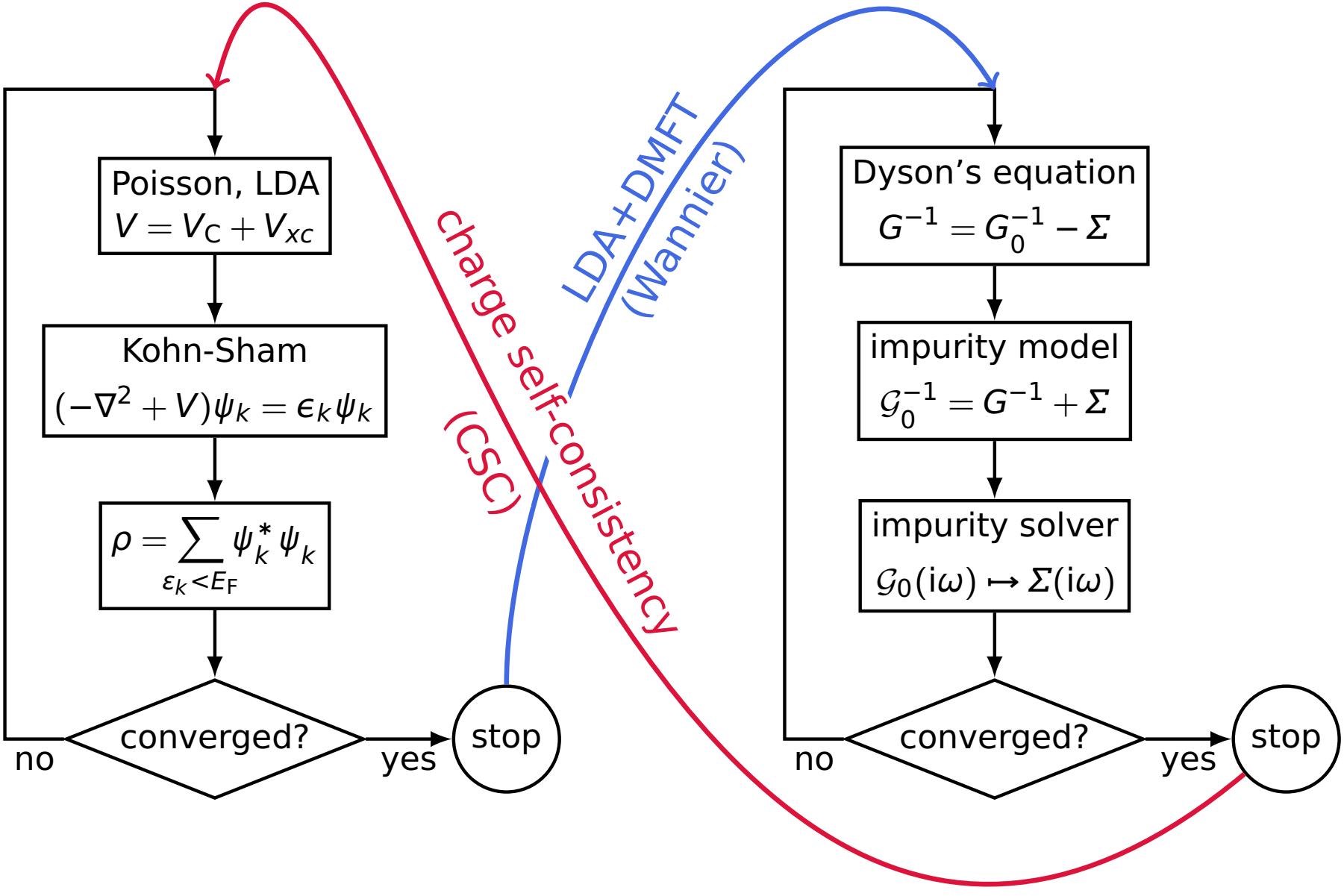




A Tale of Two Cycles



A Tale of Two Cycles



CSC for LAPW+MLWF

[Lechermann *et al.*, PRB (2006)]

- Wien2k/W2dynamics implementation in progress (Rainer Bachleitner)
  - Wien2k-integration based on Wien2TRIQS (change occupations in `lapw2`) [Pourovskii *et al.*, PRB (2007)]

$$\rho(\boldsymbol{r}) = \frac{1}{\beta} \sum_{\mathrm{i}\omega} G(\boldsymbol{r}, \boldsymbol{r}; \mathrm{i}\omega)\, \mathrm{e}^{\mathrm{i}\omega 0^+} = \langle \boldsymbol{r} | \widehat{G} | \boldsymbol{r} \rangle$$

$$\Delta\rho(\boldsymbol{r}) = \langle \boldsymbol{r} | \widehat{G} - \widehat{G}_{\mathrm{KS}} | \boldsymbol{r} \rangle = \langle \boldsymbol{r} | \widehat{G}_{\mathrm{KS}}\, \Delta\widehat{\Sigma}\, \widehat{G} | \boldsymbol{r} \rangle$$

$$\Delta N(\boldsymbol{k}) := \frac{1}{\beta} \sum_{\mathrm{i}\omega} G_{\mathrm{KS}}(\boldsymbol{k}, \mathrm{i}\omega)\, \Delta\Sigma(\mathrm{i}\omega)\, G(\boldsymbol{k}, \mathrm{i}\omega)$$

CSC for LAPW+MLWF

[Lechermann *et al.*, PRB (2006)]

- Wien2k/W2dynamics implementation in progress (Rainer Bachleitner)
  - Wien2k-integration based on Wien2TRIQS (change occupations in `lapw2`) [Pourovskii *et al.*, PRB (2007)]

$$\rho(\boldsymbol{r}) = \frac{1}{\beta} \sum_{\mathrm{i}\omega} G(\boldsymbol{r}, \boldsymbol{r}; \mathrm{i}\omega)\, \mathrm{e}^{\mathrm{i}\omega 0^+} = \langle \boldsymbol{r} | \widehat{G} | \boldsymbol{r} \rangle$$

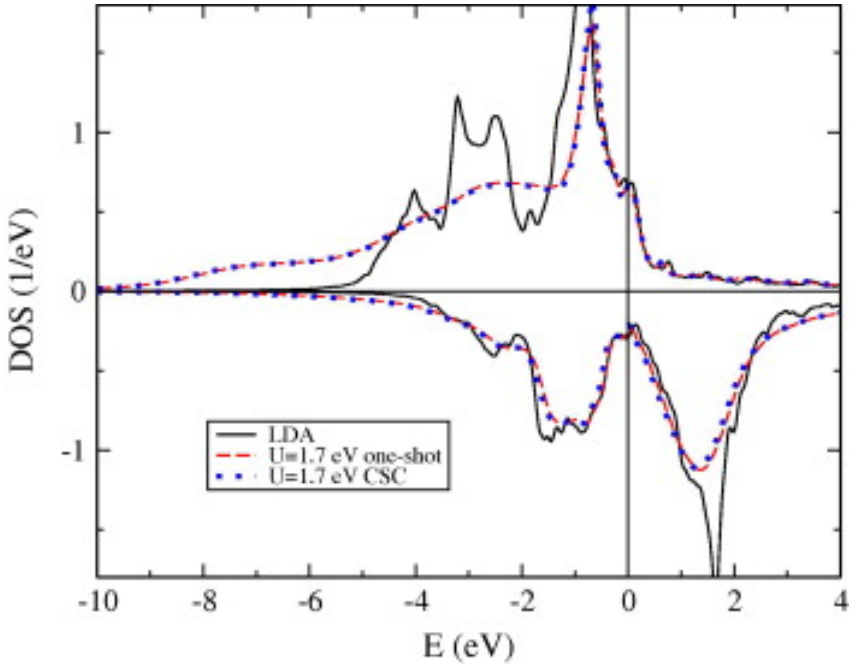
$$\Delta\rho(\boldsymbol{r}) = \langle \boldsymbol{r} | \widehat{G} - \widehat{G}_{\mathrm{KS}} | \boldsymbol{r} \rangle = \langle \boldsymbol{r} | \widehat{G}_{\mathrm{KS}}\, \Delta\widehat{\Sigma}\, \widehat{G} | \boldsymbol{r} \rangle$$

$$\Delta N(\boldsymbol{k}) := \frac{1}{\beta} \sum_{\mathrm{i}\omega} G_{\mathrm{KS}}(\boldsymbol{k}, \mathrm{i}\omega)\, \Delta\Sigma(\mathrm{i}\omega)\, G(\boldsymbol{k}, \mathrm{i}\omega)$$

$$E = E_{\mathrm{LDA}} + \langle \widehat{H}_U \rangle - E_{\mathrm{dc}} + \sum_{\boldsymbol{k}\alpha\alpha'} H^0_{\alpha\alpha'}(\boldsymbol{k}) \left(\langle c^+_{\boldsymbol{k}\alpha} c_{\boldsymbol{k}\alpha'} \rangle - \langle c^+_{\boldsymbol{k}\alpha} c_{\boldsymbol{k}\alpha'} \rangle_0 \right)$$

Some Results

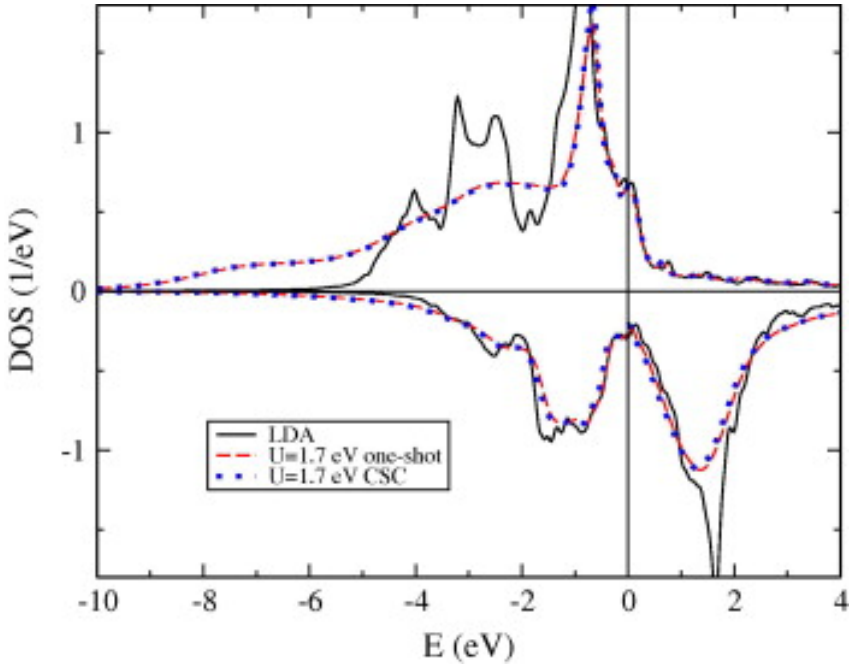
Fe (bcc):



[Grånäs *et al.*, Comp. Mater. Sci. (2012)]

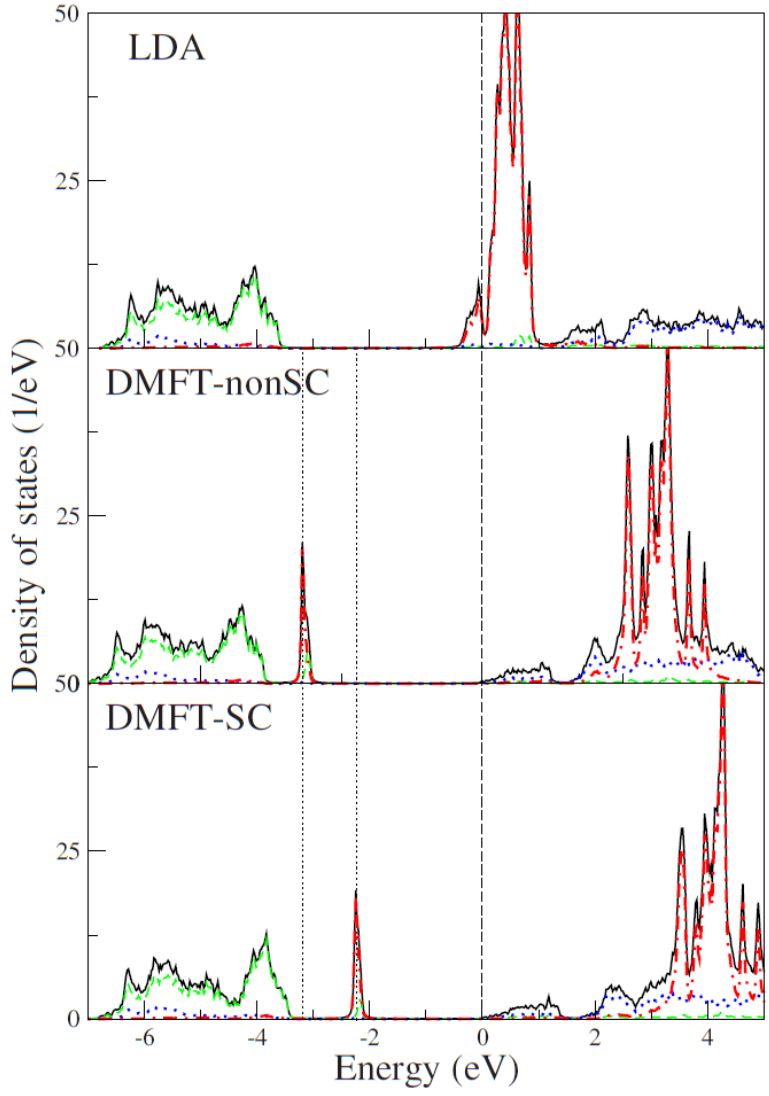
Some Results

Fe (bcc):



[Grånäs *et al.*, Comp. Mater. Sci. (2012)]

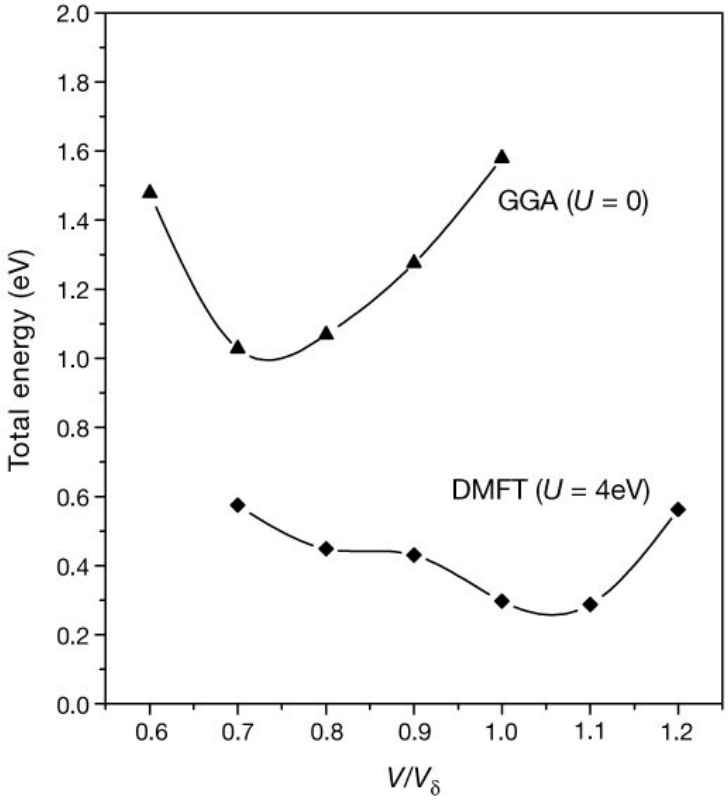
Ce_2O_3:



[Pourovskii *et al.*, PRB (2007)]

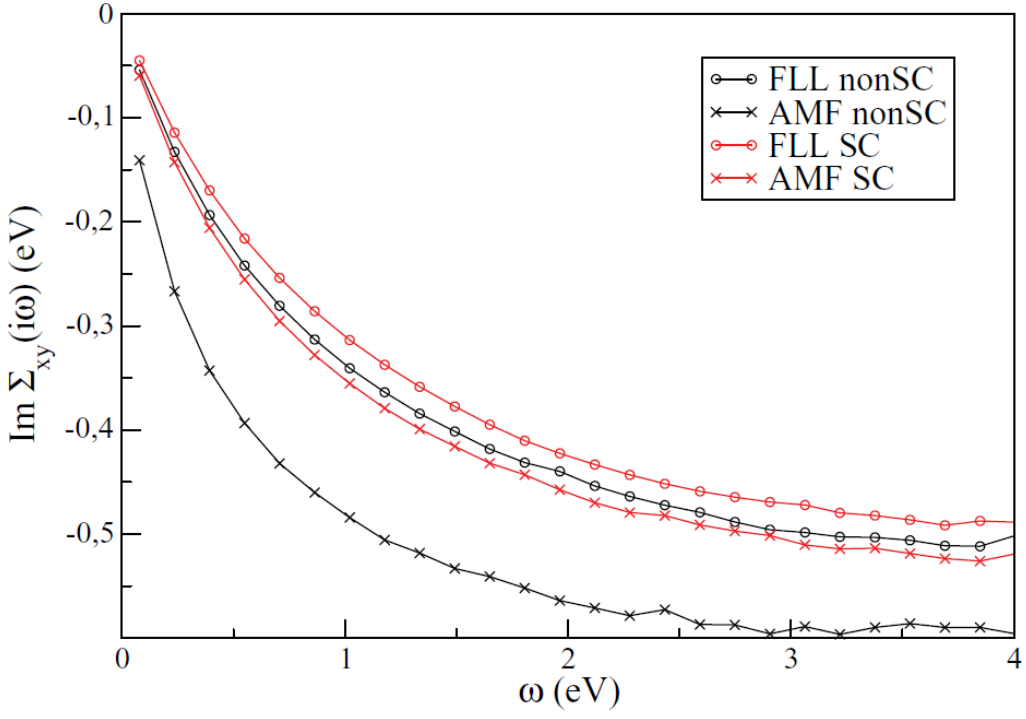
Some More Results

Pu volume:



[Savrasov *et al.*, Nature (2001)]

interplay with double-counting (LaFeAsO):



[Aichhorn *et al.*, PRB (2011)]

Conversation Piece

- when is charge self-consistency important?
  - − symmetry
  - \+ total energies (structure optimization)
- open problems
  - disentanglement and interpolation of $V_{\boldsymbol{k}}$
  - optimal protocol to reach LDA-DMFT self-consistency?
- generalization to other many-body methods
  - *GW*+DMFT
  - ab initio DΓA

Bibliography

- Savrasov, Kotliar, and Abrahams, Nature 410, 793 (2001); Savrasov and Kotliar, PRB 69, 245101 (2004)
  - LMTO implementation, total energies
  - volume increase in Pu (25% $\delta \rightarrow \alpha$)
  - "spectral density functional theory"
- Minár *et al.*, PRB 72, 045125 (2005)
  - KKR+DMFT
  - Fe_xNi_{1-x}
- Anisimov et al., PRB 71, 125119 (2005)
  - Wannier functions; LMTO
  - $SrVO_3$, V_2O_3
- Lechermann *et al.*, PRB 74, 125120 (2006)
  - Wannier functions; theory for CSC (no implementation)
- Pourovskii, Amadon, Biermann, and Georges, PRB 76, 235101 (2007)
  - LMTO, total energies
  - Ce_2O_3, γ-Ce
- Haule, Yee, and Kim, PRB 81, 195107 (2010)
  - LAPW & LMTO
  - Ce, $CeIrIn_5$, $CeCoIn_5$, $CeRhIn_5$
- Aichhorn, Pourovskii, and Georges PRB 84, 054529 (2011)
  - LAPW, projector Wannier functions; total energies
  - LaFeAsO (As height optimized)
- Amadon, J. Phys.: Condens. Mat. 24, 075604 (2012)
  - plane wave/PAW, total energies
  - Ce, Ce_2O_3, Pu_2O_3
- Grånäs *et al.*, Comp. Mater. Sci. 55, 295 (2012)
  - FP-LMTO, total energies
  - Fe, $SmCo_5$