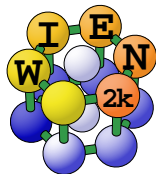# Methods available in WIEN2k for the treatment of exchange and correlation effects

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Outline of the talk

- ▶ Introduction
- ▶ Semilocal functionals:
  - ▶ GGA and MGGA
  - ▶ mBJ potential (for band gap)
  - ▶ Input file case.in0
- ▶ Methods for van der Waals systems:
  - ▶ DFT-D3
  - ▶ Nonlocal functionals
- ▶ On-site methods for strongly correlated d and f electrons:
  - ▶ DFT+U
  - ▶ Hybrid functionals
- ▶ Hybrid functionals

Total energy in Kohn-Sham DFT[1]

$$E_{\text{tot}} = \underbrace{\frac{1}{2}\sum_i \int |\nabla\psi_i(\mathbf{r})|^2\, d^3r}_{T_{\text{s}}} + \underbrace{\frac{1}{2}\int\int \frac{\rho(\mathbf{r})\rho(\mathbf{r}')}{|\mathbf{r}-\mathbf{r}'|}\, d^3r d^3r'}_{E_{\text{ee}}} + \underbrace{\int v_{\text{en}}(\mathbf{r})\rho(\mathbf{r})d^3r}_{E_{\text{en}}}$$

$$+ \underbrace{\frac{1}{2}\sum_{\substack{A,B\\A\neq B}} \frac{Z_A Z_B}{|\mathbf{R}_A-\mathbf{R}_B|}}_{E_{\text{nn}}} + \textcolor{red}{E_{\text{xc}}}$$

- T_{s} : kinetic energy of the non-interacting electrons
- E_{ee} : repulsive electron-electron electrostatic Coulomb energy
- E_{en} : attractive electron-nucleus electrostatic Coulomb energy
- E_{nn} : repulsive nucleus-nucleus electrostatic Coulomb energy
- $E_{\text{xc}} = E_{\text{x}} + E_{\text{c}}$: exchange-correlation energy
  Approximations for E_{xc} have to be used in practice
  $\implies$ The reliability of the results depends mainly on E_{xc}

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[1] W. Kohn and L. J. Sham, Phys. Rev. **140**, A1133 (1965)

Approximations for E_{xc} (Jacob's ladder[1])

$$E_{xc} = \int \epsilon_{xc}(\mathbf{r})\, d^3r$$
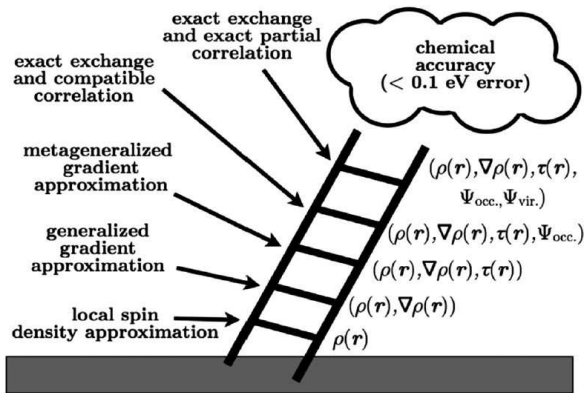
The accuracy, but also the computational cost, increase when climbing up the ladder

[1] J. P. Perdew *et al.*, J. Chem. Phys. **123**, 062201 (2005)

Kohn-Sham Schrödinger equations

Minimization of E_{tot} leads to

$$\left(-\frac{1}{2}\nabla^2 + v_{\text{ee}}(\mathbf{r}) + v_{\text{en}}(\mathbf{r}) + \hat{v}_{\text{xc}}(\mathbf{r})\right)\psi_i(\mathbf{r}) = \epsilon_i\psi_i(\mathbf{r})$$

Two types of $\hat{v}_{\text{xc}}$:

- Multiplicative: $\hat{v}_{\text{xc}} = \delta E_{\text{xc}}/\delta\rho = v_{\text{xc}}$ (KS method)
  - LDA
  - GGA

- Non-multiplicative: $\hat{v}_{\text{xc}} = (1/\psi_i)\delta E_{\text{xc}}/\delta\psi_i^* = v_{\text{xc},i}$ (generalized KS[1])
  - Hartree-Fock
  - LDA+U
  - Hybrid (mixing of GGA and Hartree-Fock)
  - MGGA
  - Self-interaction corrected (Perdew-Zunger)

[1] A. Seidl *et al.*, Phys. Rev. B **53**, 3764 (1996)

Semilocal functionals: GGA

$$\epsilon_{\mathrm{xc}}^{\mathrm{GGA}}(\rho, \nabla\rho) = \epsilon_{\mathrm{x}}^{\mathrm{LDA}}(\rho) F_{\mathrm{xc}}(r_s, s)$$

where F_{xc} is the enhancement factor and

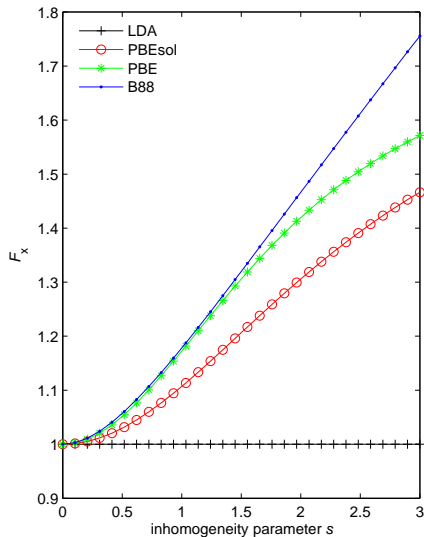$$r_s = \frac{1}{\left(\frac{4}{3}\pi\rho\right)^{1/3}} \quad \text{(Wigner-Seitz radius)}$$

$$s = \frac{|\nabla\rho|}{2\left(3\pi^2\right)^{1/3}\rho^{4/3}} \quad \text{(inhomogeneity parameter)}$$

There are two types of GGA:

- Semi-empirical: contain parameters fitted to accurate (i.e., experimental) data.

- Ab initio: All parameters were determined by using mathematical conditions obeyed by the exact functional.

Semilocal functionals: trends with GGA

Exchange enhancement factor $F_x(s) = \epsilon_x^{\text{GGA}} / \epsilon_x^{\text{LDA}}$

good for atomization energy of molecules
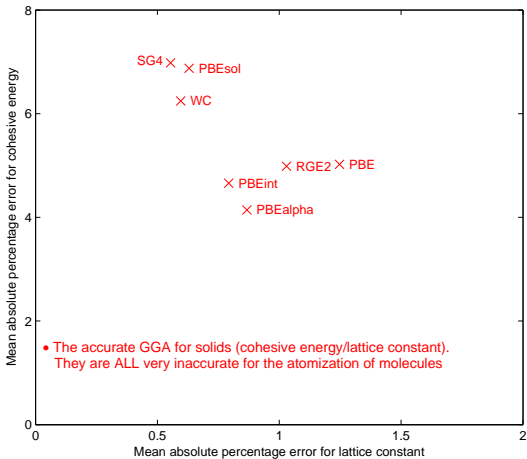
good for atomization energy of solids

good for lattice constant of solids

good for nearly nothing

Construction of an universal GGA: A failure

Test of functionals on 44 solids[1]

[1] F. Tran *et al.*, J. Chem. Phys. **144**, 204120 (2016)

Semilocal functionals: meta-GGA

$$\epsilon_{\mathrm{xc}}^{\mathrm{MGGA}}(\rho, \nabla\rho, t) = \epsilon_{\mathrm{xc}}^{\mathrm{LDA}}(\rho) F_{\mathrm{xc}}(r_s, s, \alpha)$$

- $\alpha = \frac{t - t_{\mathrm{W}}}{t_{\mathrm{TF}}}$
    - $\alpha = 1$ (region of constant electron density)
    - $\alpha = 0$ (in one- and two-electron regions very close and very far from nuclei)
    - $\alpha \gg 1$ (region between closed shell atoms)
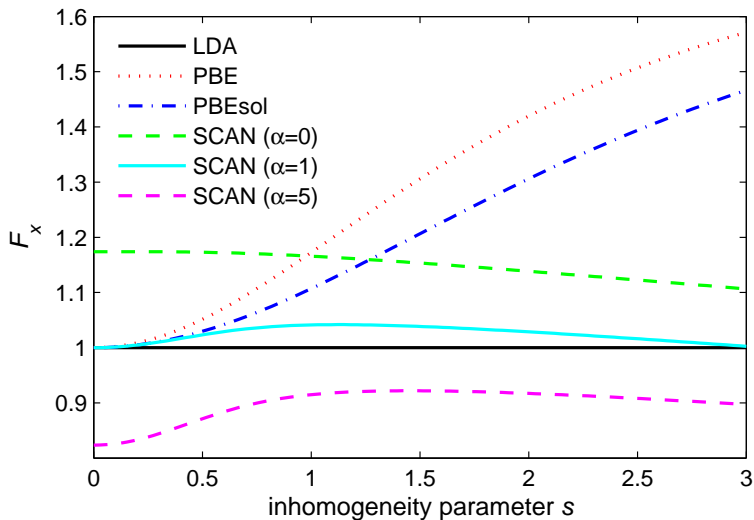$\implies$ MGGA functionals are more flexible

Example: SCAN[1] is

- as good as the best GGA for atomization energies of molecules
- as good as the best GGA for lattice constant of solids

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[1] J. Sun *et al.*, Phys. Rev. Lett. **115**, 036402 (2015)

Semilocal functionals: meta-GGA

$$F_{\mathrm{x}}(s,\alpha) = \epsilon_{\mathrm{x}}^{\mathrm{MGGA}}/\epsilon_{\mathrm{x}}^{\mathrm{LDA}}$$

Semilocal functionals: MGGA_MS2 and SCAN

Test of functionals on 44 solids[1]
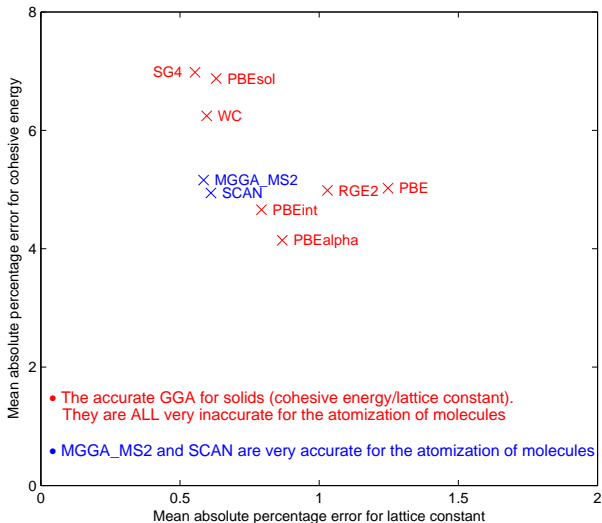
[1] F. Tran *et al.*, J. Chem. Phys. **144**, 204120 (2016)

Semilocal potential for band gap: modified Becke-Johnson

- Standard LDA and GGA functionals underestimate the band gap

- Hybrid and *GW* are much more accurate, but also much more expensive

- A cheap alternative is to use the modified Becke-Johnson (mBJ) potential:[1]

$$v_{\mathrm{x}}^{\mathrm{mBJ}}(\mathbf{r}) = c v_{\mathrm{x}}^{\mathrm{BR}}(\mathbf{r}) + (3c - 2)\frac{1}{\pi}\sqrt{\frac{5}{6}}\sqrt{\frac{t(\mathbf{r})}{\rho(\mathbf{r})}}$$

where $v_{\mathrm{x}}^{\mathrm{BR}}$ is the Becke-Roussel potential, t is the kinetic-energy density and c is given by

$$c = \alpha + \beta \left(\frac{1}{V_{\mathrm{cell}}} \int\limits_{\mathrm{cell}} \frac{|\nabla\rho(\mathbf{r})|}{\rho(\mathbf{r})} d^3 r \right)^p$$

mBJ is a MGGA potential

[1] F. Tran and P. Blaha, Phys. Rev. Lett. **102**, 226401 (2009)

Band gaps with mBJ
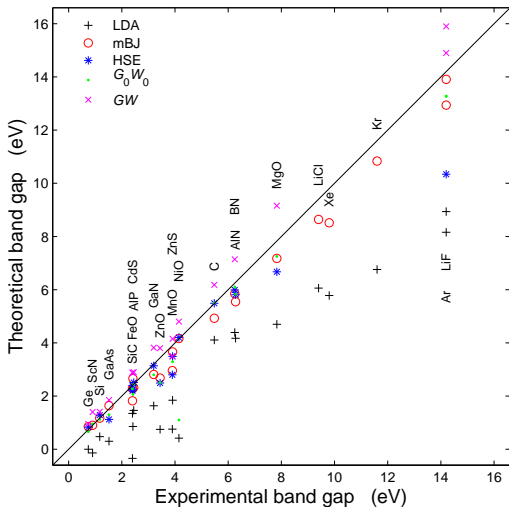
See also F. Tran and P. Blaha, J. Phys. Chem. A **121**, 3318 (2017)

How to run a calculation with the mBJ potential?

1. init_lapw (choose LDA or PBE)
2. init_mbj_lapw (create/modify files)
   2.1 automatically done: case.in0 modified and case.inm_vresp created
   2.2 run(sp)_lapw -i 1 -NI (creates case.r2v and case.vrespsum)
   2.3 save_lapw
3. init_mbj_lapw and choose one of the parametrizations:

   0: Original mBJ values[1]
   1: New parametrization[2]
   2: New parametrization for semiconductors[2]
   3: Original BJ potential[3]

4. run(sp)_lapw ...

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[1] F. Tran and P. Blaha, Phys. Rev. Lett. **102**, 226401 (2009)
[2] D. Koller *et al.*, Phys. Rev. B **85**, 155109 (2012)
[3] A. D. Becke and E. R. Johnson, J. Chem. Phys. **124**, 221101 (2006)

Input file case.in0: keywords for the xc-functional

The functional is specified at the 1st line of case.in0. Three different ways:

1. Specify a global keyword for E_x, E_c, v_x, v_c:
   - TOT XC_*NAME*

2. Specify a keyword for E_x, E_c, v_x, v_c individually:
   - TOT EX_*NAME1* EC_*NAME2* VX_*NAME3* VC_*NAME4*

3. Specify keywords to use functionals from **LIBXC**[1]:
   - TOT XC_*TYPE*_X_*NAME1* XC_*TYPE*_C_*NAME2*
   - TOT XC_*TYPE*_XC_*NAME*

   where *TYPE* is the family name: LDA, GGA or MGGA

[1] M. A. L. Marques *et al.*, Comput. Phys. Commun. **183**, 2272 (2012)
http://www.tddft.org/programs/octopus/wiki/index.php/Libxc

Input file case.in0: examples

- PBE:
  TOT XC_PBE
  or
  TOT EX_PBE EC_PBE VX_PBE VC_PBE
  or
  TOT XC_GGA_X_PBE XC_GGA_C_PBE
- mBJ (with LDA for the xc-energy):
  TOT XC_MBJ
- MGGA_MS2:
  TOT XC_MGGA_MS $\underbrace{0.504 \ 0.14601 \ 4.0}_{\kappa, c, b}$

All available functionals are listed in tables of the user's guide and in
$WIENROOT/SRC_lapw0/xc_funcs.h for **LIBXC** (if installed)

Methods for van der Waals systems

Problem with semilocal and hybrid functionals:

- They do not include London dispersion interactions $\Longrightarrow$ Results are very often qualitatively wrong for van der Waals systems

Two types of dispersion terms added to the DFT total energy:

- Pairwise term (cheap)[1]:

$$E_{c,disp}^{PW} = -\sum_{A<B} \sum_{n=6,8,10,\ldots} f_n^{damp}(R_{AB}) \frac{C_n^{AB}}{R_{AB}^n}$$

- Nonlocal term (more expensive than semilocal)[2]:

$$E_{c,disp}^{NL} = \frac{1}{2} \int \int \rho(\mathbf{r}_1) \Phi(\mathbf{r}_1,\mathbf{r}_2) \rho(\mathbf{r}_2) d^3r_1 d^3r_2$$

[1] S. Grimme, J. Comput. Chem. **25**, 1463 (2004)

[2] M. Dion *et al.*, Phys. Rev. Lett. **92**, 246401 (2004)

DFT-D3 pairwise method[1]

- **Features:**
  - Cheap
  - C_n^{AB} depend on positions of the nuclei (via coordination number)
  - Energy and forces (minimization of internal parameters)
  - 3-body term available (more important for solids than molecules)
- **Installation:**
  - Not included in WIEN2k
  - Download and compile the DFTD3 package from https://www.chemie.uni-bonn.de/pctc/mulliken-center/software/dft-d3/ copy the `dftd3` executable in `$WIENROOT`
- **Usage:**
  - Input file case.indftd3 (if not present a default one is copied automatically by **x_lapw**)
  - run(sp)_lapw -dftd3 . . .
  - case.scfdftd3 is included in case.scf

[1] S. Grimme *et al.*, J. Chem. Phys. **132**, 154104 (2010)

DFT-D3 method: input file case.indftd3

Default (and recommended) input file:

method	bj	damping function f_n^{damp}
func	default	the one in case.in0*
grad	yes	forces
pbc	yes	periodic boundary conditions
abc	yes	3-body term
cutoff	95	interaction cutoff
cnthr	40	coordination number cutoff
num	no	numerical gradient

*default will work for PBE, PBEsol, BLYP and TPSS. For other functionals, the functional name has to be specified (see dftd3.f of DFTD3 package)

DFT-D3 method: hexagonal BN[1]
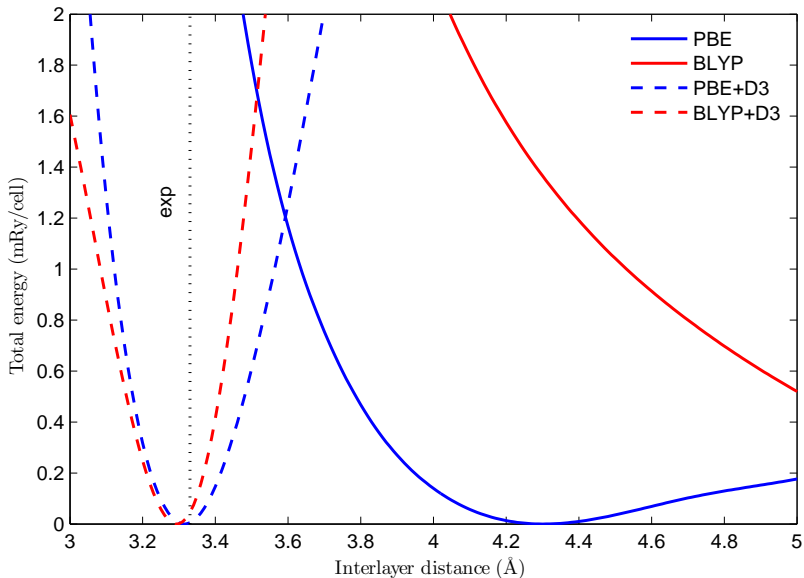
[1] F. Tran *et al.*, J. Chem. Phys. **144**, 204120 (2016)

Nonlocal vdW functionals

$$E_{c,disp}^{NL} = \frac{1}{2} \int \int \rho(\mathbf{r}_1)\Phi(\mathbf{r}_1, \mathbf{r}_2)\rho(\mathbf{r}_2)d^3r_1 d^3r_2$$

Kernels Φ proposed in the literature:

- DRSLL[1] (vdW-DF1, optB88-vdW, vdW-DF-cx0, ...):
    - Derived from ACFDT
    - Contains no adjustable parameter
- LMKLL[2] (vdW-DF2, rev-vdW-DF2):
    - Z_{ab} in DRSLL multiplied by 2.222
- rVV10[3,4]:
    - Different analytical form as DRSLL
    - Parameters: $b = 6.3$ and $C = 0.0093$
- rVV10L[5]:
    - Parameters: $b = 10.0$ and $C = 0.0093$

[1] M. Dion *et al.*, Phys. Rev. Lett. **92**, 246401 (2004)

[2] K. Lee *et al.*, Phys. Rev. B **82**, 081101(R) (2010)

[3] O. A. Vydrov and T. Van Voorhis, J. Chem. Phys. **133**, 244103 (2010)

[4] R. Sabatini *et al.*, Phys. Rev. B **87**, 041108(R) (2013)

[5] H. Peng and J. P. Perdew, Phys. Rev. B **95**, 081105(R) (2017)

Nonlocal vdW functionals in WIEN2k[1]

- Features:
  - Use the fast FFT-based method of Román-Pérez and Soler[2]:
    1. ρ is smoothed close to the nuclei (density cutoff ρ_c) $\rightarrow \rho_s$. The smaller ρ_c is, the smoother ρ_s is.
    2. ρ_s is expanded in plane waves in the whole unit cell. G_{max} is the plane-wave cutoff of the expansion.
  - Most vdW functionals from the literature are available (see user's guide)

- Usage:
  - Input file case.innlvdw ($WIENROOT/SRC_templates)
  - run(sp)_lapw -nlvdw ...
  - case.scfnlvdw is included in case.scf

- Problem:
  - **prepare_xsf** may hang

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[1] F. Tran *et al.*, Phys. Rev. B **96**, 054103 (2017)
[2] G. Román-Pérez and J. M. Soler, Phys. Rev. Lett. **103**, 096102 (2009)

Nonlocal vdW functionals: the input file case.innlvdw

1	kernel type
−0.8491	parameters of the kernel
20	plane-wave expansion cutoff GMAX
0.3	density cutoff rhoc
T	calculation of the potential (T or F)

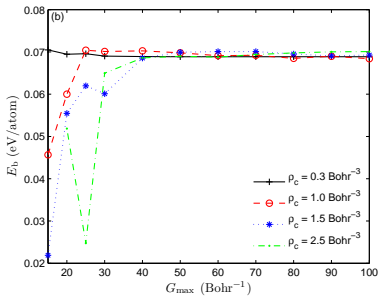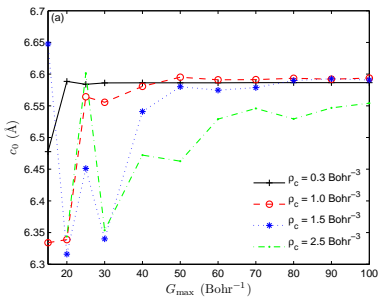**line 1** : "1" for DRSLL and LMKLL or "2" for rVV10
line 2 : "-0.8491" for DRSLL, "-1.887" for LMKLL or "6.3 0.0093" for rVV10
line 3 : Use $G_{max} = 25$ or 30 in case of numerical noise
line 4 : Eventually repeat with larger ρ_c (e.g, 0.6)
line 5 : Potential is necessary only for forces. Save computational time if set to "F"

Nonlocal vdW functionals: convergence with ρ_c and G_{max}

Strongly correlated electrons

Problem with semilocal functionals:

- They give qualitatively wrong results for solids which contain localized $3d$ or $4f$ electrons
  - The band gap is too small (zero in FeO!)
  - The magnetic moment is too small (zero in $YBa_2Cu_3O_6$!)
  - Wrong electronic configuration

Why?

- The strong on-site correlations are not correctly accounted for by semilocal functionals.

(Partial) solution to the problem:

- Combine semilocal functionals with Hartree-Fock theory:
  - DFT+U
  - Hybrid

Even better:

- LDA+DMFT (DMFT codes using WIEN2k orbitals as input exist)

On-site DFT+U and hybrid methods in WIEN2k

- For solids, the hybrid functionals are computationally very expensive.

- In WIEN2k the on-site DFT+U[1] and on-site hybrid[2,3] methods are available. These methods are approximations of the Hartree-Fock/hybrid methods

- Applied only inside atomic spheres of selected atoms and electrons of a given angular momentum ℓ.

On-site methods $\rightarrow$ As cheap as LDA/GGA.

[1] V. I. Anisimov et al., Phys. Rev. B **44**, 943 (1991)

[2] P. Novák et al., Phys. Stat. Sol. (b) **243**, 563 (2006)

[3] F. Tran et al., Phys. Rev. B **74**, 155108 (2006)

DFT+U and hybrid exchange-correlation functionals

The exchange-correlation functional is

$$E_{\text{xc}}^{\text{DFT}+U/\text{hybrid}} = E_{\text{xc}}^{\text{DFT}}[\rho] + E^{\text{onsite}}[n_{mm'}]$$

where $n_{mm'}$ is the density matrix of the correlated electrons

▶ For DFT+U both exchange and Coulomb are corrected:

$$E^{\text{onsite}} = \underbrace{E_{\text{x}}^{\text{HF}} + E_{\text{Coul}}}_{\text{correction}} - \underbrace{E_{\text{x}}^{\text{DFT}} - E_{\text{Coul}}^{\text{DFT}}}_{\text{double counting}}$$

There are several versions of the double-counting term

▶ For the hybrid methods only exchange is corrected:

$$E^{\text{onsite}} = \underbrace{\alpha E_{\text{x}}^{\text{HF}}}_{\text{corr.}} - \underbrace{\alpha E_{\text{x}}^{\text{LDA}}}_{\text{d. count.}}$$

where α is a parameter $\in [0, 1]$

How to run DFT+U and on-site hybrid calculations?

1. Create the input files:
   - case.inorb and case.indm for DFT+U
   - case.ineece for on-site hybrid functionals (case.indm created automatically):

2. Run the job (can only be run with runsp_lapw):
   - LDA+U: runsp_lapw -orb ...
   - Hybrid: runsp_lapw -eece ...

   For a calculation without spin-polarization ($\rho_\uparrow = \rho_\downarrow$):
   runsp_c_lapw -orb/eece ...

Input file case.inorb

LDA+U applied to the $4f$ electrons of atoms No. 2 and 4:

```
1 2 0                  nmod, natorb, ipr
PRATT,1.0              mixmod, amix
2 1 3                  iatom, nlorb, lorb
4 1 3                  iatom, nlorb, lorb
1                      nsic (LDA+U(SIC) used)
0.61 0.07              U J (Ry)
0.61 0.07              U J (Ry)
```

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nsic=0 for the AMF method (less strongly correlated electrons)
nsic=1 for the SIC method
nsic=2 for the HMF method

Review article : E. R. Ylvisaker *et al.*, Phys. Rev. B **79**, 035103 (2009)

Input file case.ineece

On-site hybrid functional PBE0 applied to the $4f$ electrons of atoms No. 2 and 4:

```
-12.0 2                 emin, natorb
2 1 3                   iatom, nlorb, lorb
4 1 3                   iatom, nlorb, lorb
HYBR                    HYBR/EECE
0.25                    fraction of exact exchange
```

SCF cycle of DFT+U in WIEN2k

| lapw0 | $\rightarrow v_{\mathrm{xc},\sigma}^{\mathrm{DFT}} + v_{\mathrm{ee}} + v_{\mathrm{en}}$ (case.vspup(dn), case.vnsup(dn)) |

| orb -up | $\rightarrow v_{mm'}^{\uparrow}$ (case.vorbup) |
| orb -dn | $\rightarrow v_{mm'}^{\downarrow}$ (case.vorbdn) |

| lapw1 -up -orb | $\rightarrow \psi_{n\mathbf{k}}^{\uparrow}, \epsilon_{n\mathbf{k}}^{\uparrow}$ (case.vectorup, case.energyup) |
| lapw1 -dn -orb | $\rightarrow \psi_{n\mathbf{k}}^{\downarrow}, \epsilon_{n\mathbf{k}}^{\downarrow}$ (case.vectordn, case.energydn) |

| lapw2 -up | $\rightarrow \rho_{\mathrm{val}}^{\uparrow}$ (case.clmvalup) |
| lapw2 -dn | $\rightarrow \rho_{\mathrm{val}}^{\downarrow}$ (case.clmvaldn) |

| lapwdm -up | $\rightarrow n_{mm'}^{\uparrow}$ (case.dmatup) |
| lapwdm -dn | $\rightarrow n_{mm'}^{\downarrow}$ (case.dmatdn) |

| lcore -up | $\rightarrow \rho_{\mathrm{core}}^{\uparrow}$ (case.clmcorup) |
| lcore -dn | $\rightarrow \rho_{\mathrm{core}}^{\downarrow}$ (case.clmcordn) |

| mixer | $\rightarrow$ mixed ρ^{σ} and $n_{mm'}^{\sigma}$ |

Hybrid functionals

- On-site hybrid functionals can be applied only to localized electrons
- Full hybrid functionals are necessary (but expensive) for solids with delocalized electrons (e.g., in sp-semiconductors)

Two types of full hybrid functionals available in WIEN2k[1]:

- unscreened:

$$E_{\mathrm{xc}} = E_{\mathrm{xc}}^{\mathrm{DFT}} + \alpha \left(E_{\mathrm{x}}^{\mathrm{HF}} - E_{\mathrm{x}}^{\mathrm{DFT}} \right)$$

- screened (short-range), $\frac{1}{|\mathbf{r}-\mathbf{r}'|} \rightarrow \frac{e^{-\lambda|\mathbf{r}-\mathbf{r}'|}}{|\mathbf{r}-\mathbf{r}'|}$:

$$E_{\mathrm{xc}} = E_{\mathrm{xc}}^{\mathrm{DFT}} + \alpha \left(E_{\mathrm{x}}^{\mathrm{SR-HF}} - E_{\mathrm{x}}^{\mathrm{SR-DFT}} \right)$$

screening leads to faster convergence with $\mathbf{k}$-points sampling

[1] F. Tran and P. Blaha, Phys. Rev. B **83**, 235118 (2011)

Hybrid functionals: technical details

- 10-1000 times more expensive than LDA/GGA
- **k**-point and MPI parallelization
- Approximations to speed up the calculations:
  - Reduced **k**-mesh for the HF potential. Example:
    For a calculation with a $12 \times 12 \times 12$ **k**-mesh, the reduced **k**-mesh for the HF potential can be:
    $6 \times 6 \times 6$, $4 \times 4 \times 4$, $3 \times 3 \times 3$, $2 \times 2 \times 2$ or $1 \times 1 \times 1$
  - Non-self-consistent calculation of the band structure
- Underlying functionals for unscreened and screend hybrid:
  - LDA
  - PBE
  - WC
  - PBEsol
  - B3PW91
  - B3LYP
- Use run_bandplothf_lapw for band structure

Hybrid functionals: input file case.inhf

Example for YS-PBE0 (similar to HSE06 from Heyd, Scuseria and Ernzerhof[1])

0.25	fraction α of HF exchange
T	screened (T, YS-PBE0) or unscreened (F, PBE0)
0.165	screening parameter λ
20	number of bands for the 2nd Hamiltonian
6	GMAX
3	lmax for the expansion of orbitals
3	lmax for the product of two orbitals
1d-3	radial integrals below this value neglected

Important: The computational time will depend strongly on the number of bands, GMAX, lmax and the number of k-points

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[1] A. V. Krukau et al., J. Chem. Phys. **125**, 224106 (2006)

How to run hybrid functionals?

1. init_lapw
2. Recommended: run(sp)_lapw for the semilocal functional
3. save_lapw
4. init_hf_lapw (this will create/modify input files)
   4.1 adjust case.inhf according to your needs
   4.2 reduced **k**-mesh for the HF potential? Yes or no
   4.3 specify the **k**-mesh
5. run(sp)_lapw -hf (-redklist) (-diaghf) ...

SCF cycle of hybrid functionals in WIEN2k

lapw0 -grr	$\rightarrow v_x^{\mathrm{DFT}}$ (case.r2v), $\alpha E_x^{\mathrm{DFT}}$ (:AEXSL)
lapw0	$\rightarrow v_{xc}^{\mathrm{DFT}} + v_{ee} + v_{en}$ (case.vsp, case.vns)
lapw1	$\rightarrow \psi_{n\mathbf{k}}^{\mathrm{DFT}}, \epsilon_{n\mathbf{k}}^{\mathrm{DFT}}$ (case.vector, case.energy)
lapw2	$\rightarrow \sum_{n\mathbf{k}} \epsilon_{n\mathbf{k}}^{\mathrm{DFT}}$ (:SLSUM)
hf	$\rightarrow \psi_{n\mathbf{k}}, \epsilon_{n\mathbf{k}}$ (case.vectorhf, case.energyhf)
lapw2 -hf	$\rightarrow \rho_{\mathrm{val}}$ (case.clmval)
lcore	$\rightarrow \rho_{\mathrm{core}}$ (case.clmcor)
mixer	$\rightarrow$ mixed ρ

Some recommendations

Before using a functional:

- read a few papers about the functional in order to know
  - for which properties or types of solids it is supposed to be reliable
  - if it is adapted to your problem
- figure out if you have enough computational ressources
  - hybrid functionals and GW require (substantially) more computational ressources (and patience)