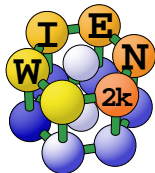


Methods available in WIEN2k for the treatment of exchange and correlation effects

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Hamilton, Canada



Outline of the talk

- ▶ Introduction
- ▶ Semilocal functionals:
 - ▶ GGA and MGGA
 - ▶ mBJ potential (for band gap)
 - ▶ Input file `case.in0`
- ▶ The DFT-D3 method for dispersion
- ▶ On-site methods for strongly correlated electrons:
 - ▶ DFT+ U
 - ▶ Hybrid functionals
- ▶ Hybrid functionals
- ▶ GW

Total energy in Kohn-Sham DFT ¹

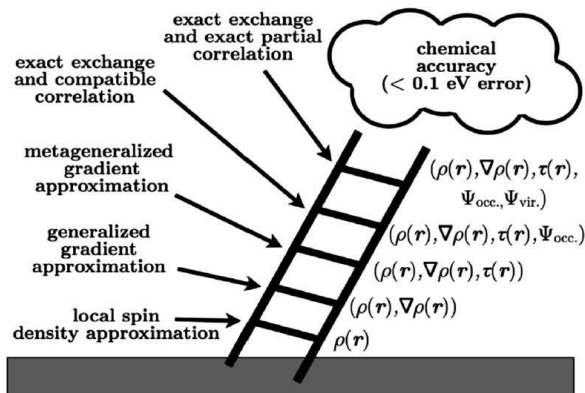
$$E_{\text{tot}} = \underbrace{\frac{1}{2} \sum_i \int |\nabla \psi_i(\mathbf{r})|^2 d^3 r}_{T_s} + \underbrace{\frac{1}{2} \int \int \frac{\rho(\mathbf{r})\rho(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} d^3 r d^3 r'}_{E_{ee}} + \underbrace{\int v_{\text{en}}(\mathbf{r})\rho(\mathbf{r})d^3 r}_{E_{en}} \\ + \underbrace{\frac{1}{2} \sum_{\substack{A,B \\ A \neq B}} \frac{Z_A Z_B}{|\mathbf{R}_A - \mathbf{R}_B|}}_{E_{nn}} + E_{\text{xc}}$$

- ▶ T_s : kinetic energy of the non-interacting electrons
- ▶ E_{ee} : electron-electron electrostatic Coulomb energy
- ▶ E_{en} : electron-nucleus electrostatic Coulomb energy
- ▶ E_{nn} : nucleus-nucleus electrostatic Coulomb energy
- ▶ $E_{\text{xc}} = E_x + E_c$: exchange-correlation energy
Approximations for E_{xc} have to be used in practice
⇒ The reliability of the results depends mainly on E_{xc} !

¹W. 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)

The 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}_{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)
 - ▶ Hartree-Fock
 - ▶ LDA+ U
 - ▶ Hybrid (mixing of GGA and Hartree-Fock)
 - ▶ MGGA
 - ▶ Self-interaction corrected (Perdew-Zunger)

Semilocal functionals: trends with GGA

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

where F_{xc} is the enhancement factor and

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

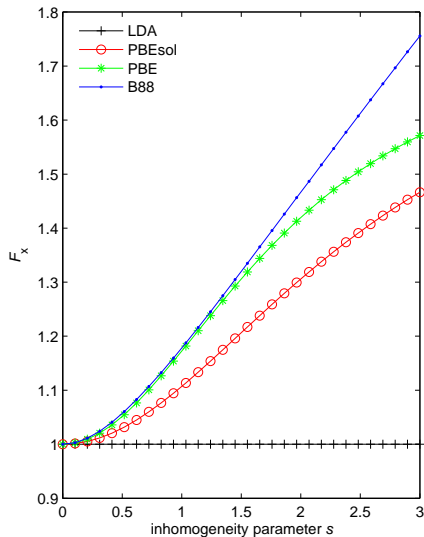
$$s = \frac{|\nabla\rho|}{2(3\pi^2)^{1/3}\rho^{4/3}} \quad (\text{inhomogeneity parameter})$$

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: GGA

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



good for atomization energy of molecules

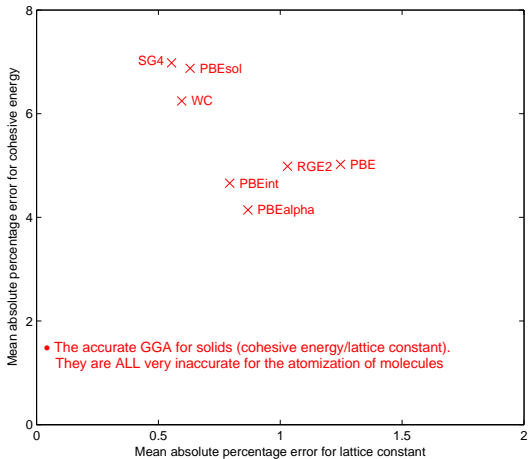
good for atomization energy of solids

good for lattice constant of solids

good for nothing

Construction of an universal GGA: A failure

Test of functionals on 44 solids¹



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

Semilocal functionals: meta-GGA

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

where F_{xc} is the enhancement factor and

- ▶ $\alpha = \frac{t-t_W}{t_{TF}}$
 - ▶ $\alpha = 1$ where the electron density is uniform
 - ▶ $\alpha = 0$ in one- and two-electron regions
 - ▶ $\alpha \gg 1$ between closed shell atoms

⇒ MGGA functionals are more flexible

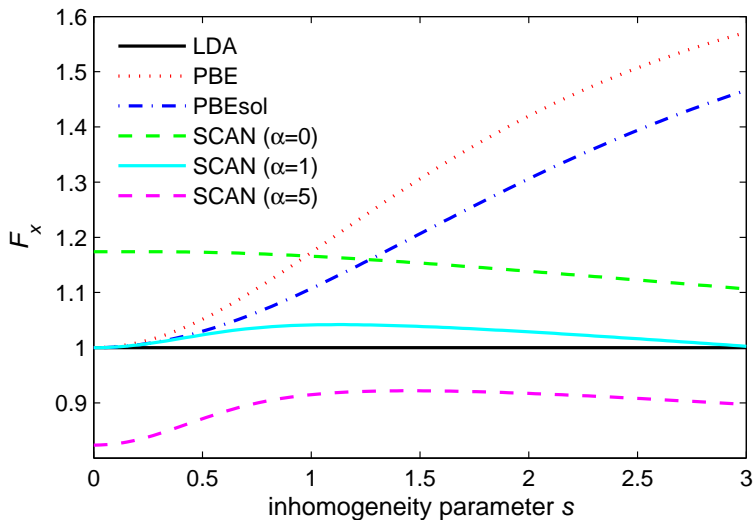
Example: SCAN¹ is

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

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

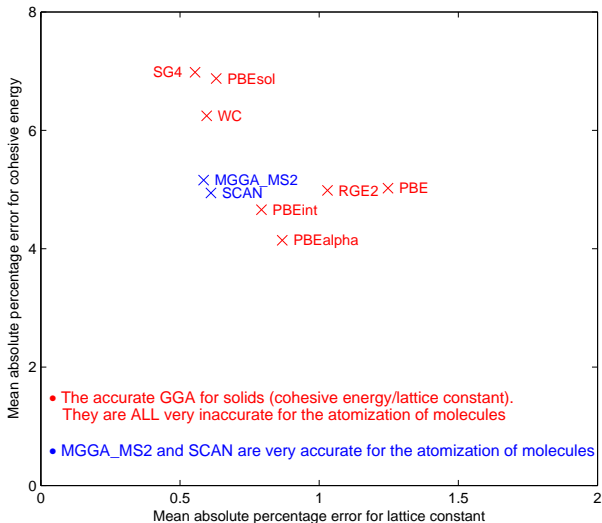
Semilocal functionals: meta-GGA

$$F_x(s, \alpha) = \epsilon_x^{\text{MGGA}} / \epsilon_x^{\text{LDA}}$$



Semilocal functionals: MGGA_MS2 and SCAN

Test of functionals on 44 solids¹



¹F. 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

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

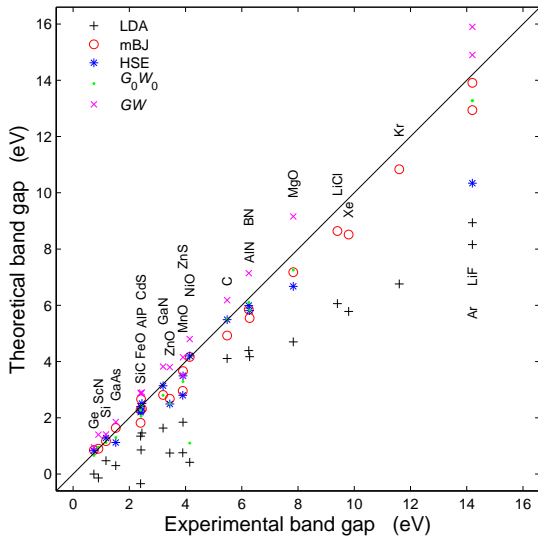
where v_x^{BR} is the Becke-Roussel potential, t is the kinetic-energy density and c is given by

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

mBJ is a MGGA potential

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

Band gaps with mBJ



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 values¹
 - 1: New parametrization²
 - 2: New parametrization for semiconductors²
 - 3: Original BJ potential³
4. `run(sp)_lapw ...`

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

²D. Koller *et al.*, *Phys. Rev. B* **85**, 155109 (2012)

³A. 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**

¹M. A. L. Marques *et al.*, *Comput. Phys. Commun.* **183**, 2272 (2012)

Input file case.in0: examples with keywords

- ▶ 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 0.504 0.14601 4.0
 κ, c, b

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

Dispersion methods for DFT

Problem with semilocal functionals:

- ▶ They do not include **London dispersion interactions**
- ▶ Results are qualitatively wrong for systems where dispersion plays a major role

Two common dispersion methods for DFT:

- ▶ Pairwise term¹:

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

- ▶ Nonlocal term²:

$$E_{c,\text{disp}}^{\text{NL}} = \frac{1}{2} \int \int \rho(\mathbf{r}) \phi(\mathbf{r}, \mathbf{r}') \rho(\mathbf{r}') d^3 r d^3 r'$$

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

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

The DFT-D3 method¹ in WIEN2k

► Features of DFT-D3:

- Very cheap (pairwise)
- C_n^{AB} depend on positions of the nuclei (via coordination number)
- Functional-dependent parameters
- Energy and forces (minimization of internal parameters)
- 3-body term

► Installation:

- Not included in WIEN2k
- Download and compile the DFTD3 package from <http://www.thch.uni-bonn.de/tc/index.php>
copy the `dftd3` executable in \$WIENROOT
- input file `case.indftd3` (if not present a default one is copied automatically)
- `run(sp)_lapw -dftd3 ...`
- `case.scfdftd3` is included in `case.scf`

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

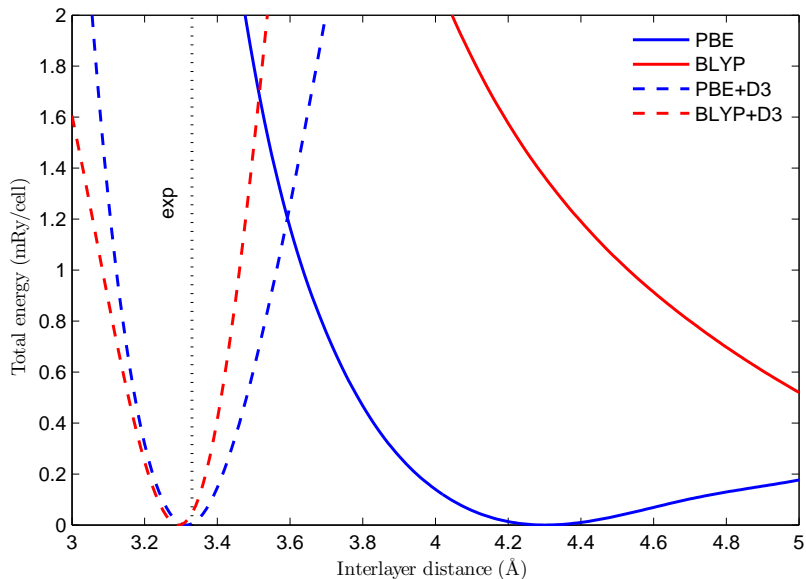
The DFT-D3 method: the input file case.indftd3

Default (and recommended) input file:

method	bj	damping function f_n^{damp}
func	default	the one in case.in0*
grad	yes	forces
pbcb	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)

The DFT-D3 method: hexagonal BN¹



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

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 or even absent like in FeO
 - ▶ The magnetic moments are too small
 - ▶ Wrong ground state

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 → **As cheap as LDA/GGA**.

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

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

³F. 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 -ecee ...`

For a calculation without spin-polarization ($\rho_{\uparrow} = \rho_{\downarrow}$):

`runsp_c_lapw -orb/ecee ...`

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)
```

nsic=0 for the AMF method (less strongly correlated electrons)

nsic=1 for the SIC method

nsic=2 for the HMF method

Input file case.ineece

On-site hybrid functional PBE0 applied to the 4*f* 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	$\rightarrow v_{xc,\sigma}^{DFT} + v_{ee} + v_{en}$ (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	$\rightarrow \psi_{nk}^{\uparrow}, \epsilon_{nk}^{\uparrow}$ (case.vectorup, case.energyup)
lapw1 -dn -orb	$\rightarrow \psi_{nk}^{\downarrow}, \epsilon_{nk}^{\downarrow}$ (case.vectordn, case.energydn)
lapw2 -up	$\rightarrow \rho_{val}^{\uparrow}$ (case.clmvalup)
lapw2 -dn	$\rightarrow \rho_{val}^{\downarrow}$ (case.clmvaldn)
lapwdm -up	$\rightarrow n_{mm'}^{\uparrow}$ (case.dmatup)
lapwdm -dn	$\rightarrow n_{mm'}^{\downarrow}$ (case.dmatdn)
lcore -up	$\rightarrow \rho_{core}^{\uparrow}$ (case.clmcorup)
lcore -dn	$\rightarrow \rho_{core}^{\downarrow}$ (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 WIEN2k¹:

- ▶ unscreened:

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

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

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

screening leads to faster convergence with **k**-points sampling

¹F. 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 screened 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 Ernzerhof¹)

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

¹A. 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

→ v_x^{DFT} (case.r2v), αE_x^{DFT} (:AEXSL)

lapw0

→ $v_{xc}^{\text{DFT}} + v_{ee} + v_{en}$ (case.vsp, case.vns)

lapw1

→ $\psi_{nk}^{\text{DFT}}, \epsilon_{nk}^{\text{DFT}}$ (case.vector, case.energy)

lapw2

→ $\sum_{nk} \epsilon_{nk}^{\text{DFT}}$ (:SLSUM)

hf

→ ψ_{nk}, ϵ_{nk} (case.vectorhf, case.energyhf)

lapw2 -hf

→ ρ_{val} (case.clmval)

lcore

→ ρ_{core} (case.clmcor)

mixer

→ mixed ρ

Calculation of quasiparticle spectra from many-body theory

- ▶ In principle the Kohn-Sham eigenvalues should be viewed as mathematical objects and not compared directly to experiment (ionization potential and electron affinity).
- ▶ The true addition and removal energies ϵ_i are calculated from the **equation of motion for the Green function**:

$$\left(-\frac{1}{2}\nabla^2 + v_{\text{en}}(\mathbf{r}) + v_{\text{H}}(\mathbf{r})\right) + \int \Sigma(\mathbf{r}, \mathbf{r}', \epsilon_i) \psi_i(\mathbf{r}') d^3 r' = \epsilon_i \psi_i(\mathbf{r})$$

- ▶ The self-energy Σ is calculated from Hedin's self-consistent equations¹:

$$\Sigma(1, 2) = i \int G(1, 4) W(1^+, 3) \Gamma(4, 2, 3) d(3, 4)$$

$$W(1, 2) = v(1, 2) + \int v(4, 2) P(3, 4) W(1, 3) d(3, 4)$$

$$P(1, 2) = -i \int G(2, 3) G(4, 2) \Gamma(3, 4, 1) d(3, 4)$$

$$\Gamma(1, 2, 3) = \delta(1, 2) \delta(1, 3) + \int \frac{\delta \Sigma(1, 2)}{\delta G(4, 5)} G(4, 6) G(7, 5) \Gamma(6, 7, 3) d(4, 5, 6, 7)$$

¹L. Hedin, Phys. Rev. **139**, A769 (1965)

The GW and G_0W_0 approximations

- ▶ **GW**: vertex function Γ in Σ set to 1:

$$\Sigma(1,2) = i \int G(1,4)W(1^+,3)\Gamma(4,2,3)d(3,4) \approx iG(1,2^+)W(1,2)$$

$$\Sigma(\mathbf{r},\mathbf{r}',\omega) = \frac{i}{2\pi} \int_{-\infty}^{\infty} G(\mathbf{r},\mathbf{r}',\omega+\omega')W(\mathbf{r},\mathbf{r}',\omega')e^{-i\delta\omega'}d\omega'$$

$$G(\mathbf{r},\mathbf{r}',\omega) = \sum_{i=1}^{\infty} \frac{\psi_i(\mathbf{r})\psi_i^*(\mathbf{r}')}{\omega - \epsilon_i - i\eta_i} \quad W(\mathbf{r},\mathbf{r}',\omega) = \int v(\mathbf{r},\mathbf{r}'')\epsilon^{-1}(\mathbf{r}'',\mathbf{r}',\omega)d^3r''$$

- ▶ **G_0W_0 (one-shot GW)**:
 G and W are calculated using the Kohn-Sham orbitals and eigenvalues. 1st order perturbation theory gives

$$\epsilon_i^{GW} = \epsilon_i^{KS} + Z(\epsilon_i^{KS})\langle\psi_i^{KS}|\Re(\Sigma(\epsilon_i^{KS})) - v_{xc}|\psi_i^{KS}\rangle$$

A few remarks on GW

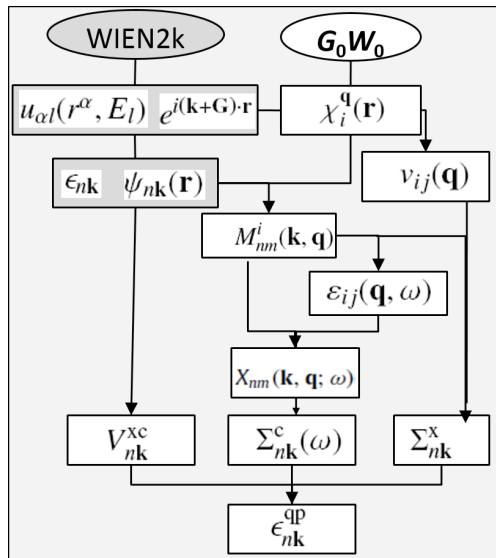
- ▶ GW calculations require very large computational resources
- ▶ G and W depend on all (occupied and unoccupied) orbitals (up to parameter e_{\max} in practice)
- ▶ GW is the state-of-the-art for the calculation of (inverse) photoemission spectra, but not for optics since excitonic effects are still missing in GW (BSE code from R. Laskowski)
- ▶ GW is more accurate for systems with weak correlations

FHI-gap: a LAPW GW code¹

- ▶ Based on the FP-LAPW basis set
- ▶ Mixed basis set to expand the GW -related quantities
- ▶ Interfaced with WIEN2k
- ▶ G_0W_0 , GW_0 @LDA/GGA(+ U)
- ▶ Parallelized
- ▶ <http://www.chem.pku.edu.cn/jianghgroup/codes/fhi-gap.html>

¹H. Jiang *et al.*, *Comput. Phys. Comput.* **184**, 348 (2013)

Flowchart of FHI-gap



How to run the FHI-gap code?

1. Run a WIEN2k SCF calculation (in `w2kdir`)
2. In `w2kdir`, execute the script `gap_init` to prepare the input files for *GW*:

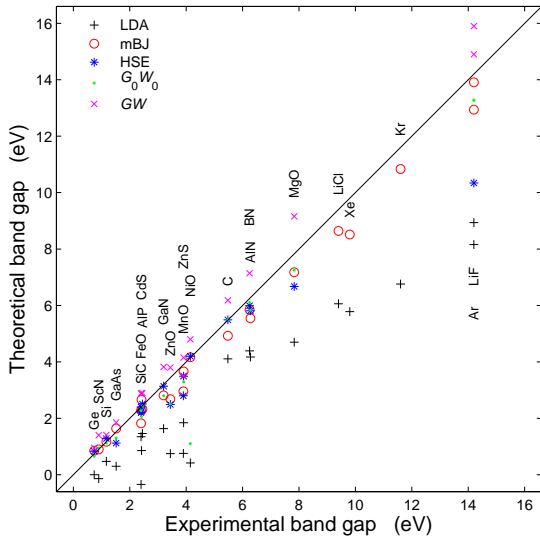
```
gap_init -d <gwdir> -nkp <nkp> -s 0/1/2 -orb -emax <emax>
```

3. Eventually modify `gwdir.ingw`
4. Execute `gap.x` or `gap-mpi.x` in `gwdir`
5. Analyse the results from:
 - 5.1 `gwdir.outgw`
 - 5.2 the plot of the DOS/band structure generated by `gap_analy`

Parameters to be converged for a GW calculation

- ▶ Usual WIEN2k parameters:
 - ▶ Size of the LAPW basis set (RK_{\max})
 - ▶ Number of **k-points** for the Brillouin zone integrations
- ▶ GW-specific parameters:
 - ▶ Size of the mixed basis set
 - ▶ Number of unoccupied states (e_{\max})
 - ▶ Number of frequencies ω for the calculation of $\Sigma = \int GWd\omega$

Band gaps



Some recommendations

Before using a method or a functional:

- ▶ Read a few papers concerning the method in order to know
 - ▶ why it has been used
 - ▶ for which properties or types of solids it is supposed to be reliable
 - ▶ if it is adapted to your problem
- ▶ Do you have enough computational resources?
 - ▶ hybrid functionals and GW require (substantially) more computational resources (and patience)