Introduction to the features of the FlapwMBPT code

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COMSCOPE
from codes to spectroscopies

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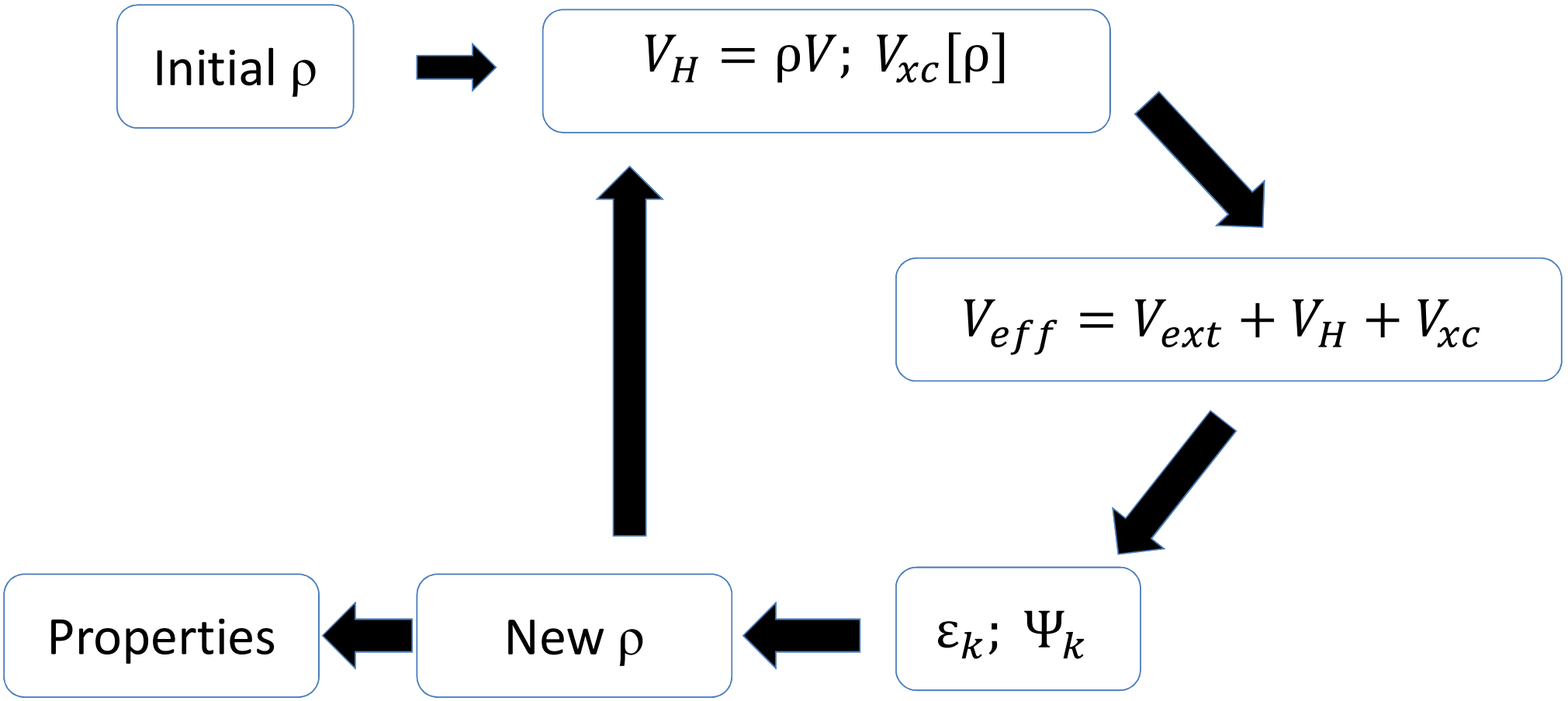
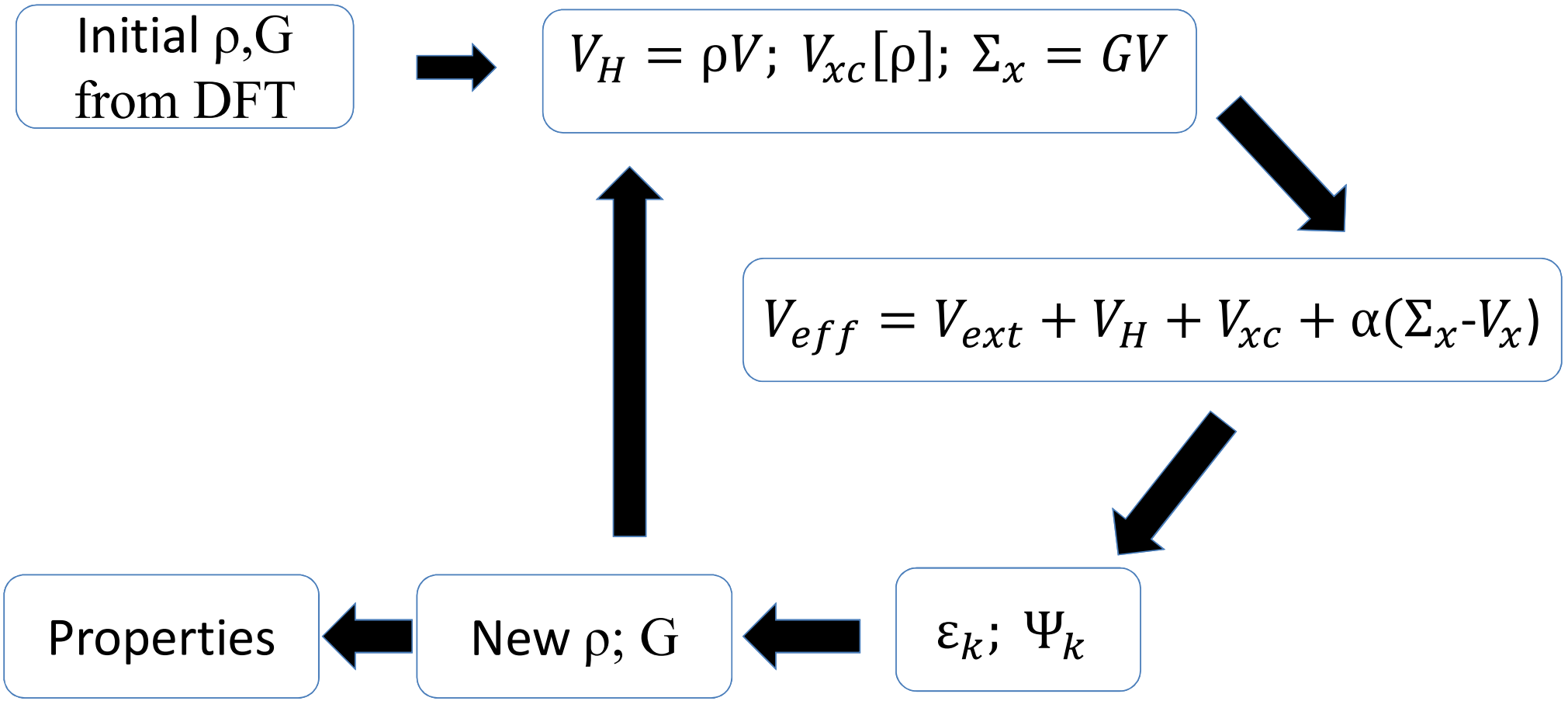
Plan

- Brief theory for the methods included in FlapwMBPT code
- General information about FlapwMBPT code
- How different methods are combined in one code
- DFT related features
- Hartree-Fock/Hybrids related features
- GW related features
- Diagrammatic approaches beyond GW approximation
- Examples of the calculations
- Hands on training

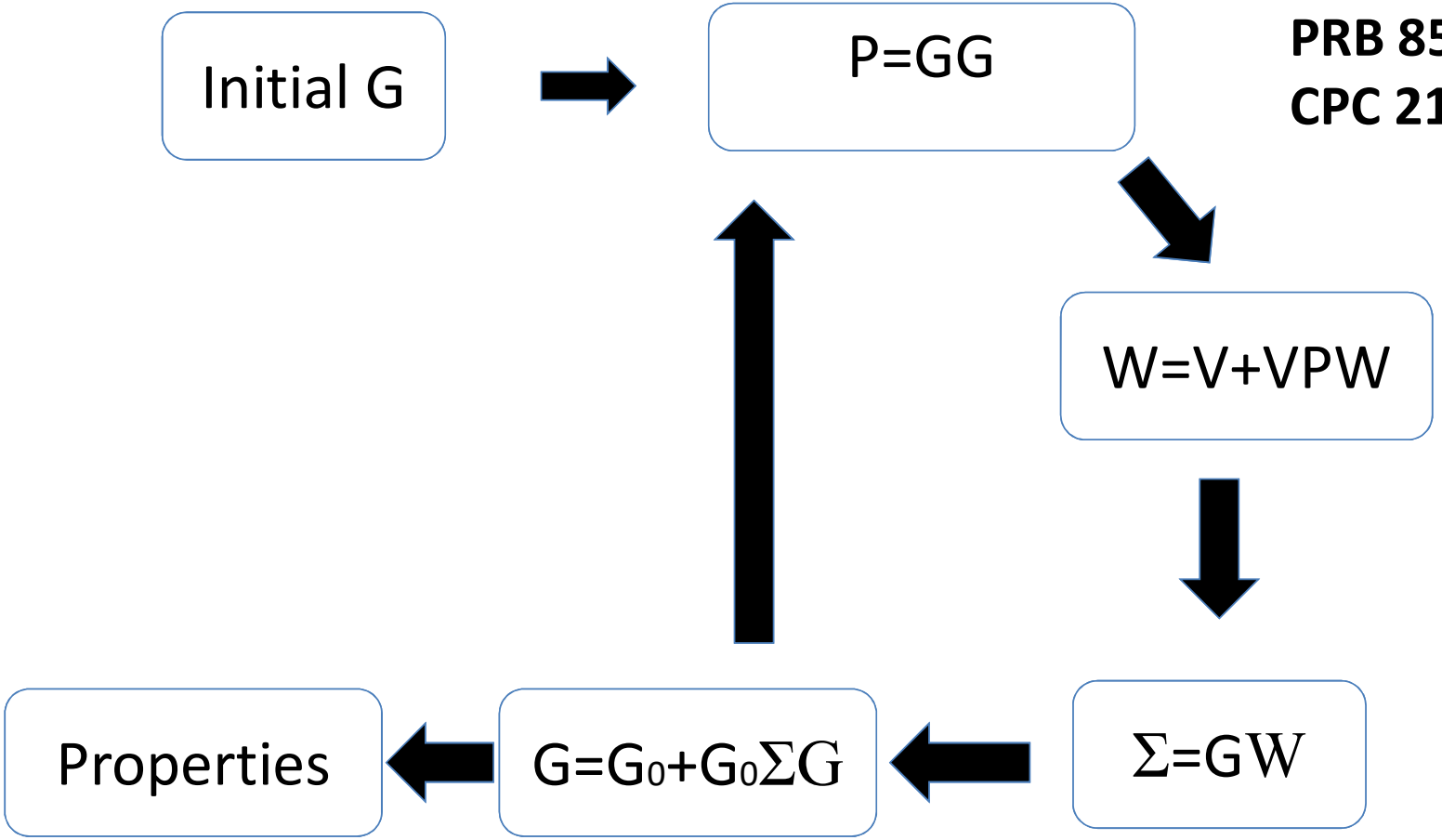
DFT


Initial ρ
$V_H = \rho V;\ V_{xc}[\rho]$
$V_{eff} = V_{ext} + V_H + V_{xc}$
$\varepsilon_k;\ \Psi_k$
New ρ
Properties

Hartree-Fock (Hybrids)

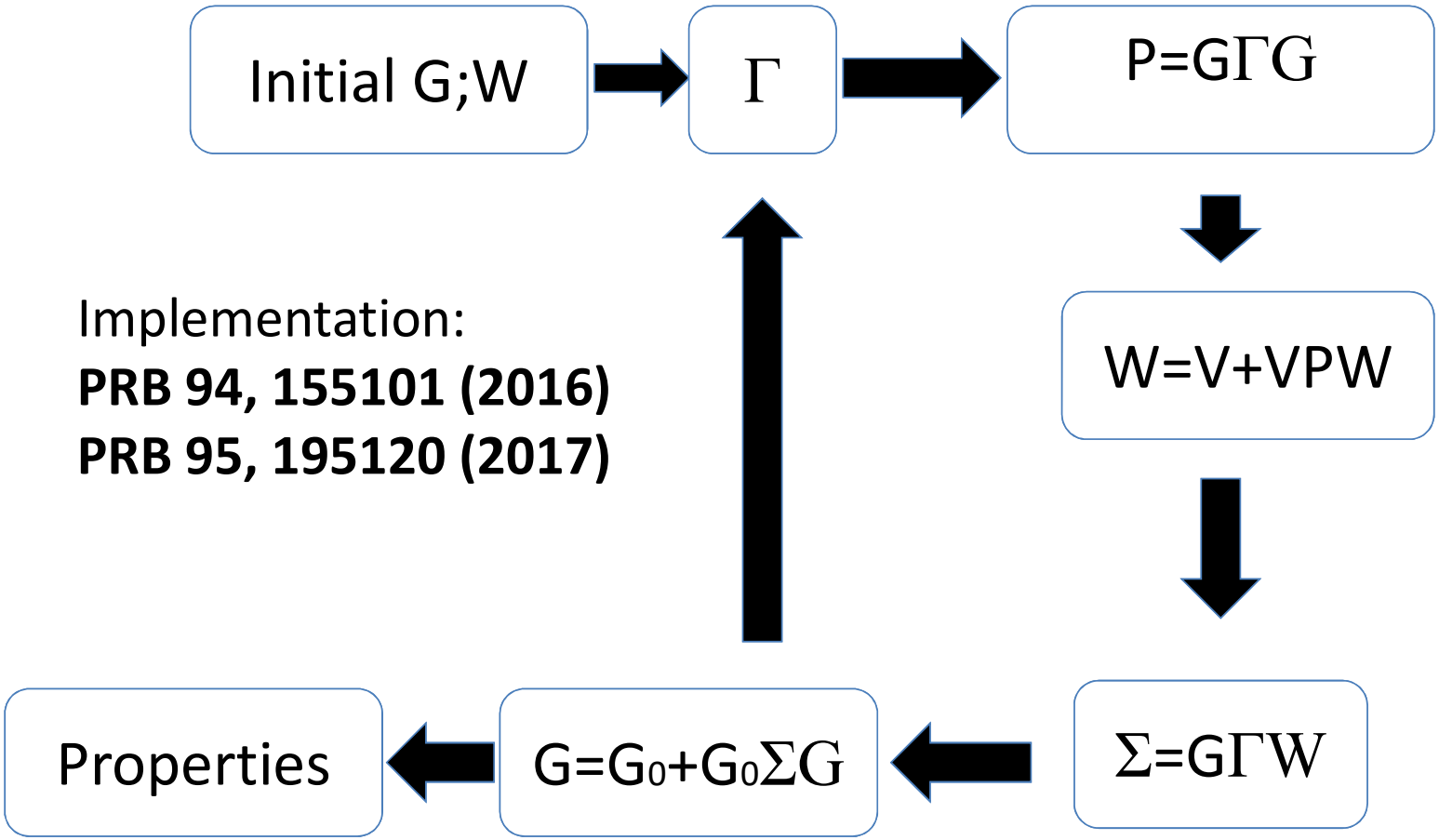


GW



Implementation:
PRB 85, 155129 (2012)
CPC 219, 407 (2017)

Vertex corrected GW



Implementation:
PRB 94, 155101 (2016)
PRB 95, 195120 (2017)

Hedin's equations (PR 139, A796 (1965))

$$\Gamma^{\alpha}(123) = \delta(12)\delta(13) + \sum_{\beta} \frac{\delta\Sigma^{\alpha}(12)}{\delta G^{\beta}(45)} G^{\beta}(46)\Gamma^{\beta}(673)G^{\beta}(75)$$

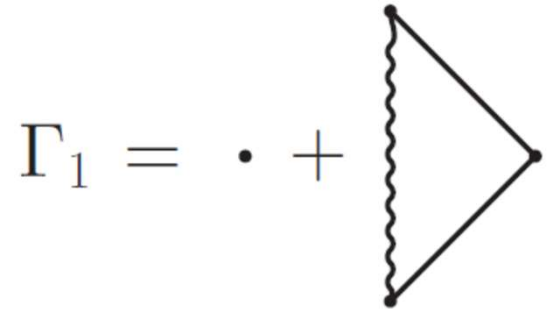
$$P(12) = \sum_{\alpha} G^{\alpha}(13)\Gamma^{\alpha}(342)G^{\alpha}(41)$$

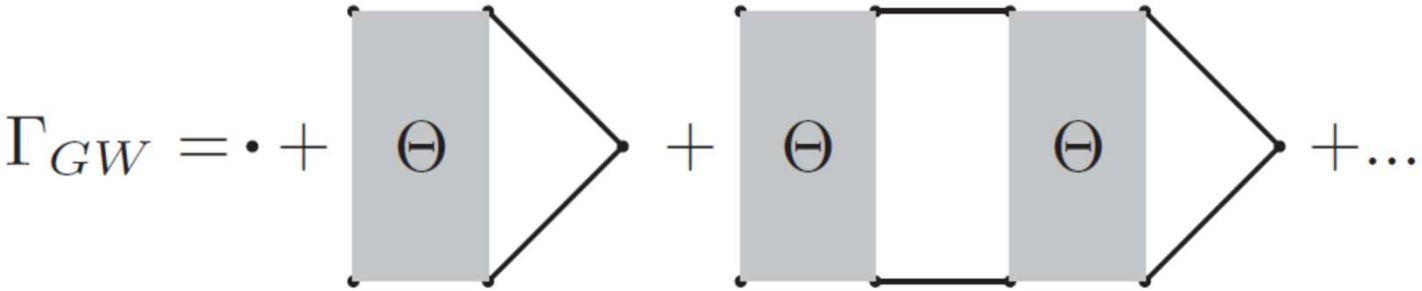
$$W(12) = V(12) + V(13)P(34)W(42)$$

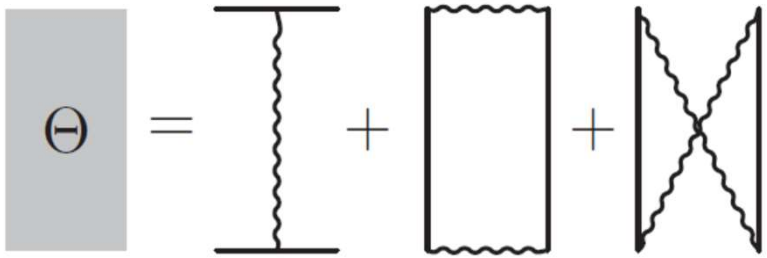
$$\Sigma^{\alpha}(12) = -G^{\alpha}(14)\Gamma^{\alpha}(425)W(51)$$

$$G^{\alpha}(12) = G_0^{\alpha}(12) + G_0^{\alpha}(13)\Sigma^{\alpha}(34)G^{\alpha}(42)$$

Approximations for the vertex



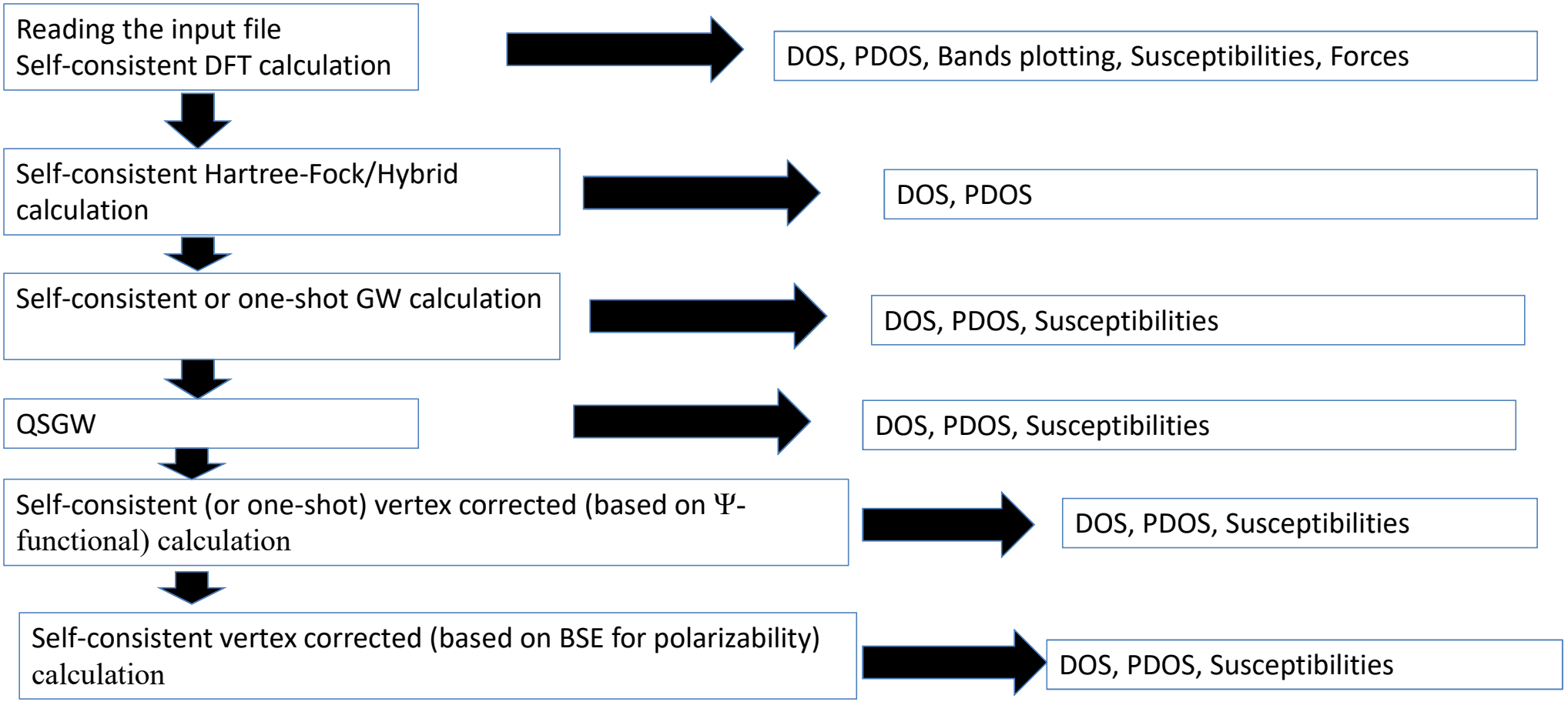




General information about FlapwMBPT

- Solid or electron gas (this talk is about solids only)
- Flexible FLAPW+LO all-electron basis set
- Non-relativistic, scalar-relativistic, or Dirac fully relativistic treatment of relativity
- Spin-polarized calculations
- MPI for parallelization
- Strictly one language (Fortran90) is used

How different methods are combined in one code



Summary of DFT related features

- Different functionals – LDA, GGA91, GGA96 (PBE)
- Can be used to generate “physical” W for subsequent GW or GWΓ

Properties available in DFT part

- Total energy: E(V), V0, B0, frozen phonons
- Atomic forces
- Susceptibilities (charge, longitudinal and transverse spin)
- One-electron spectra
- DOS, PDOS, k-resolved DOS
- Bands plotting

Summary of Hartree-Fock related features

- Hartree-Fock or Hybrids ($PBE0$, $YS-PBE0$)

(JCP 105, 9982(1996), PRB 83, 235118(2011))

- Can be used to generate “physical” W for subsequent GW or GWΓ

Properties available in Hartree-Fock part

- Total energy
- One-electron spectra
- DOS, PDOS, k-resolved DOS

Summary of GW related features

- One shot G_0W_0 or G_0W_{phys} with G_0, W_0 (W_{phys}) from DFT, Hartree-Fock, or Hybrid
- Partially sc GW_0 or GW_{phys} with W_0 (W_{phys}) from DFT, Hartree-Fock, or Hybrid
- Fully self-consistent GW
- QSGW or partial sc $QSGW_0$ or $QSGW_{phys}$
- Fully scGW can be used to generate "physical" W for subsequent $GW\Gamma$

Properties available in GW part

- Spectral functions (total, partial, k-resolved)
- Total energy (fully scGW)
- Susceptibilities

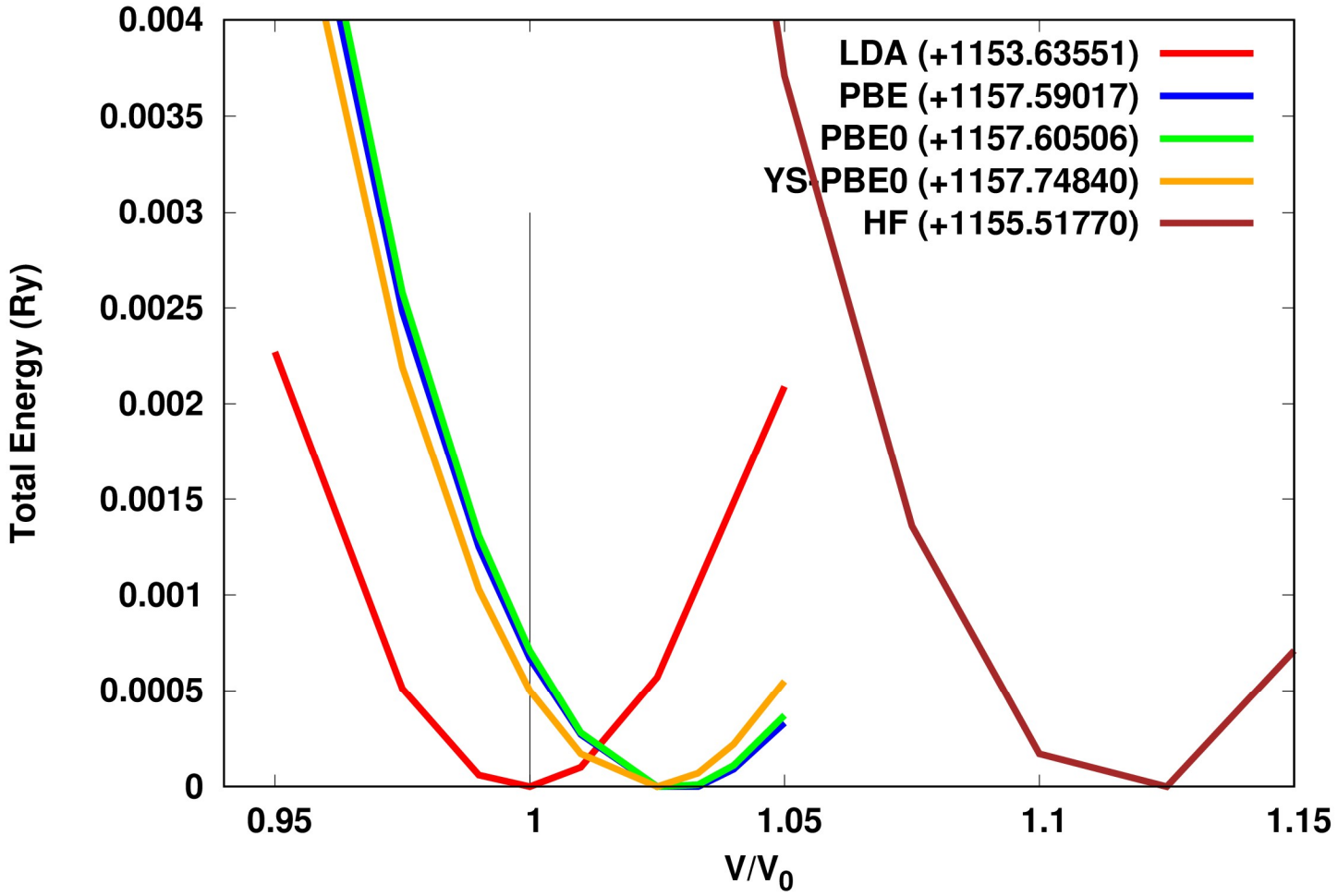
Diagrammatic approaches beyond GW

- One shot $G_0W_0\Gamma_1$ or $G_0W_{phys}\Gamma_1$ with G_0, W_0 (W_{phys}) from DFT, Hartree-Fock, Hybrid, or scGW
- Partially sc $GW_0\Gamma$ or $GW_{phys}\Gamma$ with W_0 (W_{phys}) from DFT, Hartree-Fock, Hybrid, or scGW
- Fully self-consistent $GW\Gamma$, different approaches for Γ, see PRB 94, 155101 (2016)
- Ψ-functional based scheme can be used to generate "physical" W for subsequent BSE-based scheme

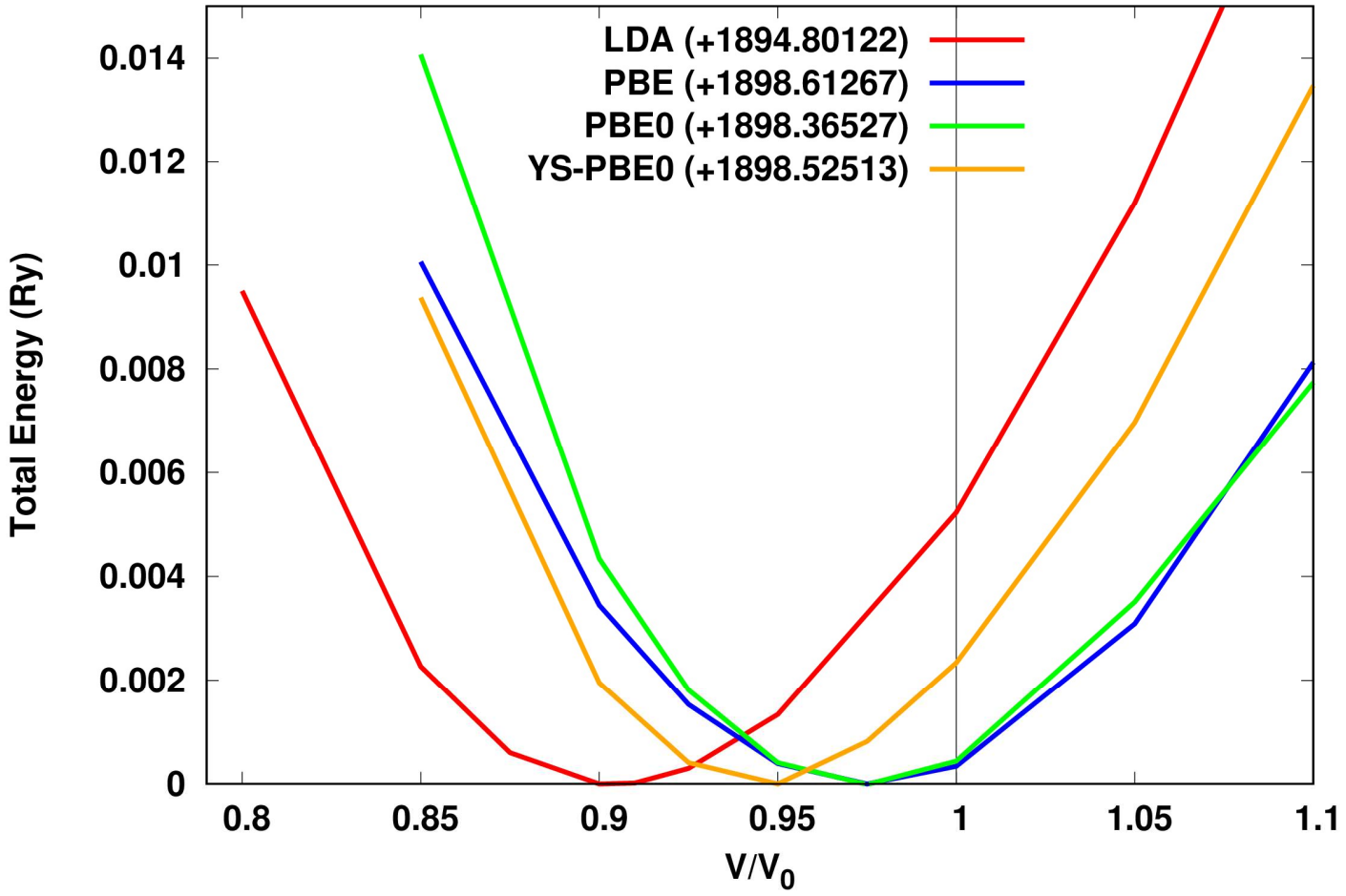
Properties available in $GW\Gamma$ part

- Spectral functions (total, partial, k-resolved)
- Total energy (Ψ-functional based schemes)
- Susceptibilities

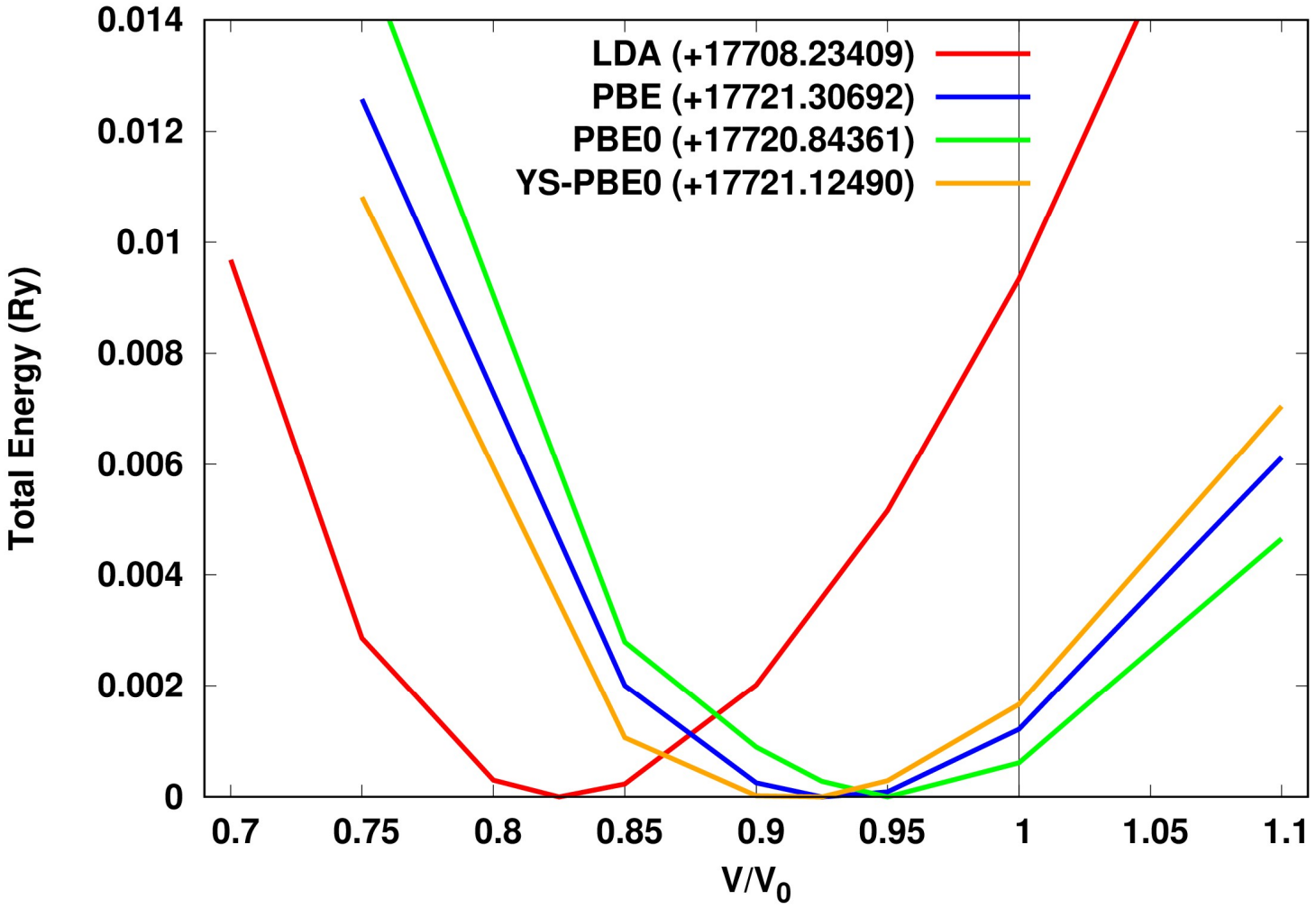
E(V) for Si (sp material)



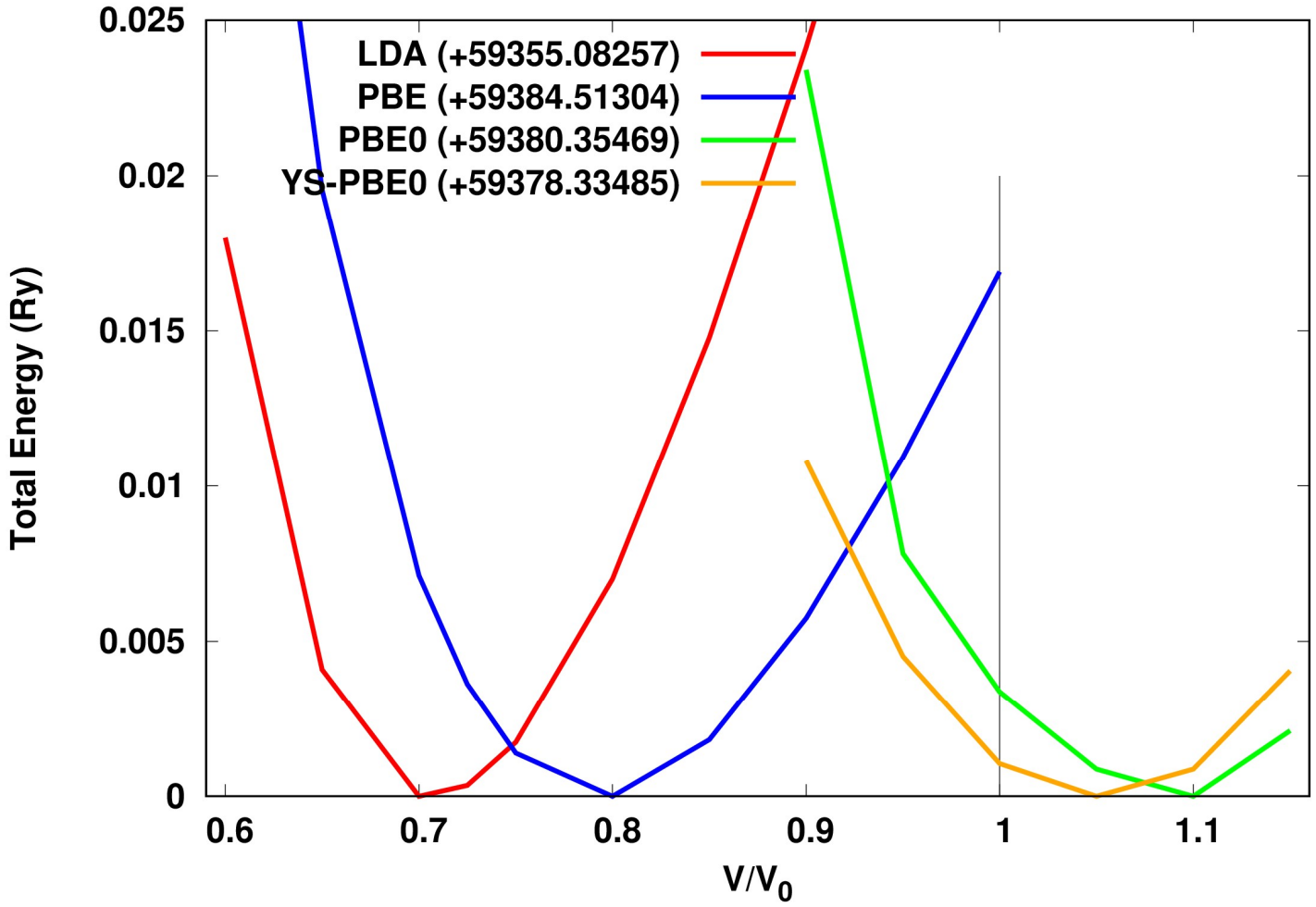
E(V) for V (3d transition metal)



E(V) for Ce (4f material)

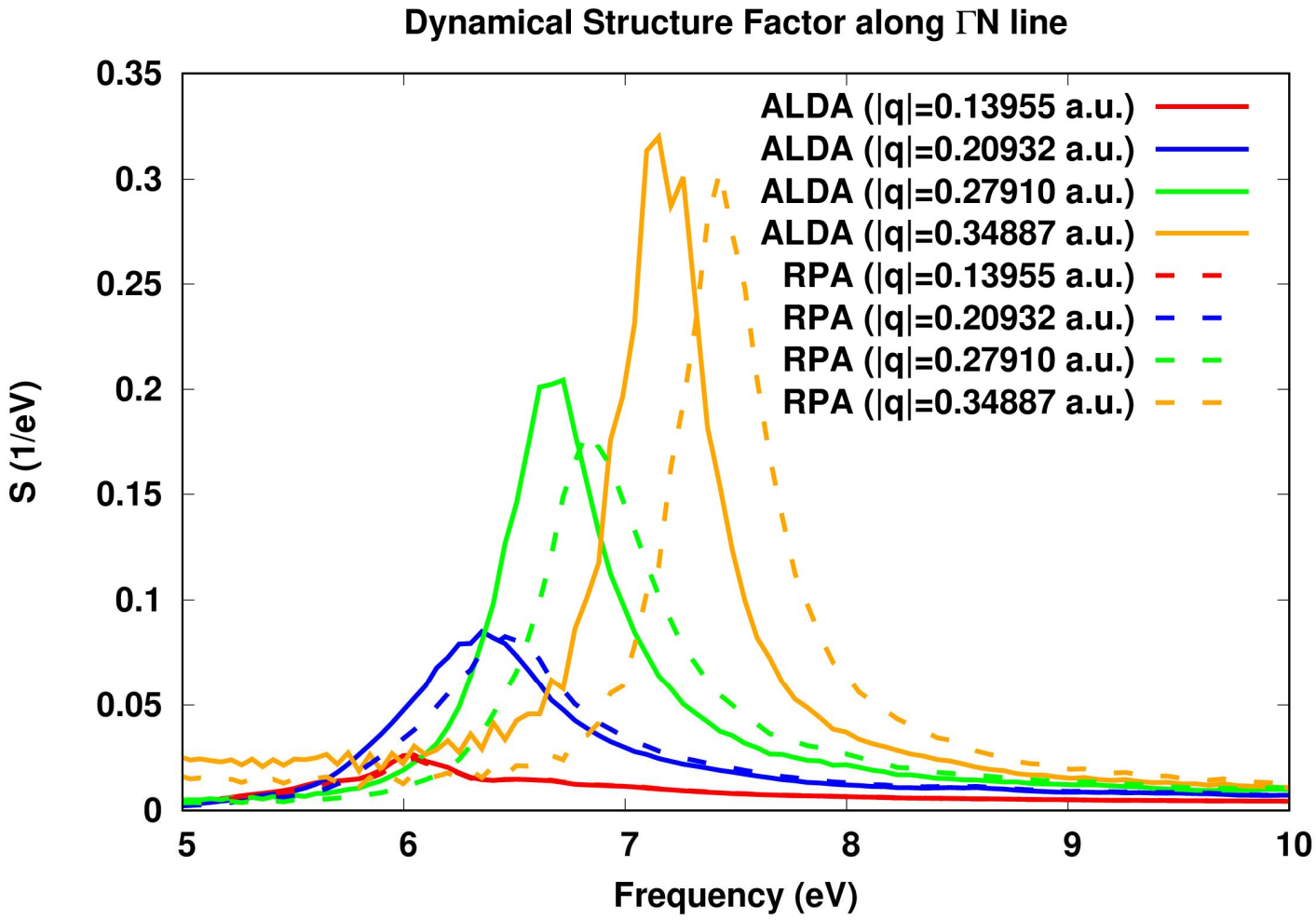


E(V) for Pu (5f material)

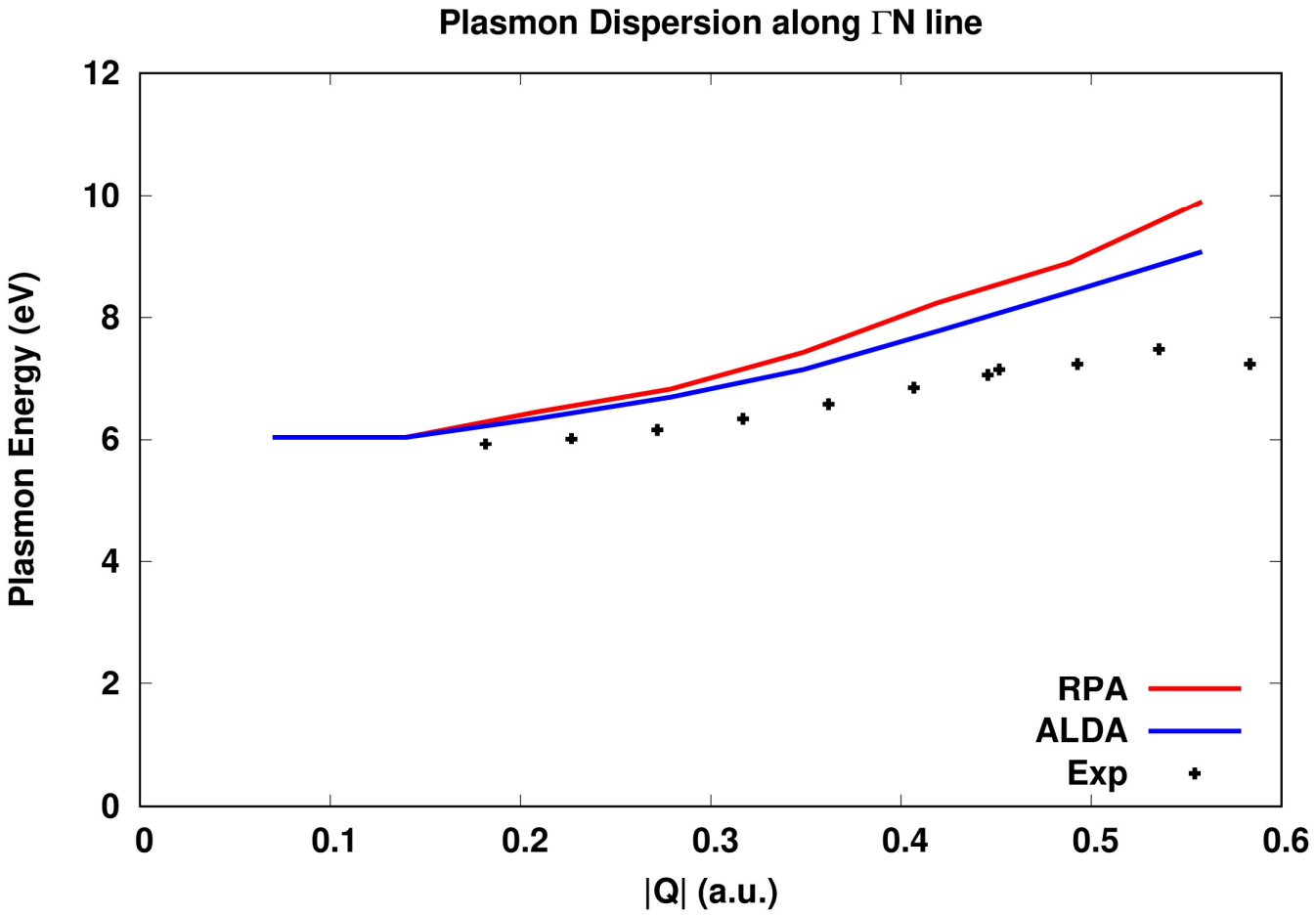


Na: Dynamical Structure Factor

$$S(\mathbf{Q},\omega) = -\frac{\hbar Q^2}{4\pi^2 e^2 n}\,\mathrm{Im}\frac{1}{\varepsilon_M(\mathbf{Q},\omega)}$$

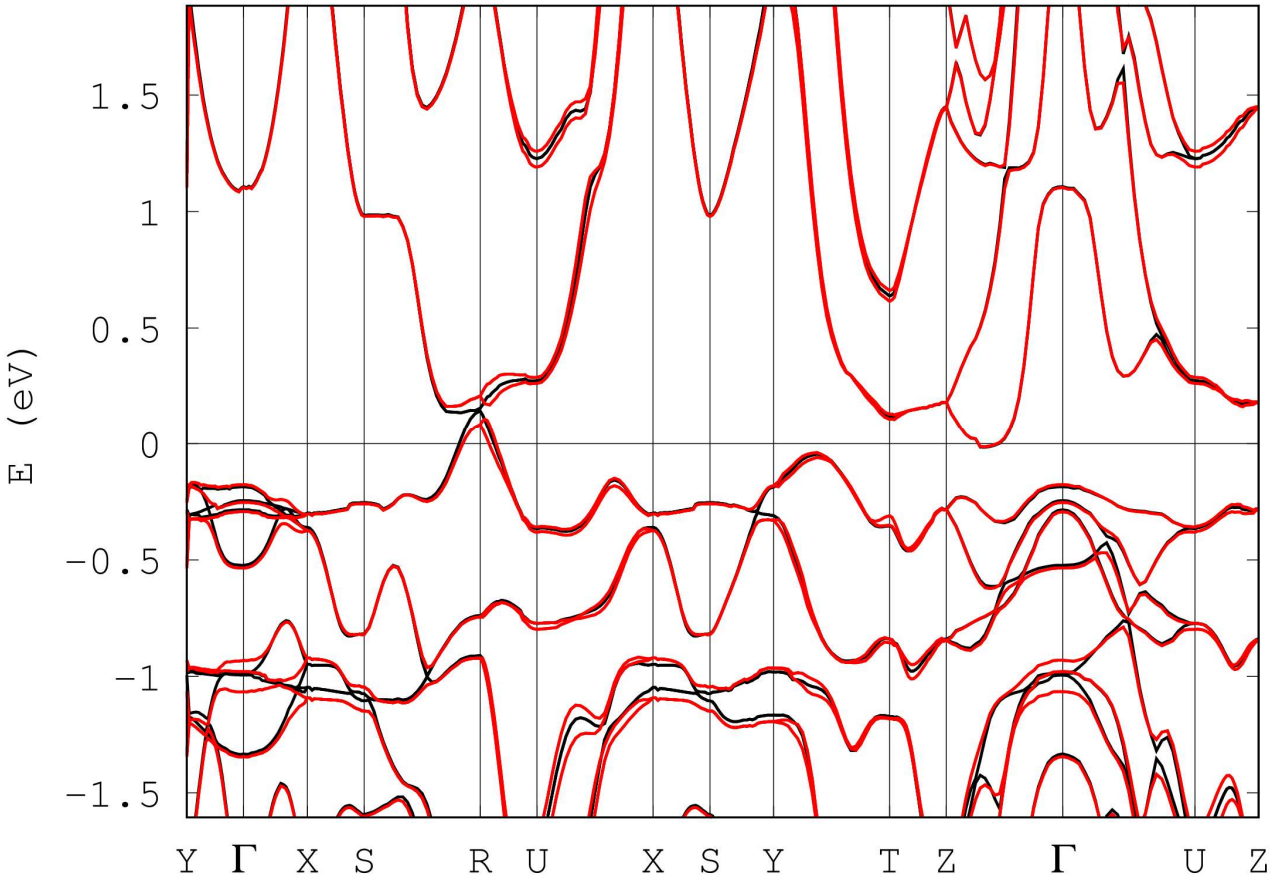


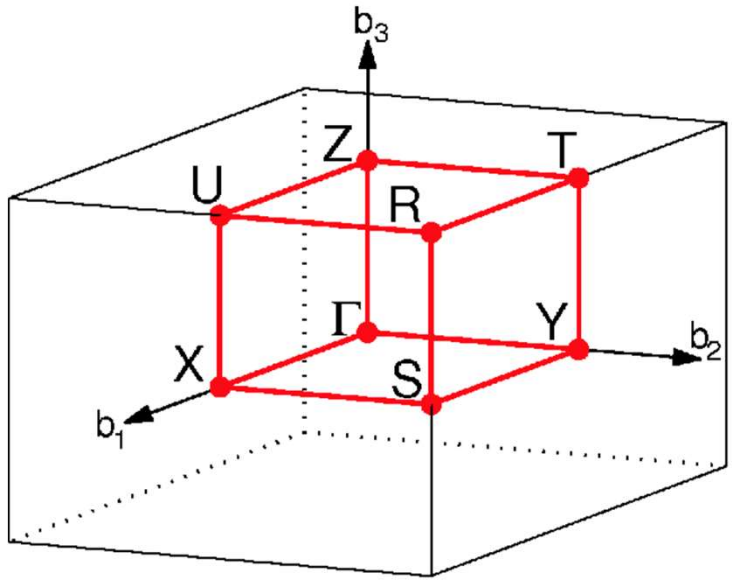
Na: Plasmon Dispersion



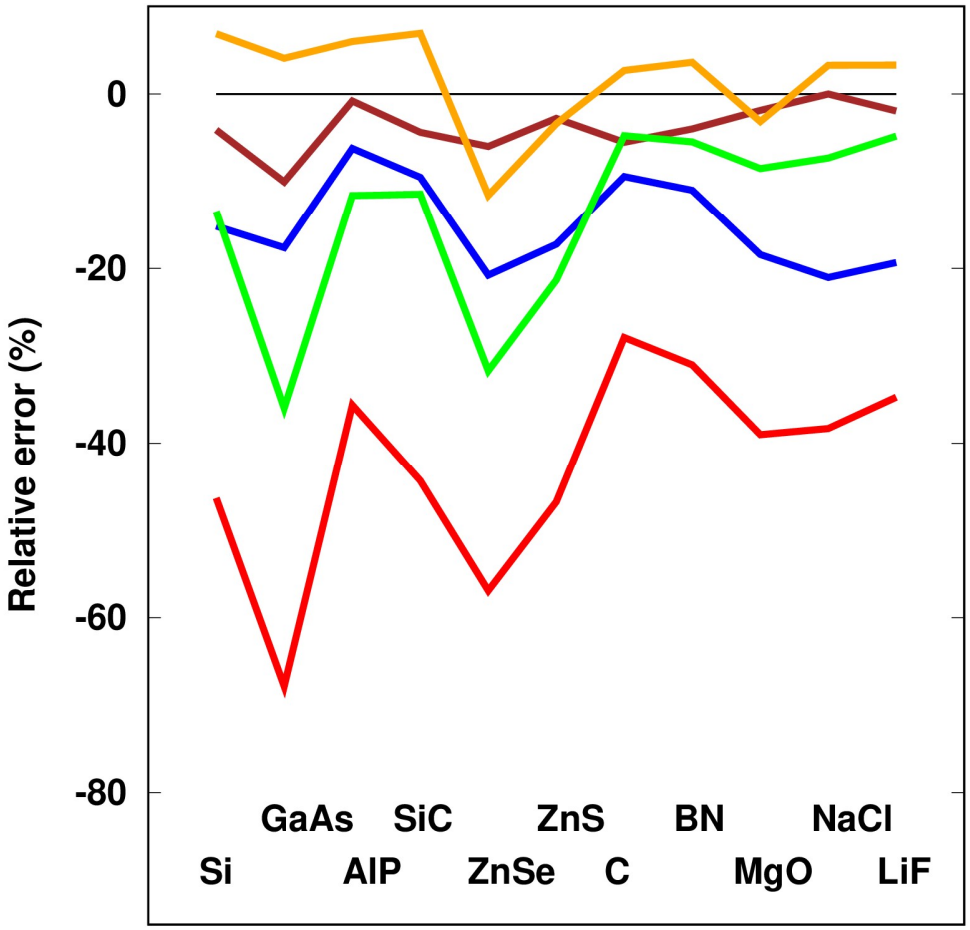
Experimental data:
PRB 84, 075109(2011)

Band plotting: FeSb2 (Orthorhombic) (role of SOI)





Band gaps: PBE and YS-PBE0 versus one shot GW



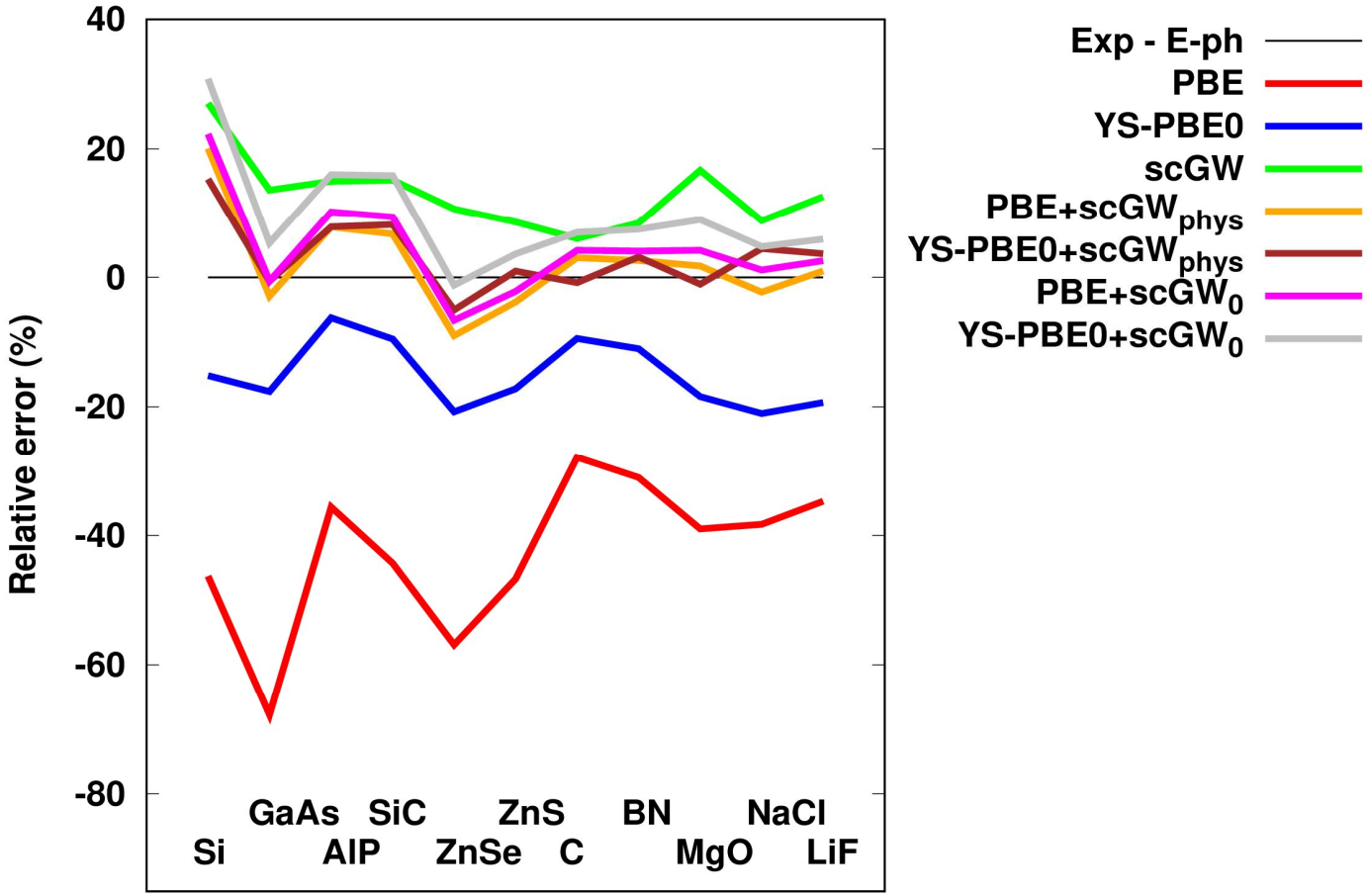
Exp - E-ph
Exp
PBE
YS-PBE0
PBE+G0W0
YS-PBE0+G0W0

Exp:
PRB 20, 624(1979)
PRB 35, 9174(1987)
PRB 53, 16283(1996)

E-ph corr-n:
PRB 89, 214304(2014)
PRL 112, 215501(2014)
RMP 77, 1173(2005)
PRB 93, 100301(2016)

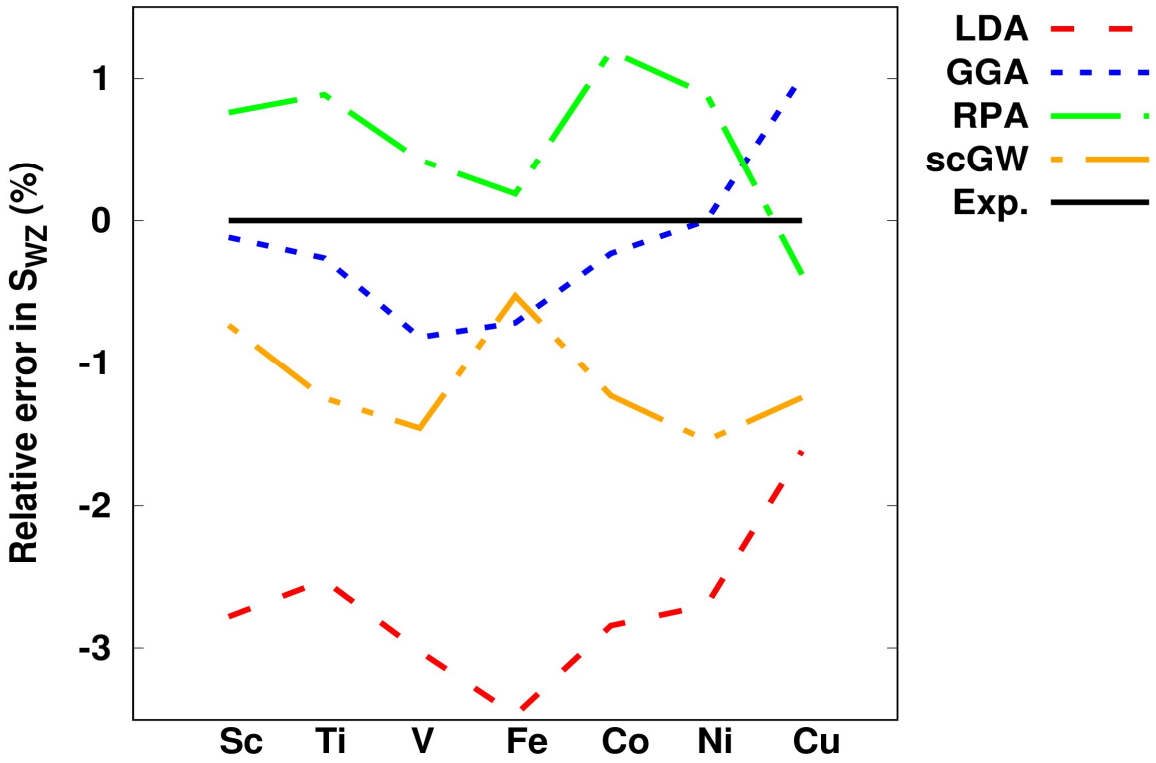
In many cases YS-PBE0 provides better starting point for G_0W_0 than PBE.

Band gaps: different flavors of scGW



Partially sc GW considerably reduces the dependence on the starting point as compared to G_0W_0. Especially for physical W.

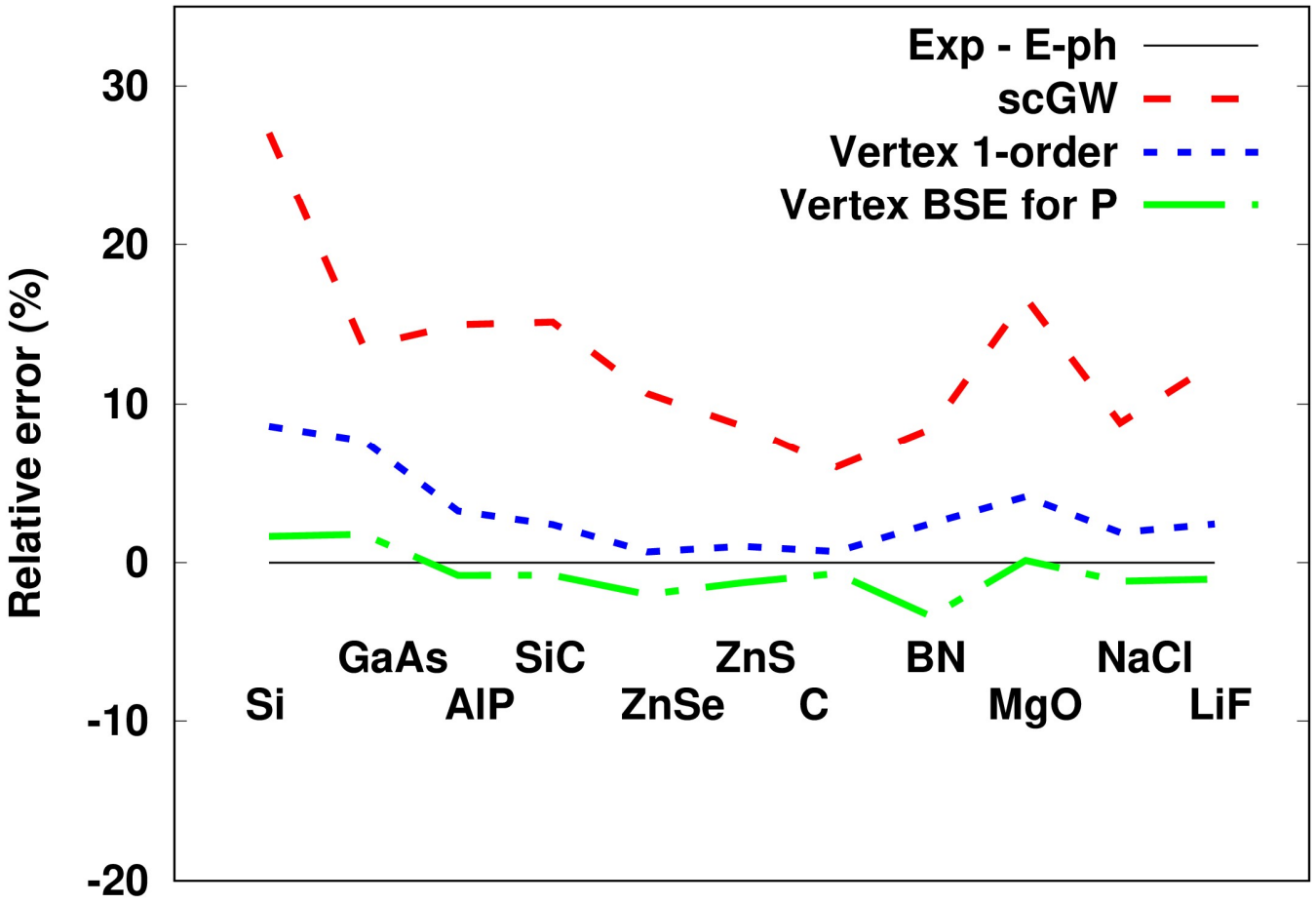
scGW for 3d metals: ground state properties



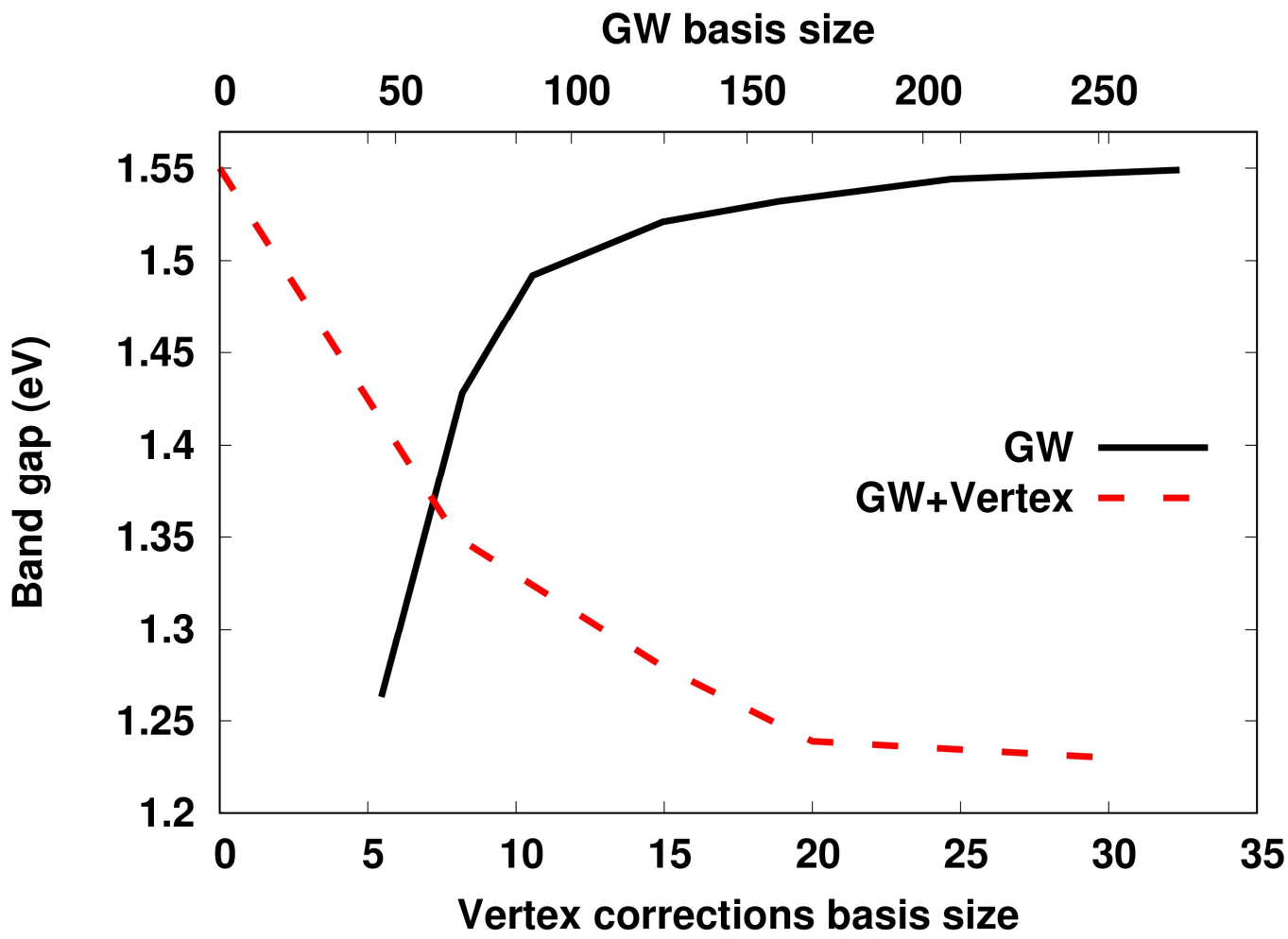
LDA, scGW:
J. Phys.: Condens. Matter 29 (2017) 465503

GGA, RPA and Exp. Data:
PRB 87, 214102 (2013)

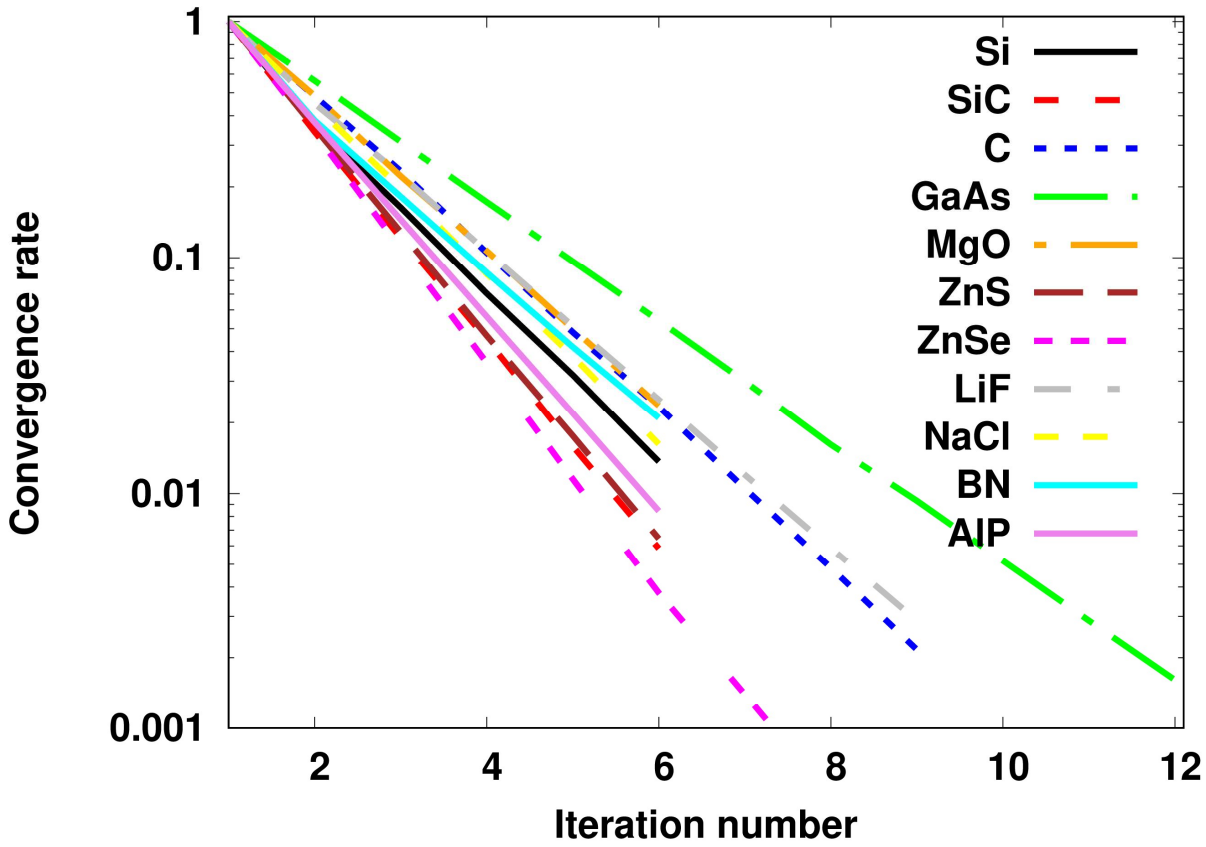
Self consistent GWΓ: Band gaps



Convergence with respect to the basis size (Si)



Convergence of the ladder sums



$$\Gamma = \mathbf{1} + \boldsymbol{WGG} + (\boldsymbol{WGG})^{2} + (\boldsymbol{WGG})^{3} + \cdots$$

Future plans

- Charge and spin susceptibilities based on hybrid functionals
- BSE for optics (based on DFT or HF (Hybrids))
- Magnetic susceptibilities in fully relativistic (Dirac equation) approach
- Linear response for phonons, electron-phonon interaction (DFT)

Hands on training (Plan)

- Basic DFT run (bands, DOS, total energy) – Si
- Spin polarized calculation - Fe
- Dirac relativistic example – δ-Pu
- Charge susceptibility – Na
- Hybrid use – LiF
- PBE+G0W0 - LiF
- QSGW - LiF
- scGW – LiF
- PBE+scGWphys - LiF
- scGWΓ – LiF
- Details about the variables in input file
  /soft/public_soft/FlapwMBPT/FlapwMBPT_Input.pdf

How to run the code

- go to **/soft/public_soft/FlapwMBPT** directory
- copy **./EXAMPLES** in your directory
- **module load apw/2018**

- In order to run the code, go in any of the subdirectories and perform:
- **sbatch sub.sh**
- The results will go in the same subdirectory. There are also precalculated ./TEST subdirectories for comparison

Basic DFT run - Si

```
TEXT    *** band structure calculation of Si  ***
CONTROL  iter_dft 10  iter_hf 0  iter_gw 0 iter_qp  0
       iter_psi 0  iter_bsp  0
       restart_begin  0 restart_end   0
       admix 0.4  adspin 0.7 adm_gw 0.6 acc_it_gw 0.8
       iexch 205 scal_spin 1.0 psi_fncl_use  1
       nproc_tau  1 nproc_k  1 nproc_pbr   1
       irel 0 clight 274.074 rel_interst F
       temperature  300.0
FILES
 allfile 'si'
SYM symgen 'I:T(0.25,0.25,0.25)_R4Z:T(0.25,0.25,0.25)_R3D_'
STRUCTURE  par 10.26122  nsort  1  istruc  3
    b_a 1.0  c_a 1.0
    a   '0.0,0.5,0.5'
    b   '0.5,0.0,0.5'
    c   '0.5,0.5,0.0'
  tau   '0.0,0.0,0.0'
REAL SPACE MESHES mdiv  20  20  20
           nrdiv  12  12  12
         nrdiv_red   4   4   4
BASIS  cut_gw_ratio 0.7 cut_vrt_ratio 1.0
     eps_pb 0.001 eps_pb_vrt 0.005
ZONES nbndf 0 nbndf_bnd   0 0
BND_PLOT n_k_div 12
DOS   emindos -0.3  emaxdos  0.3   ndos 300
    e_small 0.005 e_small_bos 0.001
K_POINT  ndiv   8   8   8  metal F k_line 111
     ndiv_c   1   1   1
     k_integral FD n_k_int 1 1 1
MULTI_SCF vv0 1.0
MAGNET  b_extval   0.0 iter_h_ext 00000
      b_ext  0.0  0.0  1.0
COULOMB eps_coul 0.0001
```

```
W   w_sc_gw scf w_sc_qp scf w_sc_psi scf w_sc_bsp scf
HARTREE-FOCK alpha_hbr 0.25 omega_hse 0.165 hybrid_type 0
VERTEX_P psi_p 60000 bse_kernel_p 6000
      iter_ladder_p  1 nu_w_stat 0
VERTEX_S psi_sig 60000 psi2_sig 60000
      iter_sigma_gwg  1
VERTEX_XI iter_ladder_xi 0 q_suscept  2
       chi_cmp 000 vrt_x_appr 000
       nrax_chi 100 freq_chi  1.0
       theta_bse GW0
OPTICS opt_mode 000000 opt_loc_fld F
TAU MESH n_tau  46  exp_tau_gw  6.0
OMEGA MESH n_omega_exa 10 n_omega_geom  30 n_omega_asy 6
        omega_geom  200.0 omega_max 900.0
NU MESH n_nu_exa 10 n_nu_geom 30  n_nu_asy  6
      nu_geom  100.0  nu_max 400.0
HEG rs  -4.0  k_inf  5.0  n_k_heg  50
ATOMIC DATE ----------------------------------------------------------
 txtel Si    z 14.0 magn_shift 0.0
 smt 2.1 h 1.d-7 nrad  900
 lmb 4  lmpb 4
 lim_pb_mt 12 10 10 10 10 10 10
 lim_pb_mt_red 6 4 4 2 2 0 0
 ntle  3  3  1  1  1  1  1
 l  augm atocc ptnl  corr idmd
 0  LOC  2.0  2.9    N   0
 0  APW  2.0  3.9    N   0
 0  LOC  0.0  4.9    N   1
 1  LOC  6.0  2.9    N   0
 1  APW  2.0  3.9    N   0
 1  LOC  0.0  4.9    N   1
 2  APW  0.0  3.9    N   0
 3  APW  0.0  4.9    N   0
 4  APW  0.0  5.9    N   0
```

Basic DFT – output files

- **out** – monitoring total energy/density convergence
- **si.out** – general output (basis set sizes, timings,…)
- **si_dft.dos** - DOS
- **si_dn_dft.dosk** – k-resolved DOS
- **siSi___sum_dft.pdos** - PDOS
- **si_dft_band_LAPW.dat** – data file for band plotting
- **si_dft_band_LAPW.gnu** – GNUPLOT file for band plotting

Spin polarized case - Fe

```
TEXT    *** band structure calculation of bcc Fe  ***
CONTROL  iter_dft  17  iter_hf  0  iter_gw 0 iter_qp  0
        iter_psi  0 iter_bsp 0
        restart_begin 0 restart_end  0
        admix 0.2  adspin 0.7 adm_gw 0.15 acc_it_gw 0.2
        iexch  5 scal_spin 1.0 psi_fncl_use 0
        nproc_tau 1 nproc_k 2 nproc_pbr   1
        irel 1 clight 274.074 rel_interst F
        temperature   300.00
FILES
  allfile 'fe'
SYM symgen 'I_R3D_R4Z_'
STRUCTURE  par  5.417731  nsort  1  istruc  2
     b_a 1.0  c_a 1.0
     a  '-0.5,0.5,0.5'
     b  '0.5,-0.5,0.5'
     c  '0.5,0.5,-0.5'
    tau  '0.0,0.0,0.0'
REAL SPACE MESHES mdiv  16  16  16
            nrdiv  10  10  10
          nrdiv_red   6   6   6
BASIS  cut_gw_ratio 0.6 cut_vrt_ratio 1.0
      eps_pb 0.001 eps_pb_vrt 0.01
ZONES nbndf  30  nbndf_bnd  0 0
BND_PLOT n_k_div 12
DOS   emindos -0.5  emaxdos  0.5   ndos 400
     e_small 0.008 e_small_bos 0.0001
K_POINT  ndiv   8   8   8  metal T k_line 110
      ndiv_c   1   1   1
      k_integral FD n_k_int 1  1  1
MULTI_SCF vv0  1.0
MAGNET  b_extval   0.0 iter_h_ext 10000
       b_ext  0.0  0.0  1.0
COULOMB eps_coul 0.001
W   w_sc_gw scf w_sc_qp scf w_sc_psi scf w_sc_bsp scf
HARTREE-FOCK alpha_hbr 0.25 omega_hse 0.165 hybrid_type 0
VERTEX_P psi_p 60000 bse_kernel_p 6000
       iter_ladder_p 1 nu_w_stat 0
VERTEX_S psi_sig 20000 psi2_sig 60000
       iter_sigma_gwg  1
VERTEX_XI iter_ladder_xi 0 q_suscept  3
        chi_cmp 000 vrt_x_appr 000
        nrax_chi  330 freq_chi  0.1
        theta_bse  _GW
OPTICS opt_mode 000000 opt_loc_fld F
TAU MESH n_tau 46 exp_tau_gw  4.0
OMEGA MESH n_omega_exa 10 n_omega_geom  30 n_omega_asy 6
        omega_geom  100.0 omega_max 600.0
NU MESH n_nu_exa 10 n_nu_geom 30  n_nu_asy  6
      nu_geom  100.0  nu_max 400.0
HEG rs  -4.0 k_inf  5.0  n_k_heg  50
ATOMIC DATE ----------------------------------------------------------
 txtel Fe    z 26.0 magn_shift 0.5
 smt 2.0 h 1.d-7 nrad  800
 lmb 4  lmpb 6
 lim_pb_mt 22 22 22 22 20 20 20
 lim_pb_mt_red 12 3 3 2 2 0 0
 ntle  3  3  2  1  1  1  1  1  1 1 1
 l  augm atocc ptnl  corr idmd
 0   LOC  2.0  3.9    N   0
 0   APW  2.0  4.9    N   0
 0   LOC  0.0  5.9    N   1
 1   LOC  6.0  3.9    N   0
 1   APW  0.0  4.9    N   0
 1   LOC  0.0  5.9    N   1
 2   APW  6.0  3.9    N   0
 2   LOC  0.0  4.9    N   1
 3   APW  0.0  4.9    N   0
 4   APW  0.0  5.9    N   0
```

Spin-polarized Fe – output files

- **out** – monitoring total energy/density convergence
- **fe.out** – general output (basis set sizes, timings,…)
- **fe_dft.dos** - DOS
- **fe_dn_dft.dosk** – k-resolved DOS (spin down)
- **fe_up_dft.dosk** – k-resolved DOS (spin up)
- **feFe___sum_dft.pdos** - PDOS
- **fe_dft_band_LAPW.dat** – data file for band plotting
- **fe_dft_band_LAPW.gnu** – GNUPLOT file for band plotting

Dirac relativistic example (δ-Pu)

```
TEXT     *** band structure calculation of Pu (FCC)  ***
CONTROL   iter_dft 40  iter_hf  0 iter_gw 0 iter_qp  0
        iter_psi  0  iter_bsp  0
        restart_begin   0 restart_end  0
        admix 0.1  adspin 0.7 adm_gw 0.2 acc_it_gw 0.35
        iexch 205 scal_spin 1.0 psi_fncl_use  1
        nproc_tau 1 nproc_k 4 nproc_pbr   1
        irel 2 clight 274.074 rel_interst T
        temperature   300.0
FILES
  allfile 'pu'
SYM symgen 'I_R4Z_R3D_'
STRUCTURE  par  8.7831  nsort  1  istruc 3
     b_a 1.0  c_a 1.0
     a   '0.0,0.5,0.5'
     b   '0.5,0.0,0.5'
     c   '0.5,0.5,0.0'
   tau   '0.0,0.0,0.0'
REAL SPACE MESHES mdiv  20  20  20
             nrdiv  12  12  12
          nrdiv_red   2   2   2
BASIS  cut_gw_ratio 0.6 cut_vrt_ratio 1.0
      eps_pb 0.0001 eps_pb_vrt 0.01
ZONES nbndf  0 nbndf_bnd 0 0
BND_PLOT n_k_div 10
DOS   emindos -1.0  emaxdos  0.8   ndos 400
     e_small 0.001 e_small_bos 0.01
K_POINT  ndiv   6   6   6  metal T k_line 011
      ndiv_c   1   1   1
      k_integral FD n_k_int 1 1 1
MULTI_SCF vv0 1.0
MAGNET  b_extval   0.0 iter_h_ext 00000
       b_ext  0.0  0.0  1.0
COULOMB eps_coul 0.0001
```

```
W   w_sc_gw scf w_sc_qp scf w_sc_psi scf w_sc_bsp scf
HARTREE-FOCK alpha_hbr 0.25 omega_hse 0.165 hybrid_type 0
VERTEX_P psi_p 66000 bse_kernel_p 6000
       iter_ladder_p  1 nu_w_stat 0
VERTEX_S psi_sig 65000 psi2_sig 60000
       iter_sigma_gwg  1
VERTEX_XI iter_ladder_xi 0 q_suscept  2
        chi_cmp 000 vrt_x_appr 000
        nrax_chi  600 freq_chi  5.0
        theta_bse GW0
OPTICS opt_mode 000000 opt_loc_fld F
TAU MESH n_tau   46 exp_tau_gw  4.0
OMEGA MESH n_omega_exa 10 n_omega_geom  30 n_omega_asy 6
         omega_geom  200.0 omega_max 800.0
NU MESH n_nu_exa 10 n_nu_geom 30  n_nu_asy  6
       nu_geom  80.0  nu_max 600.0
HEG rs -4.0 k_inf  5.0  n_k_heg  50
ATOMIC DATE --------------------------------------------------------
 txtel Pu    z 94.0 magn_shift 0.0
 smt 3.1 h 1.d-8 nrad 1200
 lmb 6  lmpb 6
 lim_pb_mt 25 22 22 20 20 20 20  10  10
 lim_pb_mt_red 5 2 2 1 1 1 1 1 1
 ntle  3  3  3  2  2  1  1  1  1  1  1
 l  augm  atocc   ptnl  corr idmd
 0   LOC  2.0  6.9     N    0
 0   APW  2.0  7.9     N    0
 0   LOC  0.0  8.9     N    1
 1   LOC  6.0  6.9     N    0
 1   APW  0.0  7.9     N    0
 1   LOC  0.0  8.9     N    1
 2   LOC 10.0  5.9     N    0
 2   APW  0.0  6.9     N    0
……………………………………………………
```

Fully relativistic run – output files

- **out** – monitoring total energy/density convergence
- **pu.out** – general output (basis set sizes, timings,…)
- **pu_dft.dos** - DOS
- **pu_dn_dft.dosk** – k-resolved DOS
- **puPu___sum_dft.pdos** - PDOS
- **pu_dft_band_LAPW.dat** – data file for band plotting
- **pu_dft_band_LAPW.gnu** – GNUPLOT file for band plotting

Charge susceptibility example (Na)

```
TEXT    *** band structure calculation of bcc Na  ***
CONTROL  iter_dft 10  iter_hf  0 iter_gw  0 iter_qp  0
        iter_psi  0  iter_bsp  0
        restart_begin  0 restart_end 0
        admix 0.7  adspin 0.7 adm_gw 0.5 acc_it_gw 0.7
        iexch 5 scal_spin 1.0 psi_fncl_use  0
        nproc_tau 1 nproc_k 4 nproc_pbr   1
        irel 0 clight 274.074 rel_interst F
        temperature   300.0
FILES
  allfile  'na'
SYM symgen 'I_R3D_R4Z_'
STRUCTURE  par  7.9593059  nsort  1  istruc  2
     b_a 1.0  c_a 1.0
     a  '-0.5,0.5,0.5'
     b  '0.5,-0.5,0.5'
     c  '0.5,0.5,-0.5'
    tau  '0.0,0.0,0.0'
REAL SPACE MESHES mdiv  10  10  10
            nrdiv   8   8   8
          nrdiv_red   2   2   2
BASIS  cut_gw_ratio 0.6 cut_vrt_ratio 1.0
      eps_pb 0.001 eps_pb_vrt 0.01
ZONES nbndf 16 nbndf_bnd  0 0
BND_PLOT n_k_div 12
DOS   emindos -0.5  emaxdos  0.5   ndos 100
     e_small 0.0005 e_small_bos 0.001
K_POINT  ndiv   8   8   8  metal T k_line 011
      ndiv_c   1   1   1
      k_integral FD n_k_int 1 1 1
MULTI_SCF vv0 1.0
MAGNET  b_extval   0.0 iter_h_ext 00000
       b_ext  0.0  0.0  1.0
COULOMB eps_coul 0.0001
W   w_sc_gw scf w_sc_qp scf w_sc_psi scf w_sc_bsp scf
HARTREE-FOCK alpha_hbr 0.25 omega_hse 0.165 hybrid_type 0
VERTEX_P psi_p 00000 bse_kernel_p 0000
       iter_ladder_p  4 nu_w_stat 0
VERTEX_S psi_sig 20000 psi2_sig 60000
       iter_sigma_gwg  2
VERTEX_XI iter_ladder_xi 0 q_suscept  15
        chi_cmp 100 vrt_x_appr 001
        nrax_chi  360 freq_chi  1.0
        theta_bse GW0
OPTICS opt_mode 000000 opt_loc_fld F
TAU MESH n_tau   46 exp_tau_gw  4.0
OMEGA MESH n_omega_exa 10 n_omega_geom  30 n_omega_asy 6
         omega_geom  80.0 omega_max 600.0
NU MESH n_nu_exa 10 n_nu_geom 30  n_nu_asy  6
       nu_geom  80.0  nu_max 600.0
HEG rs  -4.0 k_inf  5.0  n_k_heg  50
ATOMIC DATA ----------------------------------------
  txtel Na    z 11.0 magn_shift 0.0
  smt 3.44 h 1.d-6 nrad 600
  lmb 4 lmpb 4
  lim_pb_mt 15 12 12 12 10 10 10
  lim_pb_mt_red   3  2  1  0  0  0  0
  ntle  2  2  1  1  1  1  1
  l  augm  atocc   ptnl  corr idmd
  0   LOC  2.0  2.9     N    0
  0   APW  1.0  3.9     N    0
  1   LOC  6.0  2.9     N    0
  1   APW  0.0  3.9     N    0
  2   APW  0.0  3.9     N    0
  3   APW  0.0  4.9     N    0
  4   APW  0.0  5.9     N    0
```

Charge susceptibility example – output files

…….

- **na_K_points** – list of K-points
- **na___00DynSTRFact.dft** – Dynamical Structure Factor
- **na___00EPSm1.dft** – Inverse Dielectric function
- **na___00RSP.dft** – Response function

Hybrid functional (LiF)

```
TEXT    *** band structure calculation of LiF (B1)  ***
CONTROL   iter_dft 14  iter_hf  10  iter_gw 0 iter_qp  0
        iter_psi 0  iter_bsp  0
        restart_begin  0 restart_end   0
        admix 0.3  adspin 0.7 adm_gw 0.3 acc_it_gw 0.6
        iexch 205 scal_spin 1.0 psi_fncl_use  0
        nproc_tau  1 nproc_k  4 nproc_pbr   1
        irel 0 clight 274.074 rel_interst F
        temperature  300.0
FILES
 allfile 'lif'
SYM symgen 'I_R3D_R4Z_'
STRUCTURE  par  7.60804  nsort  2  istruc  3
     b_a 1.0  c_a 1.0
     a   '0.0,0.5,0.5'
     b   '0.5,0.0,0.5'
     c   '0.5,0.5,0.0'
   tau   '0.0,0.0,0.0'
        '0.5,0.5,.5'
REAL SPACE MESHES mdiv  12  12  12
            nrdiv  10  10  10
          nrdiv_red   4   4   4
BASIS  cut_gw_ratio 0.65 cut_vrt_ratio 1.0
      eps_pb 0.001 eps_pb_vrt 0.01
ZONES nbndf   0 nbndf_bnd  0  0
BND_PLOT n_k_div 2
DOS   emindos -2.0  emaxdos  2.0   ndos 600
     e_small 0.005 e_small_bos 0.04
K_POINT  ndiv   4   4   4  metal F k_line 001
      ndiv_c   1   1   1
      k_integral FD n_k_int 1 1 1
MULTI_SCF vv0  1.0
MAGNET  b_extval   0.0 iter_h_ext 00000
       b_ext  0.0  0.0  1.0
COULOMB eps_coul 0.0001
W   w_sc_gw scf w_sc_qp scf w_sc_psi scf w_sc_bsp scf
HARTREE-FOCK alpha_hbr 0.25 omega_hse 0.165 hybrid_type 3
VERTEX_P psi_p 60000 bse_kernel_p 0000
       iter_ladder_p  6 nu_w_stat 0
VERTEX_S psi_sig 60000 psi2_sig 60000
       iter_sigma_gwg  1
VERTEX_XI iter_ladder_xi 0 q_suscept  2
        chi_cmp 000 vrt_x_appr 000
        nrax_chi 100 freq_chi  1.0
        theta_bse GW0
OPTICS opt_mode 000000 opt_loc_fld F
TAU MESH n_tau  46  exp_tau_gw  4.0
OMEGA MESH n_omega_exa 10 n_omega_geom  30 n_omega_asy 6
        omega_geom  200.0 omega_max 900.0
NU MESH n_nu_exa 10 n_nu_geom 30  n_nu_asy  6
      nu_geom  100.0  nu_max 400.0
HEG rs  -4.0  k_inf  5.0  n_k_heg  50
ATOMIC DATE ------------------------------------------------------------
 txtel Li    z  3.0 magn_shift 0.0
 smt 1.8 h 1.d-6 nrad  600
 lmb 4  lmpb 4
 lim_pb_mt= 12 10 10 10 10
 lim_pb_mt_red 6 4 4 3 3 0 0
 ntle  2  1  1  1  1  1
 l  augm atocc ptnl  corr idmd
 0   LOC  2.0  1.9     N    0  ……
 txtel _F    z  9.0 magn_shift 0.0
 smt 1.8 h 1.d-6 nrad  600
 lmb 4  lmpb 4
 lim_pb_mt= 12 10 10 10 10
 lim_pb_mt_red 6 4 4 3 3 0 0
 ntle=  1  1  1  1  1  1
 l  augm atocc ptnl  corr idmd
 0   APW  2.0  2.9     N    0 ……..
```

Hybrid functional example – output files

- **……..**
- **lif_hf.dos** – DOS for hybrid functional
- **lif_dn_hf.dosk** – k-resolved DOS for hybrid
- **lifLi___sum_hf.pdos** – hybrid functional PDOS for Li
- **lif_F___sum_hf.pdos** – hybrid functional PDOS for F
- **lif___Sigma_X_band_x.hf** – Exchange Self Energy
- **lif__hf_x.eig** – hybrid functional one electron energies

PBE+G0W0 (LiF)

```
TEXT    *** band structure calculation of LiF (B1)  ***
CONTROL  iter_dft 14  iter_hf  0  iter_gw -1 iter_qp  0
        iter_psi 0  iter_bsp  0
        restart_begin  0 restart_end   0
        admix 0.3  adspin 0.7 adm_gw 0.3 acc_it_gw 0.6
        iexch 205 scal_spin 1.0 psi_fncl_use  0
        nproc_tau  4 nproc_k  1 nproc_pbr   1
        irel 0 clight 274.074 rel_interst F
        temperature  300.0
FILES
 allfile 'lif'
SYM symgen 'I_R3D_R4Z_'
STRUCTURE  par  7.60804  nsort  2  istruc  3
    b_a 1.0  c_a 1.0
    a   '0.0,0.5,0.5'
    b   '0.5,0.0,0.5'
    c   '0.5,0.5,0.0'
  tau   '0.0,0.0,0.0'
       '0.5,0.5,.5'
REAL SPACE MESHES mdiv  12  12  12
           nrdiv  10  10  10
         nrdiv_red   4   4   4
BASIS  cut_gw_ratio 0.65 cut_vrt_ratio 1.0
     eps_pb 0.001 eps_pb_vrt 0.01
ZONES nbndf   0 nbndf_bnd  1   8
BND_PLOT n_k_div 2
DOS   emindos -2.0  emaxdos  2.0   ndos 600
    e_small 0.005 e_small_bos 0.04
K_POINT  ndiv   4   4   4  metal F k_line 001
     ndiv_c   1   1   1
     k_integral FD n_k_int 1 1 1
MULTI_SCF vv0  1.0
MAGNET  b_extval   0.0 iter_h_ext 00000
      b_ext  0.0  0.0  1.0
COULOMB eps_coul 0.0001
W   w_sc_gw scf w_sc_qp scf w_sc_psi scf w_sc_bsp scf
HARTREE-FOCK alpha_hbr 0.25 omega_hse 0.165 hybrid_type 3
VERTEX_P psi_p 60000 bse_kernel_p 0000
       iter_ladder_p  6 nu_w_stat 0
VERTEX_S psi_sig 60000 psi2_sig 60000
       iter_sigma_gwg  1
VERTEX_XI iter_ladder_xi 0 q_suscept  2
        chi_cmp 000 vrt_x_appr 000
        nrax_chi 100 freq_chi  1.0
        theta_bse GW0
OPTICS opt_mode 000000 opt_loc_fld F
TAU MESH n_tau  46  exp_tau_gw  4.0
OMEGA MESH n_omega_exa 10 n_omega_geom  30 n_omega_asy 6
       omega_geom  200.0 omega_max 900.0
NU MESH n_nu_exa 10 n_nu_geom 30  n_nu_asy  6
      nu_geom  100.0  nu_max 400.0
HEG rs  -4.0  k_inf  5.0  n_k_heg  50
ATOMIC DATE ----------------------------------------------------------
 txtel Li    z  3.0 magn_shift 0.0
 smt 1.8 h 1.d-6 nrad  600
 lmb 4  lmpb 4
 lim_pb_mt= 12 10 10 10 10 10 10
 lim_pb_mt_red 6 4 4 3 3 0 0
 ntle  2  1  1  1  1  1
 l  augm atocc ptnl  corr idmd
 0   LOC  2.0  1.9    N    0  ……
 txtel _F    z  9.0 magn_shift 0.0
 smt 1.8 h 1.d-6 nrad  600
 lmb 4  lmpb 4
 lim_pb_mt= 12 10 10 10 10 10 10
 lim_pb_mt_red 6 4 4 3 3 0 0
 ntle=  1  1  1  1  1  1
 l  augm atocc ptnl  corr idmd
 0   APW  2.0  2.9    N    0 ……..
```

G_0W_0 example – output files

- **…….**
- **lif_Nu_Q____P_Re.gw** – P as a function of Matsubara freq-cy
- **lif_dn_gw.dosk** – k-resolved DOS for G_0W_0
  lifLi___sum_gw.pdos – G_0W_0 PDOS for Li
- **lif_F___sum_gw.pdos** – G_0W_0 PDOS for F
- **lif_mbpt.eig** – list of G_0W_0 one electron energies and self energy components

QSGW (LiF)

```
TEXT    *** band structure calculation of LiF (B1)  ***
CONTROL   iter_dft 14  iter_hf  0  iter_gw 0 iter_qp  10
        iter_psi 0  iter_bsp  0
        restart_begin  0 restart_end   0
        admix 0.3  adspin 0.7 adm_gw 0.3 acc_it_gw 0.6
        iexch 205 scal_spin 1.0 psi_fncl_use  0
        nproc_tau  4 nproc_k  1 nproc_pbr   1
        irel 0 clight 274.074 rel_interst F
        temperature  300.0
FILES
  allfile 'lif'
SYM symgen 'I_R3D_R4Z_'
STRUCTURE  par  7.60804  nsort  2  istruc  3
     b_a 1.0  c_a 1.0
     a   '0.0,0.5,0.5'
     b   '0.5,0.0,0.5'
     c   '0.5,0.5,0.0'
    tau   '0.0,0.0,0.0'
        '0.5,0.5,.5'
REAL SPACE MESHES mdiv  12  12  12
             nrdiv  10  10  10
           nrdiv_red   4   4   4
BASIS  cut_gw_ratio 0.65 cut_vrt_ratio 1.0
      eps_pb 0.001 eps_pb_vrt 0.01
ZONES nbndf   0 nbndf_bnd  0  0
BND_PLOT n_k_div 2
DOS   emindos -2.0  emaxdos  2.0   ndos 600
     e_small 0.005 e_small_bos 0.04
K_POINT  ndiv   4   4   4  metal F k_line 001
      ndiv_c   1   1   1
      k_integral FD n_k_int 1 1 1
MULTI_SCF vv0  1.0
MAGNET  b_extval   0.0 iter_h_ext 00000
       b_ext  0.0  0.0  1.0
COULOMB eps_coul 0.0001
W   w_sc_gw scf w_sc_qp scf w_sc_psi scf w_sc_bsp scf
HARTREE-FOCK alpha_hbr 0.25 omega_hse 0.165 hybrid_type 0
VERTEX_P psi_p 60000 bse_kernel_p 0000
        iter_ladder_p  6 nu_w_stat 0
VERTEX_S psi_sig 60000 psi2_sig 60000
        iter_sigma_gwg  1
VERTEX_XI iter_ladder_xi 0 q_suscept  2
         chi_cmp 000 vrt_x_appr 000
         nrax_chi 100 freq_chi  1.0
         theta_bse GW0
OPTICS opt_mode 000000 opt_loc_fld F
TAU MESH n_tau  46  exp_tau_gw  4.0
OMEGA MESH n_omega_exa 10 n_omega_geom  30 n_omega_asy 6
          omega_geom  200.0 omega_max 900.0
NU MESH n_nu_exa 10 n_nu_geom 30  n_nu_asy  6
        nu_geom  100.0  nu_max 400.0
HEG rs  -4.0  k_inf  5.0  n_k_heg  50
ATOMIC DATE ----------------------------------------------------------
  txtel Li    z  3.0 magn_shift 0.0
  smt 1.8 h 1.d-6 nrad  600
  lmb 4  lmpb 4
  lim_pb_mt= 12 10 10 10 10 10 10
  lim_pb_mt_red 6 4 4 3 3 0 0
  ntle  4  3  2  2  1  1  1
  l  augm atocc ptnl  corr idmd
  0   LOC  2.0  1.9     N    0  ……
  txtel _F    z  9.0 magn_shift 0.0
  smt 1.8 h 1.d-6 nrad  600
  lmb 4  lmpb 4
  lim_pb_mt= 12 10 10 10 10 10 10
  lim_pb_mt_red 6 4 4 3 3 0 0
  ntle=  3  3  2  2  1  1  1
  l  augm atocc ptnl  corr idmd
  0   APW  2.0  2.9     N    0 ……..
```

QSGW example – output files

- **……..**
- **lif_qp.dos** – DOS for QSGW
- **lif_dn_qp.dosk** – k-resolved DOS for QSGW
- **lifLi___sum_qp.pdos** – QSGW PDOS for Li
- **lif_F___sum_qp.pdos** – QSGW PDOS for F
- **lif_Nu_Q____P_Re.qp** – P as a function of Matsubara freq-cy
- **lif_Im_sigc_w_band_k.qp** – Im part of Sigma_corr
- **lif_Re_sigc_w_band_k.qp** – Re part of Sigma_corr
- **lif__qp_x.eig** – QSGW one electron energies
- **lif_Z_factor_band_k_x.qp** – Renorm Z-factor

scGW (LiF)

```
TEXT    *** band structure calculation of LiF (B1)  ***
CONTROL  iter_dft 14  iter_hf  0  iter_gw 10 iter_qp  10
       iter_psi 0  iter_bsp  0
       restart_begin  0 restart_end   0
       admix 0.3  adspin 0.7 adm_gw 0.3 acc_it_gw 0.6
       iexch 205 scal_spin 1.0 psi_fncl_use  0
       nproc_tau  4 nproc_k  1 nproc_pbr   1
       irel 0 clight 274.074 rel_interst F
       temperature  300.0
FILES
 allfile 'lif'
SYM symgen 'I_R3D_R4Z_'
STRUCTURE  par  7.60804  nsort  2  istruc  3
    b_a 1.0  c_a 1.0
    a   '0.0,0.5,0.5'
    b   '0.5,0.0,0.5'
    c   '0.5,0.5,0.0'
  tau   '0.0,0.0,0.0'
       '0.5,0.5,.5'
REAL SPACE MESHES mdiv  12  12  12
           nrdiv  10  10  10
         nrdiv_red   4   4   4
BASIS  cut_gw_ratio 0.65 cut_vrt_ratio 1.0
     eps_pb 0.001 eps_pb_vrt 0.01
ZONES nbndf   0 nbndf_bnd  0  0
BND_PLOT n_k_div 2
DOS   emindos -2.0  emaxdos  2.0   ndos 600
    e_small 0.005 e_small_bos 0.04
K_POINT  ndiv   4   4   4  metal F k_line 001
     ndiv_c   1   1   1
     k_integral FD n_k_int 1 1 1
MULTI_SCF vv0  1.0
MAGNET  b_extval   0.0 iter_h_ext 00000
      b_ext  0.0  0.0  1.0
COULOMB eps_coul 0.0001
W   w_sc_gw scf w_sc_qp scf w_sc_psi scf w_sc_bsp scf
HARTREE-FOCK alpha_hbr 0.25 omega_hse 0.165 hybrid_type 0
VERTEX_P psi_p 60000 bse_kernel_p 0000
       iter_ladder_p  6 nu_w_stat 0
VERTEX_S psi_sig 60000 psi2_sig 60000
       iter_sigma_gwg  1
VERTEX_XI iter_ladder_xi 0 q_suscept  2
        chi_cmp 000 vrt_x_appr 000
        nrax_chi 100 freq_chi  1.0
        theta_bse GW0
OPTICS opt_mode 000000 opt_loc_fld F
TAU MESH n_tau  46  exp_tau_gw  4.0
OMEGA MESH n_omega_exa 10 n_omega_geom  30 n_omega_asy 6
        omega_geom  200.0 omega_max 900.0
NU MESH n_nu_exa 10 n_nu_geom 30  n_nu_asy  6
      nu_geom  100.0  nu_max 400.0
HEG rs  -4.0  k_inf  5.0  n_k_heg  50
ATOMIC DATE ----------------------------------------------------------
 txtel Li    z  3.0 magn_shift 0.0
 smt 1.8 h 1.d-6 nrad  600
 lmb 4  lmpb 4
 lim_pb_mt= 12 10 10 10 10 10 10
 lim_pb_mt_red 6 4 4 3 3 0 0
 ntle  4  3  2  2  1  1  1
 l  augm atocc ptnl  corr idmd
 0   LOC  2.0  1.9     N    0  ……
 txtel _F    z  9.0 magn_shift 0.0
 smt 1.8 h 1.d-6 nrad  600
 lmb 4  lmpb 4
 lim_pb_mt= 12 10 10 10 10 10 10
 lim_pb_mt_red 6 4 4 3 3 0 0
 ntle=  3  3  2  2  1  1  1
 l  augm atocc ptnl  corr idmd
 0   APW  2.0  2.9     N    0 ……..
```

scGW example – output files

- **……..**
- **lif_gw.dos** – Spectral function (SF) for scGW
- **lif_dn_gw.dosk** – k-resolved SF for scGW
- **lifLi__Chain_gw.pdos** – scGW PSF for Li
- **lif_F__Chain_gw.pdos** – scGW PSF for F
- **lif_Nu_Q____P_Re.gw** – P as a function of Matsubara freq-cy
- **lif_Im_sigc_w_band_k.gw** – Im part of Sigma_corr
- **lif_Re_sigc_w_band_k.gw** – Re part of Sigma_corr

  lif_Z_factor_band_k_x.gw – Renorm Z-factor

PBE+scGW$_{phys}$ (LiF)

```
TEXT    *** band structure calculation of LiF (B1)  ***
CONTROL  iter_dft 14  iter_hf  0  iter_gw 10 iter_qp  10
        iter_psi 0  iter_bsp  0
        restart_begin  0 restart_end   0
        admix 0.3  adspin 0.7 adm_gw 0.3 acc_it_gw 0.6
        iexch 205 scal_spin 1.0 psi_fncl_use  0
        nproc_tau  4 nproc_k  1 nproc_pbr   1
        irel 0 clight 274.074 rel_interst F
        temperature  300.0
FILES
 allfile 'lif'
SYM symgen 'I_R3D_R4Z_'
STRUCTURE  par  7.60804  nsort  2  istruc  3
     b_a 1.0  c_a 1.0
     a   '0.0,0.5,0.5'
     b   '0.5,0.0,0.5'
     c   '0.5,0.5,0.0'
   tau   '0.0,0.0,0.0'
         '0.5,0.5,.5'
REAL SPACE MESHES mdiv  12  12  12
            nrdiv  10  10  10
          nrdiv_red   4   4   4
BASIS  cut_gw_ratio 0.65 cut_vrt_ratio 1.0
      eps_pb 0.001 eps_pb_vrt 0.01
ZONES nbndf   0 nbndf_bnd  0  0
BND_PLOT n_k_div 2
DOS   emindos -2.0  emaxdos  2.0   ndos 600
     e_small 0.005 e_small_bos 0.04
K_POINT  ndiv   4   4   4  metal F k_line 001
      ndiv_c   1   1   1
      k_integral FD n_k_int 1 1 1
MULTI_SCF vv0  1.0
MAGNET  b_extval   0.0 iter_h_ext 00000
       b_ext  0.0  0.0  1.0
COULOMB eps_coul 0.0001
W   w_sc_gw non w_sc_qp scf w_sc_psi scf w_sc_bsp scf
HARTREE-FOCK alpha_hbr 0.25 omega_hse 0.165 hybrid_type 0
VERTEX_P psi_p 60000 bse_kernel_p 6000
       iter_ladder_p  6 nu_w_stat 0
VERTEX_S psi_sig 60000 psi2_sig 60000
       iter_sigma_gwg  1
VERTEX_XI iter_ladder_xi 0 q_suscept  2
        chi_cmp 000 vrt_x_appr 000
        nrax_chi 100 freq_chi  1.0
        theta_bse GW0
OPTICS opt_mode 000000 opt_loc_fld F
TAU MESH n_tau  46  exp_tau_gw  4.0
OMEGA MESH n_omega_exa 10 n_omega_geom  30 n_omega_asy 6
        omega_geom  200.0 omega_max 900.0
NU MESH n_nu_exa 10 n_nu_geom 30  n_nu_asy  6
      nu_geom  100.0  nu_max 400.0
HEG rs  -4.0  k_inf  5.0  n_k_heg  50
ATOMIC DATE ------------------------------------------------------------
 txtel Li    z  3.0 magn_shift 0.0
 smt 1.8 h 1.d-6 nrad  600
 lmb 4  lmpb 4
 lim_pb_mt= 12 10 10 10 10 10 10
 lim_pb_mt_red 6 4 4 3 3 0 0
 ntle  4  3  2  2  1  1  1
 l  augm atocc ptnl  corr idmd
 0   LOC  2.0  1.9     N    0  ……
 txtel _F    z  9.0 magn_shift 0.0
 smt 1.8 h 1.d-6 nrad  600
 lmb 4  lmpb 4
 lim_pb_mt= 12 10 10 10 10 10 10
 lim_pb_mt_red 6 4 4 3 3 0 0
 ntle=  3  3  2  2  1  1  1
 l  augm atocc ptnl  corr idmd
 0   APW  2.0  2.9     N    0 ……..
```

PBE+scGW$_{phys}$ example – output files

- **…….. Similar to scGW output:**
- **lif_gw.dos** – Spectral function (SF)
- **lif_dn_gw.dosk** – k-resolved SF
- **lifLi__Chain_gw.pdos** – PSF for Li
- **lif_F__Chain_gw.pdos** – PSF for F
- **lif_Nu_Q____P_Re.gw** – P as a function of Matsubara freq-cy
- **lif_Im_sigc_w_band_k.gw** – Im part of Sigma_corr
- **lif_Re_sigc_w_band_k.gw** – Re part of Sigma_corr

  lif_Z_factor_band_k_x.gw – Renorm Z-factor

scGWΓ (LiF)

```
TEXT    *** band structure calculation of LiF (B1)  ***
CONTROL  iter_dft 14  iter_hf  0  iter_gw  2 iter_qp  0
       iter_psi 10  iter_bsp  0
       restart_begin  0 restart_end   0
       admix 0.3  adspin 0.7 adm_gw 0.3 acc_it_gw 0.6
       iexch 205 scal_spin 1.0 psi_fncl_use  0
       nproc_tau  4 nproc_k  1 nproc_pbr   1
       irel 0 clight 274.074 rel_interst F
       temperature  300.0
FILES
 allfile 'lif'
SYM symgen 'I_R3D_R4Z_'
STRUCTURE  par  7.60804  nsort  2  istruc  3
    b_a 1.0  c_a 1.0
    a   '0.0,0.5,0.5'
    b   '0.5,0.0,0.5'
    c   '0.5,0.5,0.0'
  tau   '0.0,0.0,0.0'
       '0.5,0.5,.5'
REAL SPACE MESHES mdiv  12  12  12
           nrdiv  10  10  10
         nrdiv_red  4   4   4
BASIS  cut_gw_ratio 0.65 cut_vrt_ratio 1.0
     eps_pb 0.001 eps_pb_vrt 0.01
ZONES nbndf   0 nbndf_bnd  1  10
BND_PLOT n_k_div 2
DOS   emindos -2.0  emaxdos  2.0   ndos 600
    e_small 0.005 e_small_bos 0.04
K_POINT  ndiv   4   4   4  metal F k_line 001
     ndiv_c  2  2  2
     k_integral FD n_k_int 1 1 1
MULTI_SCF vv0  1.0
MAGNET  b_extval   0.0 iter_h_ext 00000
      b_ext  0.0  0.0  1.0
COULOMB eps_coul 0.0001
W   w_sc_gw scf w_sc_qp scf w_sc_psi scf w_sc_bsp scf
HARTREE-FOCK alpha_hbr 0.25 omega_hse 0.165 hybrid_type 0
VERTEX_P psi_p 60000 bse_kernel_p 0000
       iter_ladder_p  6 nu_w_stat 0
VERTEX_S psi_sig 60000 psi2_sig 60000
       iter_sigma_gwg  1
VERTEX_XI iter_ladder_xi 0 q_suscept  2
        chi_cmp 000 vrt_x_appr 000
        nrax_chi 100 freq_chi  1.0
        theta_bse GW0
OPTICS opt_mode 000000 opt_loc_fld F
TAU MESH n_tau  46  exp_tau_gw  4.0
OMEGA MESH n_omega_exa 10 n_omega_geom  30 n_omega_asy 6
        omega_geom  200.0 omega_max 900.0
NU MESH n_nu_exa 10 n_nu_geom 30  n_nu_asy  6
      nu_geom  100.0  nu_max 400.0
HEG rs  -4.0  k_inf  5.0  n_k_heg  50
ATOMIC DATE ----------------------------------------------------------
 txtel Li    z  3.0 magn_shift 0.0
 smt 1.8 h 1.d-6 nrad  600
 lmb 4  lmpb 4
 lim_pb_mt= 12 10 10 10 10 10 10
 lim_pb_mt_red 6 4 4 3 3 0 0
 ntle  4  3  2  2  1  1  1
 l  augm atocc ptnl  corr idmd
 0   LOC  2.0  1.9    N    0  ……
 txtel _F    z  9.0 magn_shift 0.0
 smt 1.8 h 1.d-6 nrad  600
 lmb 4  lmpb 4
 lim_pb_mt= 12 10 10 10 10 10 10
 lim_pb_mt_red 6 4 4 3 3 0 0
 ntle=  3  3  2  2  1  1  1
 l  augm atocc ptnl  corr idmd
 0   APW  2.0  2.9    N    0 ……..
```

scGWΓ example – output files

- **…….**
- **lif_gwg.dos** – Spectral function (SF) for scGWΓ
- **lif_dn_gwg.dosk** – k-resolved SF for scGWΓ
- **lifLi__Chain_gwg.pdos** – scGWΓ PSF for Li
- **lif_F__Chain_gwg.pdos** – scGWΓ PSF for F
- **lif_Nu_Q____P_Re.gwg** – P as a function of Matsubara freq-cy
- **lif_Im_sigc_w_band_k.gwg** – Im part of Sigma_corr
- **lif_Re_sigc_w_band_k.gwg** – Re part of Sigma_corr

  lif_Z_factor_band_k_x.gwg – Renorm Z-factor

Getting the source

In order to obtain the latest version of the code:

Contact Andrey Kutepov (akutepov@bnl.gov)

Brief description of your plans on using the code would be very helpful.

In case you are using it, the reports on any bugs and problems would be very helpful too.