1) Input file of a DFT calculation with PBE0(X=1/7), performed with pw.x (Quantum Espresso version 6.3)

```
&control
   calculation='scf'
   restart_mode='from_scratch',
   prefix='fe',
   pseudo_dir = './ '
   outdir='./',
   wf_collect=.true.
   verbosity = 'high'
/
 &system
   ibrav = 5,
   celldm(1) = 10.255, celldm(4)=.561146108
   nat  = 10,
   ntyp = 3,
   ecutwfc = 60
   ecutfock = 60
   nspin=2,
   nbnd=300,
   starting_magnetization(1)=0.5,
   starting_magnetization(2)=-0.5,
   occupations='smearing', degauss=0.001,
   force_symmorphic=.true.
   input_dft='pbe0', nqx1 = 2, nqx2 = 2, nqx3 = 2,
   exx_fraction=0.1429
   x_gamma_extrapolation = .true.
   exxdiv_treatment='gygi-baldereschi'
   nosym=.true.
 &ions
 /
 &cell
 /
 ATOMIC_SPECIES
 Au  55.85 Fe_ONCV_PBE-1.0_noghost.upf
 Ag  55.85 Fe_ONCV_PBE-1.0_noghost.upf
 O 15.999  08_O.oncvpsp.upf
ATOMIC_POSITIONS (crystal)
Ag     0.353421986        0.353421986        0.353421986
Au     0.146577999        0.146577999        0.146577999
Ag     0.646578014        0.646578014        0.646578014
Au     0.853421986        0.853421986        0.853421986
O      0.946735978        0.553264022        0.250000000
O      0.553264022        0.250000000        0.946735978
O      0.750000000        0.053264000        0.446736008
O      0.446736008        0.750000000        0.053264000
O      0.053264000        0.446736008        0.750000000
O      0.250000000        0.946735978        0.553264022
K_POINTS automatic
4 4 4 0 0 0
```

2) Input file of a GW calculation performed with epsilon.cplx.x (BerkeleyGW version 1.2)

```
epsilon_cutoff 40.0
```

number_bands 300

begin qpoints
0.000500000 0.000250000 -0.000250000 1.0 1
0.000000000 0.000000000 0.250000000 1.0 0
0.000000000 0.000000000 0.500000000 1.0 0
0.000000000 0.000000000 0.750000000 1.0 0
0.000000000 0.250000000 0.000000000 1.0 0
0.000000000 0.250000000 0.250000000 1.0 0
0.000000000 0.250000000 0.500000000 1.0 0
0.000000000 0.250000000 0.750000000 1.0 0
0.000000000 0.500000000 0.000000000 1.0 0
0.000000000 0.500000000 0.250000000 1.0 0
0.000000000 0.500000000 0.500000000 1.0 0
0.000000000 0.500000000 0.750000000 1.0 0
0.000000000 0.750000000 0.000000000 1.0 0
0.000000000 0.750000000 0.250000000 1.0 0
0.000000000 0.750000000 0.500000000 1.0 0
0.000000000 0.750000000 0.750000000 1.0 0
0.250000000 0.000000000 0.000000000 1.0 0
0.250000000 0.000000000 0.250000000 1.0 0
0.250000000 0.000000000 0.500000000 1.0 0
0.250000000 0.000000000 0.750000000 1.0 0
0.250000000 0.250000000 0.000000000 1.0 0
0.250000000 0.250000000 0.250000000 1.0 0
0.250000000 0.250000000 0.500000000 1.0 0
0.250000000 0.250000000 0.750000000 1.0 0
0.250000000 0.500000000 0.000000000 1.0 0
0.250000000 0.500000000 0.250000000 1.0 0
0.250000000 0.500000000 0.500000000 1.0 0
0.250000000 0.500000000 0.750000000 1.0 0
0.250000000 0.750000000 0.000000000 1.0 0
0.250000000 0.750000000 0.250000000 1.0 0
0.250000000 0.750000000 0.500000000 1.0 0
0.250000000 0.750000000 0.750000000 1.0 0
0.500000000 0.000000000 0.000000000 1.0 0
0.500000000 0.000000000 0.250000000 1.0 0
0.500000000 0.000000000 0.500000000 1.0 0
0.500000000 0.000000000 0.750000000 1.0 0
0.500000000 0.250000000 0.000000000 1.0 0
0.500000000 0.250000000 0.250000000 1.0 0
0.500000000 0.250000000 0.500000000 1.0 0
0.500000000 0.250000000 0.750000000 1.0 0
0.500000000 0.500000000 0.000000000 1.0 0
0.500000000 0.500000000 0.250000000 1.0 0
0.500000000 0.500000000 0.500000000 1.0 0
0.500000000 0.500000000 0.750000000 1.0 0
0.500000000 0.750000000 0.000000000 1.0 0
0.500000000 0.750000000 0.250000000 1.0 0
0.500000000 0.750000000 0.500000000 1.0 0
0.500000000 0.750000000 0.750000000 1.0 0
0.750000000 0.000000000 0.000000000 1.0 0
0.750000000 0.000000000 0.250000000 1.0 0
0.750000000 0.000000000 0.500000000 1.0 0
0.750000000 0.000000000 0.250000000 1.0 0
0.750000000 0.000000000 0.500000000 1.0 0

```
  0.750000000  0.000000000  0.750000000   1.0 0
  0.750000000  0.250000000  0.000000000   1.0 0
  0.750000000  0.250000000  0.250000000   1.0 0
  0.750000000  0.250000000  0.500000000   1.0 0
  0.750000000  0.250000000  0.750000000   1.0 0
  0.750000000  0.500000000  0.000000000   1.0 0
  0.750000000  0.500000000  0.250000000   1.0 0
  0.750000000  0.500000000  0.500000000   1.0 0
  0.750000000  0.500000000  0.750000000   1.0 0
  0.750000000  0.750000000  0.000000000   1.0 0
  0.750000000  0.750000000  0.250000000   1.0 0
  0.750000000  0.750000000  0.500000000   1.0 0
  0.750000000  0.750000000  0.750000000   1.0 0
end
```

3) Input file of a GW calculation performed with sigma.cplx.x (BerkeleyGW version 1.2)

```
number_bands 300

band_index_min 49
band_index_max 53

screening_semiconductor
exact_static_ch 1

dont_use_vxcdat

spin_index_min 1

begin kpoints
  0.000000000  0.000000000  0.000000000   1.0
  0.000000000  0.000000000  0.250000000   1.0
  0.000000000  0.000000000 -0.500000000   1.0
  0.000000000  0.250000000  0.250000000   1.0
  0.000000000  0.250000000 -0.500000000   1.0
  0.000000000  0.250000000 -0.250000000   1.0
  0.000000000 -0.500000000  0.250000000   1.0
  0.000000000 -0.500000000 -0.500000000   1.0
  0.250000000  0.250000000  0.250000000   1.0
  0.250000000  0.250000000 -0.500000000   1.0
  0.250000000  0.250000000 -0.250000000   1.0
  0.250000000 -0.500000000 -0.500000000   1.0
  0.250000000 -0.500000000 -0.250000000   1.0
 -0.500000000 -0.500000000 -0.500000000   1.0
end
```

4) Input file of a BSE calculation performed with kernel.cplx.x (BerkeleyGW version 1.2)

```
number_val_bands 24
number_cond_bands 14

use_symmetries_coarse_grid
screening_semiconductor
```

5) Input file of a BSE calculation performed with absorption.cplx.x (BerkeleyGW version 1.2)

number_val_bands_coarse 24
number_cond_bands_coarse 14
number_val_bands_fine 17
number_cond_bands_fine 12

degeneracy_check_override

use_symmetries_coarse_grid
no_symmetries_fine_grid
no_symmetries_shifted_grid

screening_semiconductor

use_velocity

haydock
number_iterations 500

gaussian_broadening
energy_resolution 0.15