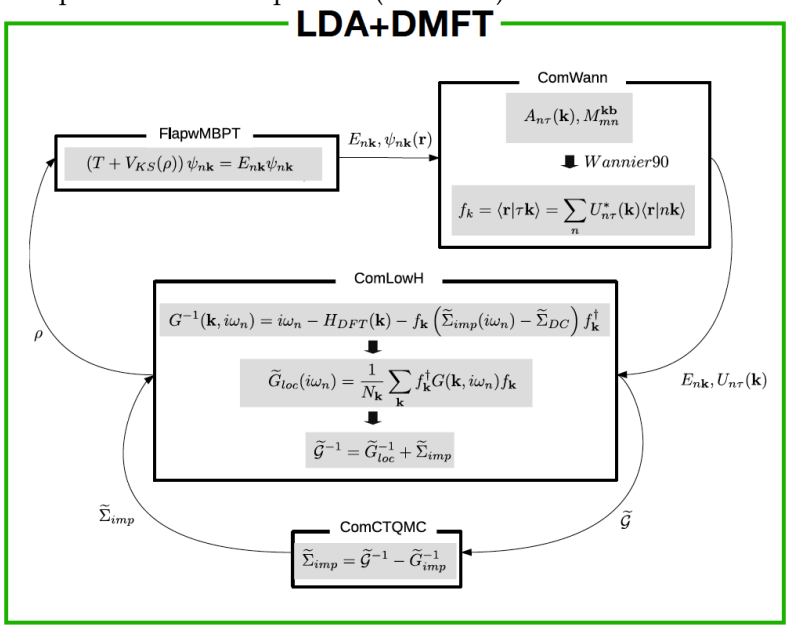
Example: FeSe

LDA+DMFT in COMSUITE

We will calculate the electronic structure of FeSe within LDA+DMFT. COMSUITE package for LDA+DMFT is composed of four components (softwares). Its work flow is described below.



1. Construction of a Kohn-Sham Hamiltonian within LDA by **FlapwMBPT** (see https://doi.org/10.1016/j.cpc.2017.06.012)
2. Construction of the atom-centered local basis set spanning the low energy Hilbert space by **ComWann utilizing Wannier90 package**
3. Wannier interpolation of the mean-field Hamiltonian and solving the DMFT self-consistent equation by **ComLowH** and **ComCTQMC**
4. Updating the electron density

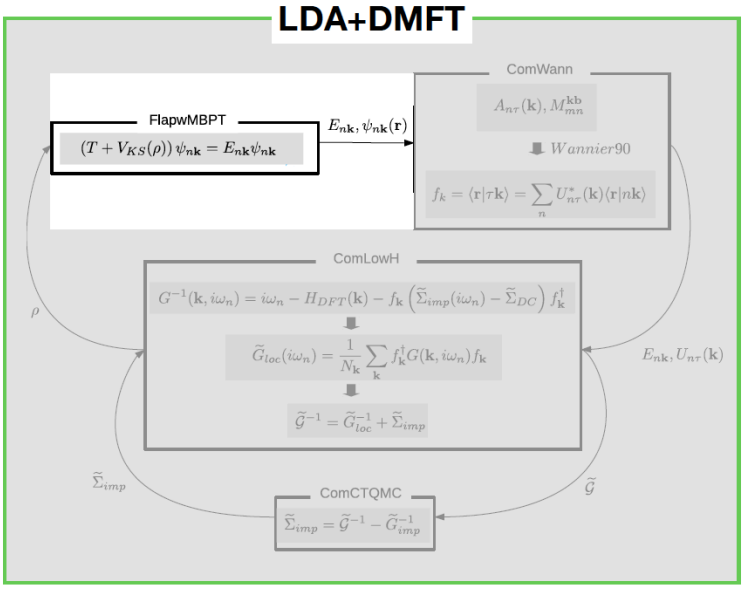
These components (software) along with Wannier90 library are located at install_directory ('install_directory' is described in 'Build and Install' section in Installation of COMSUITE page). To access COMSUITE executables, you should export bin path in your startup shell script.

```
export COMSUITE_BIN=install_directory/bin
```

This tutorial consists of three parts: LDA prerun, LDA+DMFT run, and analysis.

FeSe LDA prerun

To run LDA+DMFT, we start with the LDA prerun (unshaded part of following figure).



To start the LDA calculation, you need to create a directory named "lda" (or a name of your own choice). Note that this name should be specified in 'comdmft.ini' as will be explained in the next section. Having done this, move to the created directory:

```
$ mkdir lda
$ cd lda
```

Create an input file "ini" using FeSe cif file by executing cif2matdelab.py:

```
$ $COMSUITE_BIN/cif2matdelab.py –m dft –k 2 FeSe.cif
```

The generated ini file of FeSe looks as follows:

```
TEXT band structure calculation
CONTROL   iter_dft= 80  iter_hf=  0  iter_gw=  0 iter_qp=  0
          admix=0.100  adspin=0.700 adm_gw=0.050 acc_it_gw=0.10
          iexch=005 scal_spin= 1.0000
          nproc_tau=   1 nproc_k=  30
          irel=1 clight=274.074e+00 rel_interst=F irel_core=1
          temperature=    900.00  restart=F
FILES
  allfile=mdl
SYM symgen=I_R2Z:T(0.5,0.5,0.0)_R2Y:T(0.0,0.5,0.0)_MX:T(0.5,0.0,0.0)_M(-0.5,0.5,0.0)_
STRUCTURE  par=  1.0000000  natom=  4 nsort=  2 istruct= -5
      is=  1  1  2  2
      b/a= 1.000000  c/a= 1.000000
      a=   7.1288060000000000   0.0000000000000000   0.0000000000000000
      b=   0.0000000000000000   7.1288060000000000   0.0000000000000000
      c=   0.0000000000000000   0.0000000000000000  10.4345836706000000
    tau=  -0.2500000000000000   0.2500000000000000   0.0000000000000000
    tau=   0.2500000000000000  -0.2500000000000000   0.0000000000000000
    tau=  -0.2500000000000000  -0.2500000000000000   0.2673000000000000
    tau=   0.2500000000000000   0.2500000000000000  -0.2673000000000000
REAL SPACE MESHES mdiv=  14   14   22
                  nrdiv=  12   12   18
BASIS  cut_lapw_ratio=0.610 cut_pb_ratio=0.980
       eps_pb=1.e-03
ZONES nbndf=   0
DOS   emindos=-15.000  emaxdos= 15.000   ndos=  800
      n_cont_frac=  30 e_small=2.e-02
      dos= T           bandstructure= T
K_POINT  ndiv=   6   6   4  metal=T n_k_div=  9 k_line=010
MULTI_SCF vv0=  1.00
MAGNET  b_extval=   0.000000 iter_h_ext=0000100
        b_ext=  0.000  0.000  1.000
TAU MESH n_tau=   62 n_tau_int=  900
OMEGA MESH n_omega_exa=   29 n_omega_asy=   18 omega_max=  200.00
          interp_omega_d= 2
NU MESH n_nu_exa=   29 n_nu_asy=   18 nu_max=  200.00
        interp_nu_d= 2
ATOMIC DATA ------------------------------------------------------------
  txtel=fe    z= 26.0 magn_shift= 0.000
  smt= 2.50000 h= 0.0120 nrad= 1216 z_dop=0.000
  lmb= 4  lmpb= 4
  lim_pb_mt= 30 30 30 30 30
  ntle=  3  3  2  2  2  1  1  1  1
  l  augm  atocc   ptnl  corr idmd
  0   LOC  2.000  3.950     N    0
  0   APW  0.000  4.800     N    0
  0   LOC  0.000  5.800     N    1
  1   LOC  6.000  3.950     N    0
  1   APW  0.000  4.800     N    0
  1   LOC  0.000  5.800     N    1
  2   APW  8.000  3.800     L    0
  2   LOC  0.000  4.950     N    1
  3   APW  0.000  4.800     N    0
  3   LOC  0.000  5.800     N    1
  4   APW  0.000  5.800     N    0
  4   LOC  0.000  6.800     N    1
  txtel=se    z= 34.0 magn_shift= 0.000
  smt= 2.10000 h= 0.0120 nrad= 1216 z_dop=0.000
  lmb= 4  lmpb= 4
  lim_pb_mt= 30 30 30 30 30
  ntle=  2  2  3  2  2  1  1  1  1
  l  augm  atocc   ptnl  corr idmd
  0   APW  2.000  4.800     N    0
  0   LOC  0.000  5.800     N    1
  1   APW  4.000  4.800     N    0
  1   LOC  0.000  5.800     N    1
  2   LOC 10.000  3.950     N    0
  2   APW  0.000  4.800     N    0
  2   LOC  0.000  5.950     N    1
  3   APW  0.000  4.800     N    0
  3   LOC  0.000  5.800     N    1
  4   APW  0.000  5.800     N    0
  4   LOC  0.000  6.800     N    1
```

One should modify several input keywords as follows:

- iter_dft: The number of DFT iterations. Set to 80.
- admix: charge mixing in DFT iterations. Set to 0.100.
- nproc_tau: The number of MPI processes associated with imaginary time and frequency. Set to 1. For the details on the MPI parallization in FlapwMBPT, please go to FlapwMBPT homepage (https://www.bnl.gov/cmpmsd/flapwmbpt).
- nproc_k: The number of MPI processes associated with parallelization over Brillouin zone k-points. For the present case, set to 30. For the details on the MPI parallization in FlapwMBPT, please goto FlapwMBPT homepage (https://www.bnl.gov/cmpmsd/flapwmbpt).
- temperature: Temperature in K. Set to 900
- mdiv: The real space mesh in the unit cell used for electronic density, Hartree potential, and LDA exchange-correlation potential evaluations. Set to [14 14 22].
- nrdiv: The real space mesh associated with the interstitial product basis. Set to [12 12 18]
- ndiv: The number of k-mesh in Brillouin zone. 6 × 6 × 4 k-mesh for the present case.

Note also that the total number of MPI processes is nproc_tau × nproc_k which is 30 for the present case.

We also modified Fe and Se muffin-tin basis information for a better convergence. One should modify the muffin-tin basis set information in ATOMIC DATA as figure shown above. For the muffin-tin basis set format, please go to FlapwMBPT homepage (https://www.bnl.gov/cmpmsd/flapwmbpt).

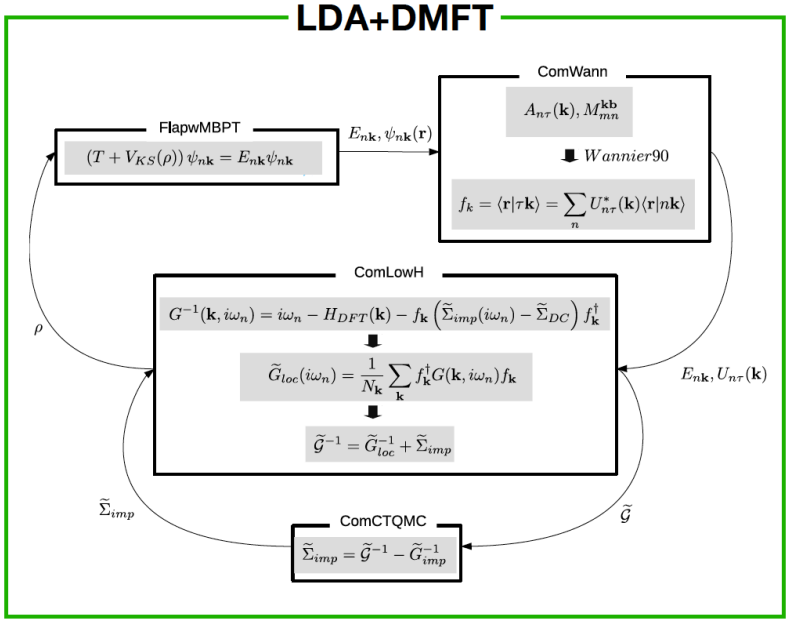
The next step is to run LDA by executing rspflapw.exe. An example of job script to run rspflapw.exe using SLURM is

```
#!/bin/bash -l
#SBATCH -J temp
#SBATCH -p regular
#SBATCH -N 1
#SBATCH -e temp.%j.err
#SBATCH -o temp.%j.out
#SBATCH -L SCRATCH
#SBATCH -C haswell
#SBATCH -t 05:00:00
srun -n 30 $COMSUITE_BIN/rspflapw.exe
```

The total number of processes should be 30 as specified in ini file.

FeSe LDA+DMFT run

Once the prerun is finished successfully, the next step is to run the LDA+DMFT calculation (the entire part of the figure below). To run LDA+DMFT, the input file named "comdmft.ini" is needed (see input file section). The calculation of FeSe within LDA+DMFT reads output data from the LDA prerun. If you specify the prerun path in comdmft.ini (e.g., '../lda' in this case) correctly, it will read necessary data automatically



To run LDA+DMFT, move to your work folder, then create lda_dmft folder (you can name what you want) and move to the folder as follows:

```
$ cd ..
$ mkdir lda_dmft
$ cd lda_dmft
```

Then create comdmft.ini (see input file section) file for LDA+DMFT calculation and execute 'comdmft.py' python file in $COMSUITE_BIN. An example of job script using SLURM is

```
#!/bin/bash -l
#SBATCH -J temp
#SBATCH -q regular
#SBATCH -N 12
#SBATCH -e temp.%j.err
#SBATCH -o temp.%j.out
#SBATCH -L SCRATCH
#SBATCH -C haswell
```

```
#SBATCH -t 05:00:00
$COMSUITE_BIN/comdmft.py
```

Here ‘comdmft.py’ is a python script which controls LDA+DMFT calculation. Based on the ‘comdmft.ini’ input file, ‘comdmft.py’ generates all necessary input files to run individual programs and execute jobs.

Input file (comdmft.ini)

In order to perform LDA+DMFT calculation, we need only a single input file ‘comdmft.ini’. This input file should be written in python dictionary format. All dictionary keys are in small letters. ‘comdfmt.ini’ is composed of three python dictionaries: ‘control’, ‘wan_hmat’, and ‘imp’:

```
control={'initial_lattice_dir'      : '../lda',
        'method'              : 'lda+dmft',
        'spin_orbit'          : False,
        'mpi_prefix': "srun -n 160",
        'impurity_problem':[[1, ‘d’],[2, 'd']],
        'impurity_problem_equivalence':[1,1],
        }

wan_hmat={
       'kgrid': [15, 15, 10],
       'froz_win_min': -10.0,
       'froz_win_max': 10.0,
                  }

imp={'temperature'          : 300, # temperature (in K)
    '1':
    {
   'F0': 5.0,
   'F2': 6.89230769231,
   'F4': 4.30769230769 ,
   'nominal_n': 6.0,
   'impurity_matrix': [
        [1,0,0,0,0],
        [0,2,0,0,0],
        [0,0,3,0,0],
        [0,0,0,2,0],
        [0,0,0,0,4]
        ],
    ‘thermalization_time’: 1,
    ‘measurement_time’: 10,
    ‘green_cutoff’:  10
    ‘coulomb’: 'full',
    }
    }
```

■ **In Control**

These fields contain basic parameters to control LDA+DMFT run.

- 'initial_lattice_dir' : '../lda'
  Enter the path which contains LDA output such as Kohn-Sham eigenvalue and eigenfunctions. It is the LDA prerun folder.

- ‘method’ : ‘lda+dmft’
  Either lda+dmft or lqsgw+dmft. Currently COMSUITE has these two options. Choose ‘lda+dmft’ for the present work (LDA+DMFT approximation).

- 'spin_orbit': False
  Enter True of False. If False, correlated orbitals correspond to cubic spherical harmonics

$$Y_{lm} = \begin{cases} \frac{i}{\sqrt{2}}\left(Y_l^{-|m|} - (-1)^m Y_l^{|m|}\right), & m < 0 \\ Y_l^0, & m = 0 \\ \frac{1}{\sqrt{2}}\left(Y_l^{-|m|} + (-1)^m Y_l^{|m|}\right), & m > 0 \end{cases}$$

where Y_l^m is a spherical harmonics.
if True, correlated orbitals chosen at each correlated atom correspond spin-angular functions |l,i,m>

$$\Omega_{l,i=\pm\frac{1}{2},m} = \sum_{s\pm 1/2} C_{i,s}^{l,m} Y_l^{m-s}(\hat{r}) u_s$$

where u_s is a spinor, and $C_{i,s}^{l,m} = \langle l, m-s, \frac{1}{2}, s | l+i, m \rangle$.

- 'mpi_prefix': 'srun -n 160'
  MPI prefix used for FlapwMBPT, ComLowH, ComWann, and ComCTQMC. If a different prefix is required for individual program, specifiy the number using 'mpi_prefix_lattice','mpi_prefix_lowh', 'mpi_prefix_wannier', and 'mpi_prefix_impurity'. Note that 160 is the number of total processes we want to use for the present case.

- 'impurity_problem': [[1,'d'], [2,'d']]
  A python list to specify correlated orbitals. The first and second indices indicates the atom index and shell type, respectively. Atom index: in the order listed in the "../lda/coord.xsf".
  Shell index is either "d" or "f". Here, two Fe-d shells are treated as an impurity problem.

- 'impurity_problem_equivalence': [1,1]
  Equivalence of each impurity problem. The value is identified by a positive integer starting from 1. If this value is the same, they are equivalent.

- 'restart': False
  Enter True or False. If True, it will resume the calculation from the previous LDA+DMFT run. The default value is False.

- 'mpi_prefix_lowh':
  MPI prefix for ComLowH. The default value is the one specified in control['mpi_prefix']

- 'mpi_prefix_impurity':
  MPI prefix for the impurity solver. The default value is the one specified in control['mpi_prefix']

- 'mpi_prefix_wannier':
  MPI prefix for ComWann. The default value is the one specified in control['mpi_prefix'].

- 'sigma_mix_ratio':
  Self-energy linear mixing ratio. You can specify any number within 0.0 – 1.0. The default value is 0.5.

- 'max_iter_num_impurity':
  Maximum iteration for the DMFT self-consistent loop. The default value is 50.

- 'proj_win_min':
  Low-energy cutoff to renormalize the projectors. The default value is the one specified in wan_hmat['dis_win_min']

- 'proj_win_max':
  High-energy cutoff to renormalize the projectors. The default value is the one specified in wan_hmat['dis_win_max']

■ **In wan_hmat**:
These fields define frozen window, disentanglement window, and ab initio calculation from which maximally localized Wannier functions (MLFWs) are constructed.

- 'kgrid': [15,15,10]
  Crystal momentum grid for the wannier interpolation of LDA band structure.

- 'froz_win_min': -10.0 eV
  Lower boundary of the inner (frozen) window in eV.

- 'froz_win_max': 10.0 eV
  Upper boundary of the inner (frozen) window in eV.

- 'dis_win_min':
  Lower boundary of the outer (disentanglement) window in eV. The default value is same with wan_hmat['froz_win_min']

- 'dis_win_max':
  Upper boundary of the outer (disentanglement) window in eV. The default value is wan_hmat['froz_win_max'] +40.0

- 'num_iter':
  The number of minimization step for the wannierization process. (gauge dependent part of total spreading). The default value is 0.

- 'dis_num_iter':
  The number of minimization step for the disentanglement process. (gauge independent part of total spreading). The default value is 100.

■ **In imp**:
These fields are related with the Monte-Carlo algorithm and sampling of observables.

- 'temperature': 300
  Simulation temperature in K

- 'F0', 'F2', 'F4': The values of Slater integrals in eV. Note that for "f" shells, 'F0', 'F2', 'F4', and 'F6' should be specified.

- 'nominal_n': Nominal occupancy associated with the impurity shell. This value is required since we adopt the so-called "nominal double counting" for LDA+DMFT which reads:

  $$\tilde{\Sigma}^{DC} = U(N_0 - \frac{1}{2}) - J(\frac{N_0}{2} - \frac{1}{2})$$

  where N_0 is the nominal occupancy specified by 'nominal_n'.

- For each distinct impurity problem indexed by the value in control ["impurity_problem_equivalence"],
  - 'impurity_matrix': [
    [1,0,0,0,0],
    [0,2,0,0,0], 1: d_{xy}
    [0,0,3,0,0], 2: d_{yz}, d_{xz}
    [0,0,0,2,0], 3: d_{z^2}
    [0,0,0,0,4] 4: $d_{x^2-y^2}$
    ],
    Equivalence of the matrix element of the hybridization function and impurity self-energy. Starting from "1", you can set any positive number. If these values are the same, hybridization function and impurity self-energy will be identical for those. If the element in the matrix is zero, then it will not be sampled by the impurity solver. Each column and row correspond to the Wannier orbitals in the following order $|xy\rangle, |yz\rangle, |z^2\rangle, |xz\rangle, |x^2-y^2\rangle$ if control['spin_orbit']==False. If control['spin_orbit']==True, the most rapidly changing index is "m" and the next one is "i". They are sorted in ascending order. For the case of "f" shell, for example, they are ordered as: $|3,-0.5, -2.5\rangle, |3,-0.5, -1.5\rangle, |3,-0.5, -0.5\rangle, |3,-0.5, 0.5\rangle, |3,-0.5, 1.5\rangle, |3,-0.5, 2.5\rangle, |3,0.5, -3.5\rangle, |3,0.5, -2.5\rangle, |3,0.5,-1.5\rangle, |3,0.5, -0.5\rangle, |3,0.5, 0.5\rangle, |3,0.5, 1.5\rangle, |3,0.5, 2.5\rangle, |3,0.5, 3.5\rangle,$

- 'thermalization_time': 1,
  Wall time for the thermalization in minutes.

- 'measurement_time': 10,
  Wall time for the measurement in minutes.

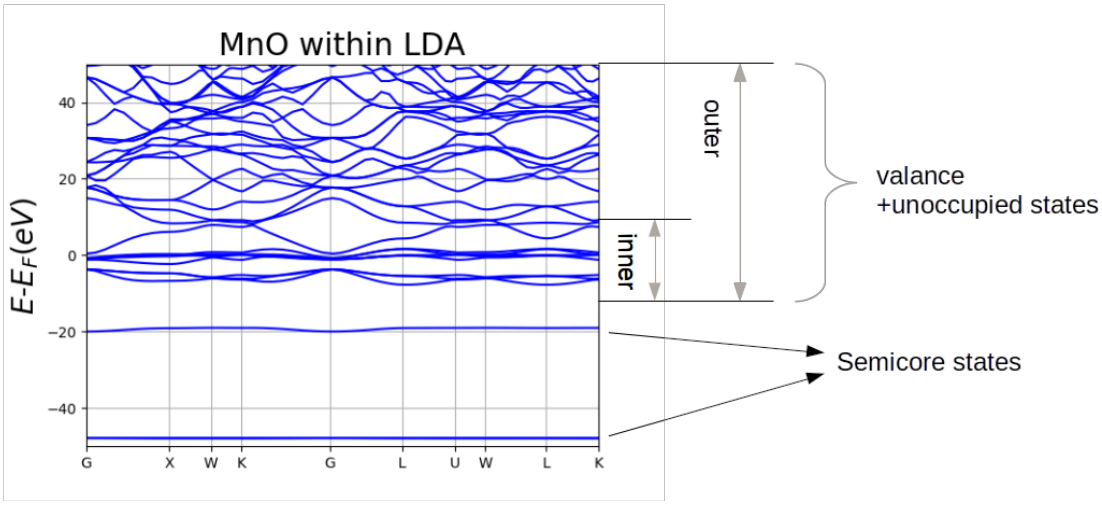
- 'green_cutoff': 10,
  Cutoff-energy in eV to sample green's function and self-energy. The values beyond this energy will be provided by analytical equations.

- 'susceptibility_cutoff': 300,
  Cutoff-energy to sample susceptibility. The default value is 300 eV.

- 'Coulomb': 'full',
  'full' or 'ising' are available. We construct Coulomb matrix in the following way.
  $$U_{m_1,m_2,m_3,m_4} = \sum_{k=0}^{2l,even} \frac{4\pi}{2k+1} F_l^k \sum_{q=-k}^{k} \langle Y_l^{m_1} | Y_k^q Y_l^{m_4} \rangle \langle Y_l^{m_2} Y_k^q | Y_l^{m_3} \rangle$$
  If 'full', no additional approximation is considered. If 'ising', only U_{abba} or U_{abab} are non-zero.

Input file (comdmft.ini)-Important concepts for wan_hmat

COMSUITE uses localized orbitals such as Wannier functions to represent the low-energy Hilbert space. To construct the Wannier functions, the inner (frozen) energy window can be set to range from E_F+'froz_win_min' to E_F+'froz_win_max', and the outer (disentanglement) energy window can range from E_F+'dis_win_min' to E_F+'dis_win_max'; see the figure below (Here we take the MnO case as an example).

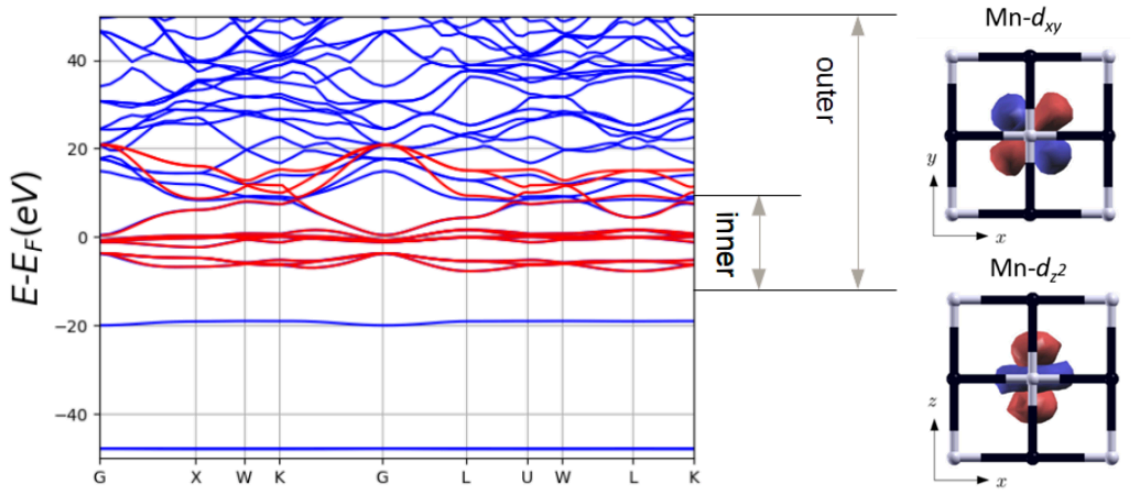


We choose initial trial orbitals $|\tau\mathbf{R}=0\rangle_t$ using MT orbitals with desired angular momentum character. The radial functions of $|\tau\mathbf{R}=0\rangle_t$ are chosen in such a way to maximize

$$\frac{1}{N_{\mathbf{k}}} \sum_{n\mathbf{k}}^{E_{min}^{inner} < E_{n\mathbf{k}} < E_{min}^{inner}} |\langle n\mathbf{k}|\tau\mathbf{k}\rangle_t|^2$$

, where $|\tau\mathbf{k}\rangle_t = \frac{1}{N_{\mathbf{k}}} \sum_{\mathbf{R}} |\tau\mathbf{R}\rangle_t e^{i\mathbf{k}\cdot\mathbf{R}}$. Among the MT orbitals above, we chosse ones which are larger than 0.15. For correlated orbitals, final wannier functions $|\tau\mathbf{R}=0\rangle_f$ usually satisfy a condition of ${}_f\langle\tau\mathbf{R}=0|\tau\mathbf{R}=0\rangle_t > 0.95$. This means that $|\tau\mathbf{R}=0\rangle_f$ are strongly localized and are regarded as atom-like wavefunctions.

The figure below shows the Wannier functions and interpolated band structure of MnO in comparison with the LDA band structure. The number of bands in the inner window is 10, while the number of bands in the outer window is 29. The number of trial orbitals is 12 (Mn-*s*, Mn-*p*, Mn-*d*, O-*p*).



Output files

COMSUITE places important output files generated from individual programs in the work directory (lda_dmft in this example). The list of files is

cmd.log
convergence.log : convergence log file
sig.dat : impurity self-energy
delta.dat : hybridization function

The format of each file and meaning of fields are introduced below. The results of FeSe LDA+DMFT calculation are presented with illustrative plots.

■ **convergence.log**

step	i_outer	i_latt	i_imp	causality	delta_rho	w_sp_min	w_sp_max	mu	std_sig	n_imp	histo_1	histo_2
wannier	1					0.50677703	2.88818561					
delta	1		1	good				-0.019280458878				
impurity_1	1		1	good					0.287717595956	6.00764	249.733784782	248.017658037
dft	2	1			5.154448e-06							
wannier	2					0.5067774	2.88818893					
delta	2		1	good				0.20448195624				
impurity_1	2		1	good					0.108398183571	6.03352	244.489908363	241.269380924
dft	3	1			0.001663299							
wannier	3					0.50688796	2.88815083					
delta	3		1	good				0.343062784144				
impurity_1	3		1	good					0.0542822907893	6.05166	239.922505082	240.530895385

- i_outer: The scf step number for a given charge density and impurity self-energy
- i_latt: The iteration number for solving Kohn-Sham equation with a given charge density obtained from ComLowH.
- i_imp: The iteration number for solving impurity problem through ComLowH + ComCTQMC
- causality: causality of hybridization function / self-energy
- delta_rho: The norm difference between the current charge density and the one from the previous scf step.
- w_sp_min: minimum spread of the Wannier functions
- w_sp_max: maximum spread of the Wannier functions
- mu: LDA+DMFT chemical potential w.r.t. LDA chemical potential
- std_sig:

$$\sqrt{\frac{\sum_i (\Sigma_i^j(i\omega_n) - \Sigma_i^{j-1}(i\omega_n))^2}{n_\omega n_{orb}}}$$

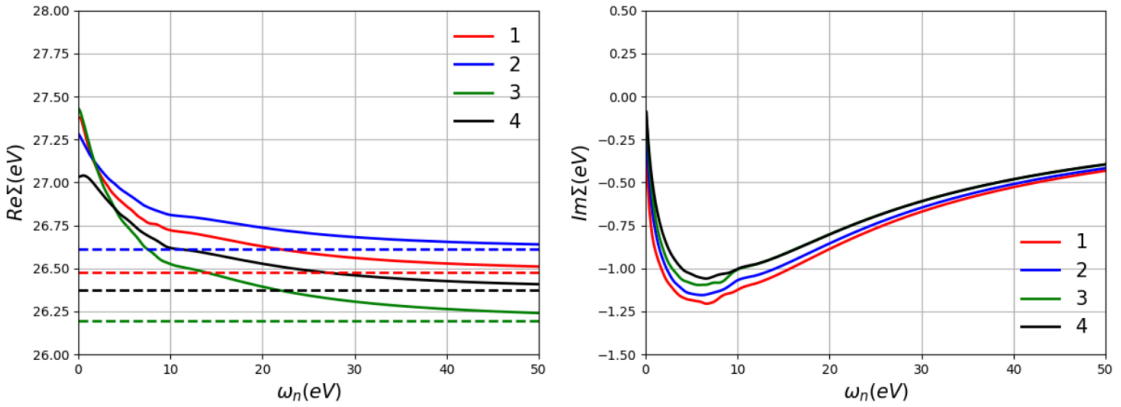
- n_imp: occupation of the impurity orbitals
- histo_1: the first moment of the perturbation order histogram
- histo_2: the second moment of the perturbation order histogram

■ **sig.dat**

'sig.dat' contains impurity self-energies. The first column lists matsubara frequencies and the next columns are real and imaginary parts of self-energies of Fe d-orbital.

# omega(eV)	Re Sig_{1,1}(eV)	Im Sig_{1,1}(eV)	Re Sig_{1,2}(eV)	Im Sig_{1,2}(eV)	Re Sig_{1,3}(eV)	Im Sig_{1,3}(eV)	Re Sig_{1,4}(eV)	Im Sig_{1,4}(eV)
0.081216424692	27.376953779216	-0.265104324996	27.277842455532	-0.177075773451	27.425998025766	-0.896745581017	27.033042807875	-0.089882158904
0.243649274076	27.377335210723	-0.516027757206	27.263135232851	-0.371165995460	27.409245675634	-0.261729717960	27.035383203165	-0.230922866262
0.406082123461	27.350541973157	-0.651404469022	27.246646297662	-0.496864677447	27.379208055544	-0.386778760189	27.039100192451	-0.336976074057
0.568514972845	27.318305180096	-0.747066591669	27.230117705542	-0.595424684452	27.348947676966	-0.489921729552	27.040624934272	-0.425962173127
0.730947822229	27.283867336136	-0.813375262193	27.213446880534	-0.671093501416	27.316278876584	-0.573829854054	27.038299684794	-0.497785452319
0.893380671613	27.249406344349	-0.860174419442	27.196383033097	-0.731505939544	27.283167710025	-0.642241108661	27.034153928540	-0.558997023966
1.055813520997	27.217499872937	-0.896115537220	27.180008692133	-0.781941528204	27.249932818533	-0.701737027931	27.028489430603	-0.611537107947
1.218246370382	27.189034943431	-0.926890068635	27.164604070524	-0.824741777617	27.216838520564	-0.751693103836	27.020998760780	-0.657759918529
1.380679219766	27.163768431266	-0.954352109219	27.150755271948	-0.861886211823	27.185414567001	-0.792034173701	27.011697700432	-0.698102246840
1.543112069150	27.139979968647	-0.978308633734	27.137567579078	-0.894546386133	27.155791097520	-0.825615737018	27.002172449123	-0.734820401891

Plots of the self-energy:



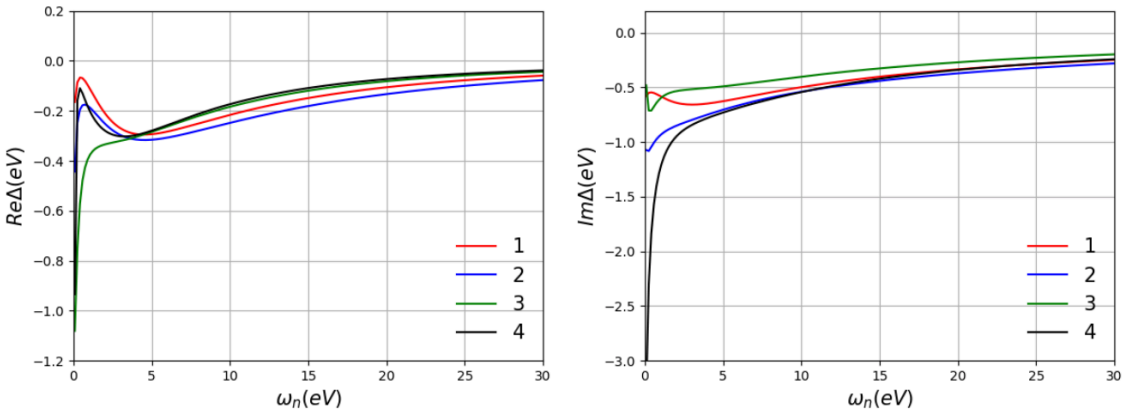
Impurity self-energy associated with the Fe-d orbitals on the imaginary frequency axis. The red, blue, green, and black lines represent Fe-d_{xy}, Fe-$d_{yz,xz}$, Fe-d_{z2}, and Fe-d_{x2-y2} characters, respectively.

■ **delta.dat**

'delta.dat' is in the same format of 'sig.dat':

# omega(eV)	Re Sig_{1,1}(eV)	Im Sig_{1,1}(eV)	Re Sig_{1,2}(eV)	Im Sig_{1,2}(eV)	Re Sig_{1,3}(eV)	Im Sig_{1,3}(eV)	Re Sig_{1,4}(eV)	Im Sig_{1,4}(eV)
0.081216424692	-0.164790827849	-0.578253170439	-0.443075833811	-1.072532593788	-1.080496117222	-0.480486426904	-0.933935326792	-3.287178965744
0.243649274076	-0.085975929071	-0.549773510856	-0.248216107607	-1.081679010133	-0.750392962889	-0.711746312504	-0.158153314833	-2.303444685780
0.406082123461	-0.067083525036	-0.545502201394	-0.195149501640	-1.045030341353	-0.573239028216	-0.712120234125	-0.109533071562	-1.838117222560
0.568514972845	-0.069107370488	-0.550932762083	-0.177851525437	-1.007352567113	-0.479545394563	-0.676744763718	-0.129348980065	-1.575849463378
0.730947822229	-0.080363493565	-0.561031721003	-0.175076998543	-0.975652597003	-0.427144505699	-0.642572465938	-0.155879527165	-1.407791078879
0.893380671613	-0.095836308888	-0.572950608252	-0.179547586463	-0.949702618977	-0.395549821259	-0.614562878212	-0.181202705616	-1.290203711398
1.055813520997	-0.113131003935	-0.585297104458	-0.187789380922	-0.928308795299	-0.375319059063	-0.592656137414	-0.203212397537	-1.202523050927

Plots of the hybridization function:



Hybridization function associated with the Fe-d orbitals on imaginary frequency axis. The red, blue, green, and black lines represent Fe-d_{xy}, Fe-$d_{yz,xz}$, Fe-d_{z2}, and Fe-d_{x2-y2} characters, respectively.

Analytical Continuation of Self-energy

To obtain the density of states (DOS), we need to perform an analytic continuation of 'sig.dat' to produce the impurity self-energy on the real frequency axis. To do this, we will adopt the maximum entropy (maxent) method. Any publicly available maxent code can be employed. For the purposes of this tutorial, however, we will use K. Haule's maxent code (freely available at http://www.physics.rutgers.edu/~haule).

To access maxent code, you should export the path to the executable in your startup shell script.

export WIEN_DMFT_ROOT=[path to Haule's code bin directory where maxent_run.py is located]

To run the maxent code, move to your working directory, create the maxent directory in the "lda_dmft" directory and then move to it:

```
$ mkdir maxent
$ cd maxent
```

By executing 'maxent_wrapper.py', we can obtain the self-energy on real axis by automatically calling maxent_run.py:

```
$ $COMSUITE_BIN/maxent_wrapper.py ../sig.dat
```

You can see its options with -h option:

```
$COMSUITE_BIN/maxent_wrapper.py –h
```

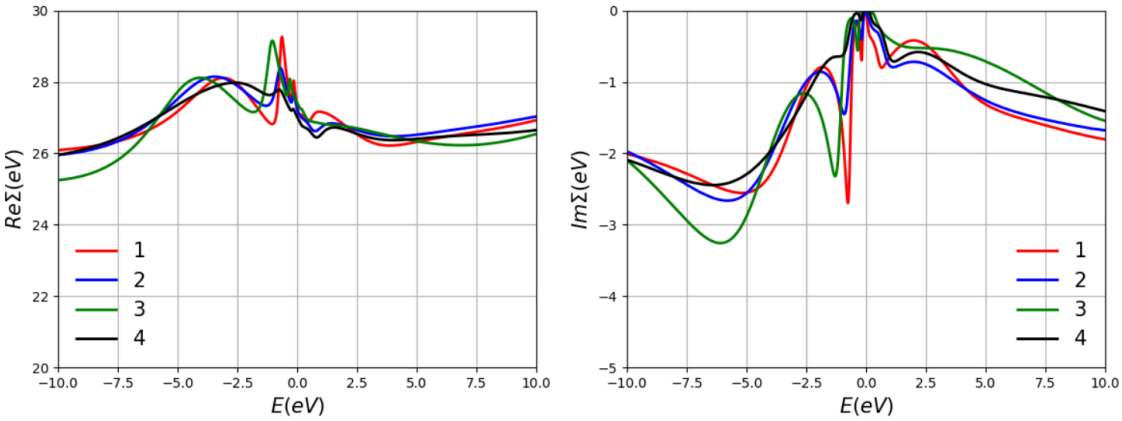
```
usage: maxent_wrapper.py [-h] sig [error]

call maxent_run.py from EDMFTF package and return self-energy on real axis. If
maxent_params.dat is not present in the directory, it generates one. The name
of the output file will be sig_realaxis.dat

positional arguments:
  sig         self-energy file on imaginary axis
  error       Errors for the maxent.Optional. Default value=0.05

optional arguments:
  -h, --help  show this help message and exit
```

Here note that in order to perform maxent, `maxent_params.dat' file is needed. This file should be written in python dictionary format as follows:

```
params={'statistics': 'fermi', # fermi/bose
        'Ntau'      : 3000,     # Number of time points
        'L'         : 70.0,     # cutoff frequency on real axis
        'Nw'        : 501,     # number of frequency points on real axis
        'gwidth'    : 140.0,  # width of gaussian
        'idg'       : 1,       # error scheme: idg=1 -> sigma=deltag ; idg=0 -> sigma=deltag*G(tau)
        'deltag'    : 0.05,   # error
        'Asteps'    : 4000,    # anealing steps
        'alpha0'    : 1000,    # starting alpha
        'x0'        : 0.01,    # low energy cutoff
        'min_ratio' : 0.001,    # condition to finish, what should be the ratio
        'iflat'     : 1,       # iflat=0 : constant model, iflat=1 : gaussian of width gwidth, iflat=2 : input using file model.dat
        'Nitt'      : 1000,    # maximum number of outside iterations
        'Nr'        : 0,       # number of smoothing runs
        'bwdth'     : 0.03,    # smoothing width
        'Nf'        : 5,      # to perform inverse Fourier, high frequency limit is computed from the last Nf points
         }
```

If 'maxent_params.dat' file is not present in the directory, maxent_wrapper.py will automatically generate the file with default options and execute subsequent jobs. If maxent is finished successfully, you will obtain analytically continued self-energy file, 'sig_realaxis.dat'. 'sig_realaxis.dat' is in the same format with 'sig.dat' except that the first column is real frequency values.

Plots of the impurity self-energy on the real frequency axis:



The impurity self-energy on the real frequency axis as obtained by using the maximum entropy method.

LDA+DMFT density of states

To obtain the DOS, we must post-process the data by executing ComLowH again. First, create a

directory for the DOS calculation in the “lda_dmft” directory and move to it:

```
$ mkdir realgrid
$ cd realgrid
```

Copy necessary files to calculate DOS and partial DOS by using prepare_realaxis.py which is in $COMSUITE_BIN folder.

```
$ $COMSUITE_BIN/prepare_realaxis.py 0.1 ../lowh/ ../wannier/ ../maxent/sig_realaxis.dat 30 30 30 -m 2
```

You can see its options with -h option:

```
$COMSUITE_BIN/prepare_realaxis.py –h
```

```
usage: prepare_realaxis.py [-h] [-m MODE]
                           broadening lowh_directory wan_directory self_energy
                           [kmesh_b1_for_dos] [kmesh_b2_for_dos]
                           [kmesh_b3_for_dos]

prepare inputs of comlowh calculation on real axis

positional arguments:
  broadening            broadening
  lowh_directory        lowh directory
  wan_directory         wannier directory
  self_energy           real-axis self-energy
  kmesh_b1_for_dos      finer kmesh along b1 axis for the DOS. Optional
  kmesh_b2_for_dos      finer kmesh along b2 axis for the DOS. Optional
  kmesh_b3_for_dos      finer kmesh along b3 axis for the DOS. Optional

optional arguments:
  -h, --help            show this help message and exit
  -m MODE, --mode MODE  If 3, code calculates spectral function along the high
                        symmetry line defined in 'kpath.dat'. If it is 2, it
                        calculates projected density of states. Default: 3
```

Run ComLowH with job submission script. An example of job script using SLURM is

```
#!/bin/bash -l
#SBATCH -J temp
#SBATCH -q debug
#SBATCH -N 1
#SBATCH -e temp.%j.err
#SBATCH -o temp.%j.out
#SBATCH -L SCRATCH
#SBATCH -C haswell
#SBATCH -t 00:30:00
srun -n 30 $COMSUITE_BIN/ComLowH
```

Having done so, you will obtain files tdos.dat and pdos.dat.

The format of tdos.dat file is:

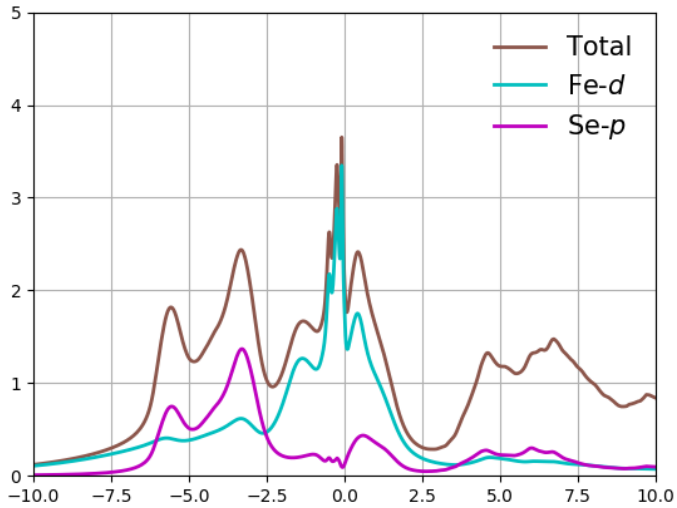
```
#       omega (eV)          TDOS (1/eV)
   -70.000000000000      0.000195619177
   -65.733023713200      0.000220852216
   -61.955278682000      0.000247384949
   -58.587128546700      0.000275509163
   -55.565331497900      0.000305078323
   -52.839027896300      0.000336222906
   -50.366851286200      0.000368858343
   -48.114812211200      0.000403221253
   -46.054723948000      0.000439643908
   -44.163014879300      0.000479094039
```

The format of pdos.dat file is:

```
#     omega (eV)              (1,0,0)             (1,1,-1)              (1,1,0)              (1,1,1)              (1,2-2)              (1,2,-1)              (1,2,0)              (1,2,1)
(1,2,2)                 (2,0,0)             (2,1,-1)              (2,1,0)              (2,1,1)              (2,2-2)              (2,2,-1)              (2,2,0)              (2,2,1)
(2,2,2)                 (3,1,-1)            (3,1,0)               (3,1,1)              (3,2-2)              (3,2,-1)             (3,2,0)               (3,2,1)              (3,2,2)
(4,1,-1)                (4,1,0)             (4,1,1)               (4,2-2)              (4,2,-1)             (4,2,0)              (4,2,1)               (4,2,2)
   -70.000000000000       0.000005939755      0.000005057305        0.000005245784       0.000005057315       0.000006792508       0.000006744313        0.000006834740       0.000006744311
0.000006830156       0.000005939755       0.000005057315       0.000005245805       0.000005057305       0.000006792506       0.000006744311       0.000006834740       0.000006744313
0.000006830156       0.000006469568       0.000006645676       0.000006469557       0.000004628600       0.000004658246       0.000004645276       0.000004658246       0.000004388215
0.000006469545       0.000006645675       0.000006469555       0.000004628616       0.000004658247       0.000004645299       0.000004658247       0.000004388215
   -65.733023713200       0.000006714454      0.000005663130        0.000005884281       0.000005663142       0.000007735440       0.000007693656        0.000007789557       0.000007693654
0.000007779381       0.000006714454       0.000005663142       0.000005884307       0.000005663130       0.000007735438       0.000007693654       0.000007789557       0.000007693656
0.000007779381       0.000007346607       0.000007555772       0.000007346595       0.000005149602       0.000005186301       0.000005168610       0.000005186301       0.000004869603
0.000007346580       0.000007555771       0.000007346592       0.000005149621       0.000005186302       0.000005168637       0.000005186302       0.000004869603
   -61.955278682000       0.000007536253      0.000006297008        0.000006553719       0.000006297022       0.000008740915       0.000008666530        0.000008797795       0.000008666528
0.000008812729       0.000007536253       0.000006297022       0.000006553751       0.000006297008       0.000008740913       0.000008666528       0.000008797795       0.000008666530
0.000008812729       0.000008282317       0.000008528090       0.000008282303       0.000005688591       0.000005733385       0.000005710025       0.000005733385       0.000005365853
0.000008282285       0.000008528090       0.000008282300       0.000005688613       0.000005733386       0.000005710057       0.000005733387       0.000005365853
   -58.587128546700       0.000008405428      0.000006958375        0.000007253559       0.000006958391       0.000009834622       0.000009732416        0.000009891220       0.000009732416
0.000009883403       0.000008405428       0.000006958391       0.000007253596       0.000006958375       0.000009834619       0.000009732414       0.000009891220       0.000009732416
0.000009883403       0.000009277528       0.000009563571       0.000009277510       0.000006244538       0.000006298553       0.000006268481       0.000006298553       0.000005875991
0.000009277490       0.000009563570       0.000009277508       0.000006244563       0.000006298554       0.000006268517       0.000006298555       0.000005875991
   -55.565331497900       0.000009322357      0.000007646758        0.000007983299       0.000007646777       0.000010967621       0.000010864515        0.000011047250       0.000010864513
0.000011046570       0.000009322357       0.000007646777       0.000007983343       0.000007646758       0.000010967618       0.000010864513       0.000011047250       0.000010864515
0.000011046570       0.000010333031       0.000010663112       0.000010333011       0.000006816480       0.000006880890       0.000006842979       0.000006880889       0.000006399075
0.000010332988       0.000010663111       0.000010333008       0.000006816508       0.000006880891       0.000006843021       0.000006880892       0.000006399075
```

- (atom index, l, m) if spin_orbit==False and (atom index, I, i,m) if spin_orbit==True.

Plot of tdos.dat and pdos.dat:



The total density of states and the projected density of states within charge self-consistent LDA+DMFT.

LDA+DMFT spectral function

To obtain spectral function, we must post-process the data by executing ComLowH again. First create a directory for the spectral function in "lda_dmft" directory and move to it:

```
$ mkdir realaxis
$ cd realaxis
```

Having done so, copy the necessary files to calculate the spectral function by using prepare_realaxis.py which is in $COMSUITE_BIT directory. Note that the option should be '-m 3'.

```
$ $COMSUITE_BIN/prepare_realaxis.py 0.1 ../lowh/ ../wannier/ ../maxent/sig_realaxis.dat -m 3
```

Then you should create a k-path file (kpath.dat) In the first line, the number of k-points is specified. In the following lings, k-points are written in terms of the reciprocal lattice vector.

```
129       # (kx,  ky,  kz)
    0.00000000   0.00000000   0.00000000
    0.00000000   0.02941176   0.00000000
    0.00000000   0.05882353   0.00000000
    0.00000000   0.08823529   0.00000000
    0.00000000   0.11764706   0.00000000
    0.00000000   0.14705882   0.00000000
    0.00000000   0.17647059   0.00000000
    0.00000000   0.20588235   0.00000000
    0.00000000   0.23529412   0.00000000
    0.00000000   0.26470588   0.00000000
```

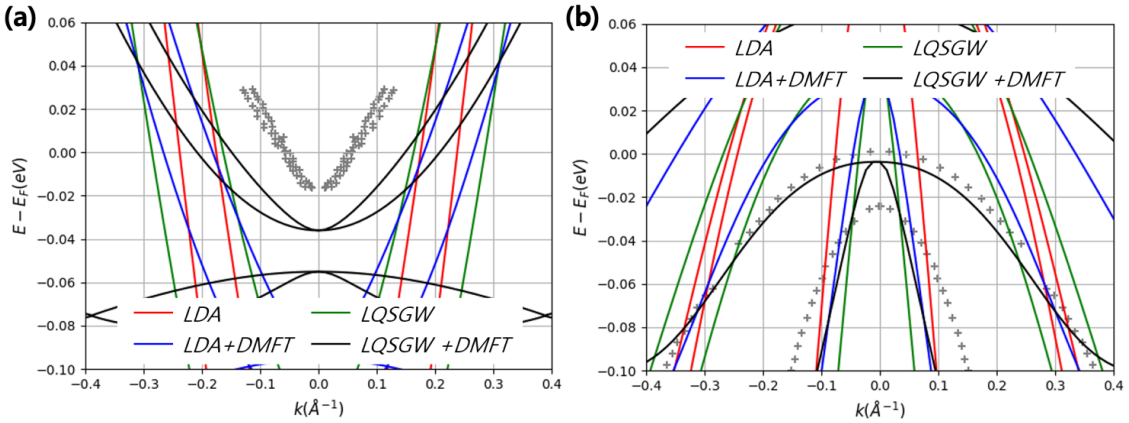
Run ComLowH with job submission script. An example of job script using SLURM is

```
#!/bin/bash -l
#SBATCH -J temp
#SBATCH -q debug
#SBATCH -N 1
#SBATCH -e temp.%j.err
#SBATCH -o temp.%j.out
#SBATCH -L SCRATCH
#SBATCH -C haswell
#SBATCH -t 00:30:00
srun -n 30 $COMSUITE_BIN/ComLowH
```

Having done so, you will have obtained a file named spectral.dat. The format of this file is

# kpoint	E (eV)	A (1/eV)
1	-70.000000000000	0.000001986280
2	-70.000000000000	0.000001986436
3	-70.000000000000	0.000001986897
4	-70.000000000000	0.000001987642
5	-70.000000000000	0.000001988636
6	-70.000000000000	0.000001989830
7	-70.000000000000	0.000001991164
8	-70.000000000000	0.000001992575
9	-70.000000000000	0.000001993999
10	-70.000000000000	0.000001995379

Plot of spectral.dat file along a high symmetry line in the first Brillouin zone.:



LDA (red lines), LQSGW (green lines), LDA+DMFT (blue lines), and LQSGW+DMFT (black lines) along (a) $\Gamma - M - \Gamma$ line (b) $M - \Gamma - M$ at $T = 300$ K. Angle resolved photoemission data at high-temperature phase ($T = 120$ K) are marked by gray plus symbols[1].

[1] M. D. Watson et al., Phys. Rev. B **91**, 155106 (2015); P. Zhang et al., Phys. Rev. B **91**, 214503 (2015)