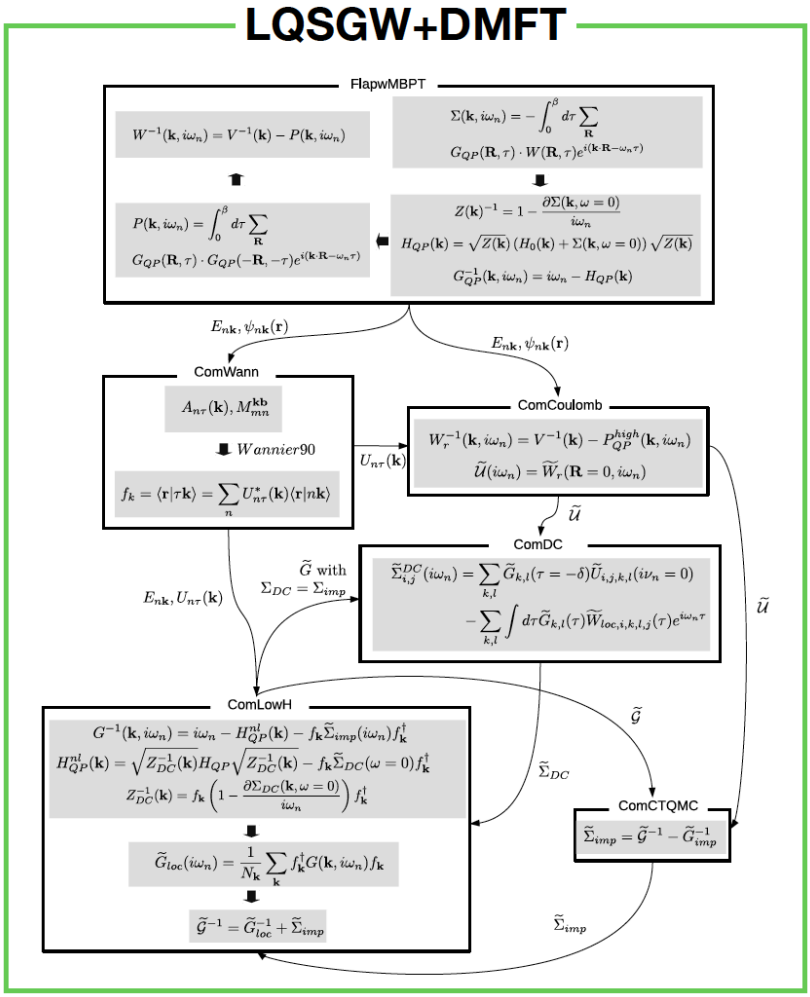
**Example: NiO**

## LQSGW+DMFT in COMSUITE

We will calculate the electronic structure of a charge transfer insulator NiO within LQSGW+DMFT. COMSUITE package for LQSGW+DMFT is composed of six components (softwares) and its work flow is described below.




1. Construction of a quasi-particle Hamiltonian within *ab initio* LQSGW 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. calculation of the bosonic Weiss field within constrained Random Phase approximation(cRPA) and evaluation of Slater's integral associated with the impurity orbitals by **ComCoulomb**
4. calculation of the double-counted self-energy associated with the impurity orbitals within local GW approximation by **ComDC**
5. Wannier interpolation of the mean-field Hamiltonian and solving the DMFT self-consistent equation by **ComLowH** and **ComCTQMC**

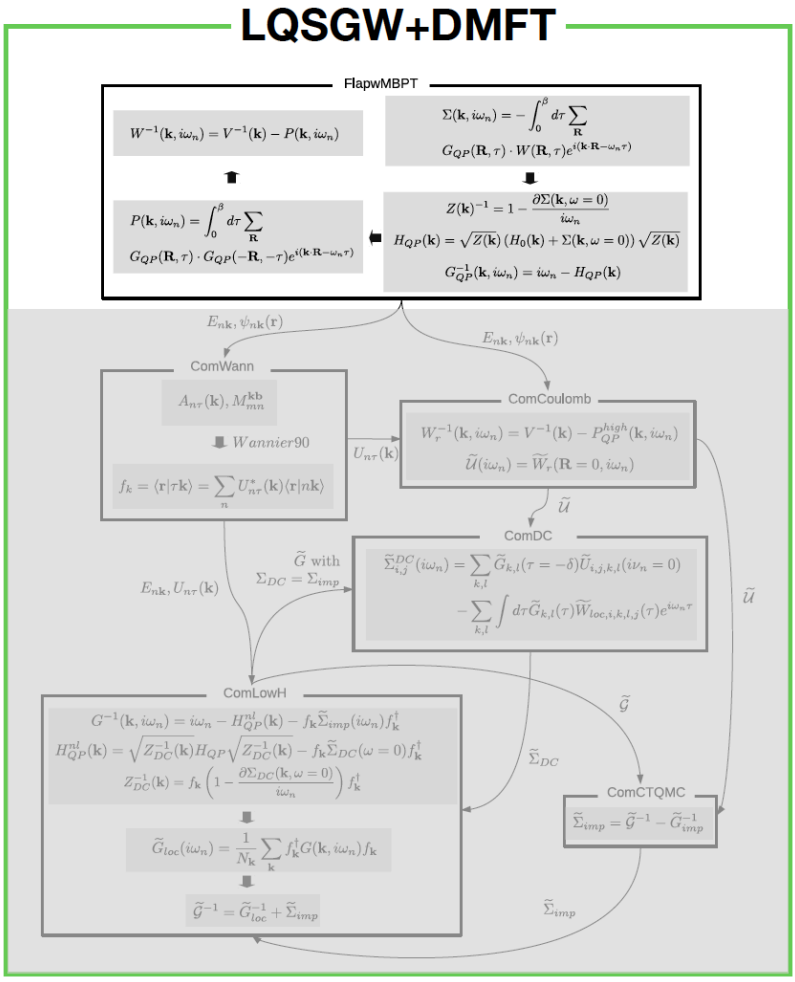
These components (software) along with Wannier90 library are located at install_directory ('install_directory' is described in 'Build and Install' section in Installation of COMSUITE page). To access COMSUITE executables, you should export above bin path in your startup shell script.

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

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

## NiO LQSGW prerun

To run LQSGW+DMFT, the first step is the LQSGW prerun (unshaded part of following figure).




To proceed with the LQSGW calculation, please create a directory named "lqsgw" in your work directory. It is possible to give this directory another name. However, it is important that this name be specified in 'comdmft.ini' (as will be explained in the next section). After doing so, cd to this directory:

```
$ mkdir lqsgw
$ cd lqsgw
```

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

```
$ $COMSUITE_BIN/cif2matdelab.py –m qp –k 3 NiO.cif
```

The generated ini file of NiO looks as follows:

```
TEXT band structure calculation
CONTROL   iter_dft=108  iter_hf=  0  iter_gw=  0 iter_qp= 40
          admix=0.100  adspin=0.700 adm_gw=0.100 acc_it_gw=0.10
          iexch=005 scal_spin= 1.0000
          nproc_tau=   24 nproc_k=   16
          irel=1 clight=274.074e+00 rel_interst=F irel_core=1
          temperature=   1000.00  restart=F
FILES
  allfile=NiO
SYM symgen=I_R4Z_R3D_
STRUCTURE  par=  7.92600000 natom=  2 nsort=  2  istruc= 3
      is=  1  2
      b/a= 1.000000  c/a= 1.000000
      a=   0.0000000000000000   0.5000000000000000   0.5000000000000000
      b=   0.5000000000000000   0.0000000000000000   0.5000000000000000
      c=   0.5000000000000000   0.5000000000000000   0.0000000000000000
    tau=   0.0000000000000000   0.0000000000000000   0.0000000000000000
    tau=   0.5000000000000000   0.5000000000000000   0.5000000000000000
REAL SPACE MESHES mdiv=  14  14  14
                  nrdiv=  10  10  10
BASIS  cut_lapw_ratio=0.610 cut_pb_ratio=0.980
       eps_pb=1.e-03
ZONES nbndf=   0
DOS   emindos=-20.000  emaxdos= 20.000   ndos=  800
      n_cont_frac=  30 e_small=2.e-02
      dos= T           bandstructure= T
K_POINT  ndiv=   6   6   6  metal=T n_k_div=  12 k_line=111
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=   46 n_tau_int=  1200
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=O1     z=  8.0 magn_shift= 0.000
  smt= 1.77000 h= 0.0200 nrad=  616 z_dop=0.000
  lmb= 6  lmpb= 6
  lim_pb_mt= 30 30 30 30 30 30 30
  ntle=  3  3  2  2  2  2  2  1  1
  l  augm  atocc   ptnl  corr idmd
  0   APW  2.000  2.800     N    0
  0   LOC  0.000  3.950     N    1
  0   LOC  0.000  4.950     N    1
  1   APW  4.000  2.800     N    0
  1   LOC  0.000  3.950     N    1
  1   LOC  0.000  4.950     N    1
  2   APW  0.000  3.800     N    0
  2   LOC  0.000  4.950     N    1
  3   APW  0.000  4.800     N    0
  3   LOC  0.000  5.950     N    1
  4   APW  0.000  5.800     N    0
  4   LOC  0.000  6.950     N    1
  5   APW  0.000  6.800     N    0
  5   LOC  0.000  7.950     N    1
  6   APW  0.000  7.800     N    0
  6   LOC  0.000  8.950     N    1
  txtel=Ni    z= 28.0 magn_shift= 0.000
  smt= 2.12000 h= 0.0200 nrad=  616 z_dop=0.000
  lmb= 6  lmpb= 6
  lim_pb_mt= 30 30 30 30 30 30 30
  ntle=  4  3  2  2  2  2  2  1  1
  l  augm  atocc   ptnl  corr idmd
  0   LOC  2.000  3.950     N    0
  0   APW  2.000  4.800     N    0
  0   LOC  0.000  5.950     N    1
  0   LOC  0.000  6.950     N    1
  1   LOC  6.000  3.950     N    0
  1   APW  0.000  4.800     N    0
  1   LOC  0.000  5.950     N    1
  2   APW  8.000  3.800     N    0
  2   LOC  0.000  4.950     N    1
  3   APW  0.000  4.800     N    0
  3   LOC  0.000  5.950     N    1
  4   APW  0.000  5.800     N    0
  4   LOC  0.000  5.950     N    1
  5   APW  0.000  6.800     N    0
  5   LOC  0.000  7.950     N    1
  6   APW  0.000  7.800     N    0
  6   LOC  0.000  8.950     N    1
```

One should modify several input keywords as follows:

- iter_dft: The number of DFT iterations. Set to 108.
- iter_qp: The number of LQSGW iterations. Set to 40.
- admix: charge mixing in DFT iterations. Set to 0.100.
- acc_it_gw: Final mixing for LQSGW iterations. Mixing is changed linearly from iteration to iteration from its initial value to its final. Set to 0.1.
- nproc_tau: The number of MPI processes associated with imaginary time and frequency. Set to 16. 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 24. For the details on the MPI parallization in FlapwMBPT, please goto FlapwMBPT homepage (https://www.bnl.gov/cmpmsd/flapwmbpt).

- mdiv: The real space mesh in the unit cell used for electronic density, Hartree potential, and LDA exchange-corrleation potential evaluations. Set to [14 14 14].
- nrdiv: The real space mesh associated with the interstitial product basis. Set to [12 12 12]
- cut_lapw_ratio: Defines the maximal value of **k +G** for the LAPW basis in the interstitial region.
- ndiv: The number of k-mesh in Brillouin zone. 6 × 6 × 6 k-mesh for the present case.
- k_line: Three numbers defying the direction in the reciprocal space for certain output purposes. Set to 111.

Note also that the total number of MPI processes is nproc_tau × nproc_k which is 384 for the present case.

We also modified Ni and O 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 LQSGW by executing rspflapw.exe. An example of job script to run rspflapw.exe using SLURM is

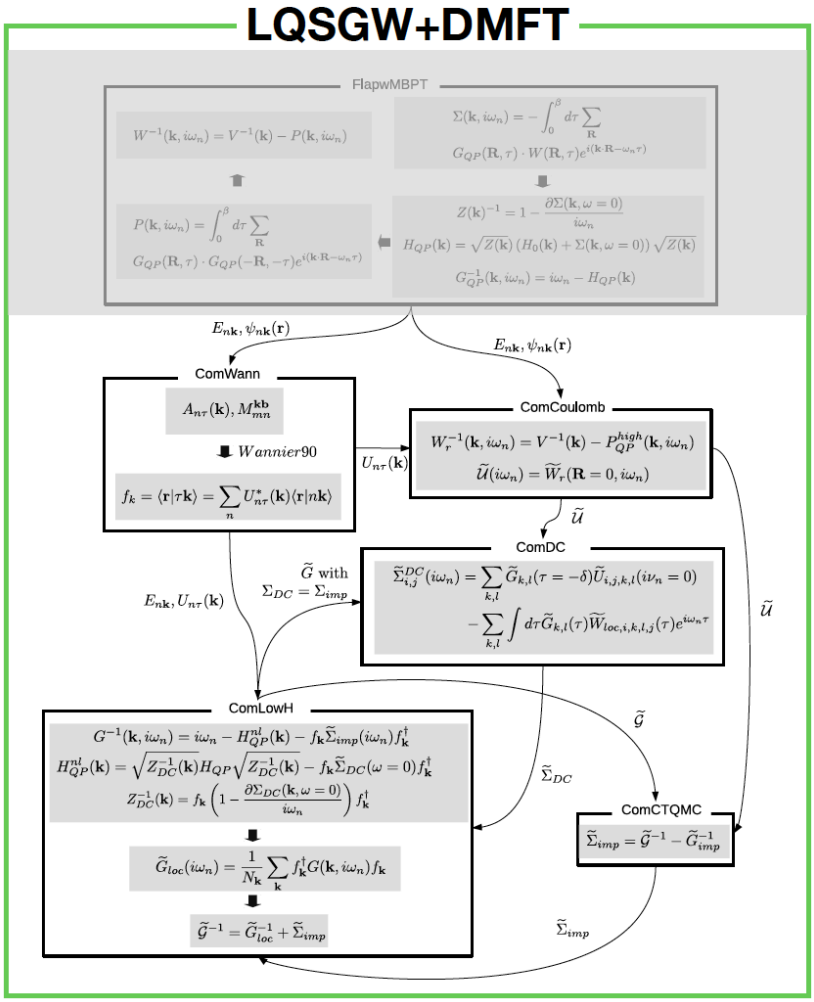
An example of job script using SLURM is

```
#!/bin/bash -l
#SBATCH -J temp
#SBATCH -p regular
#SBATCH -N 32
#SBATCH -e temp.%j.err
#SBATCH -o temp.%j.out
#SBATCH -L SCRATCH
#SBATCH -C haswell
#SBATCH -t 05:00:00
srun -n 384 $COMSUITE_BIN/rspflapw.exe
```

The total number of processes is 384 as specified in ini file. Note that rspflapw will redistribute the number of processes for double parallelization using MPI_SPLIT. If it fails the redistribution based on the input total number of processes, it will terminate the run with error message.

## NiO LQSGW+DMFT run

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




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

```
$ cd ..
$ mkdir lqsgw_dmft
$ cd lqsgw_dmft
```

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

```
#!/bin/bash -l
#SBATCH -J temp
#SBATCH -q premium
#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 the LQSGW+DMFT simulation. Based on the 'comdmft.ini' input file, 'comdmft.py' generates all the necessary input files for the individual programs (ComWann, ComCoulomb,ComDC, ComLowH and ComCTQMC) to run and execute jobs.

**Input file (comdmft.ini)**

In other to perform LQSGW+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 of 'control', 'wan_hmat' and 'imp':

```
control={'initial_lattice_dir'        : '../lqsgw',
        'method'              : 'lqsgw+dmft',
        'spin_orbit'          : False,
        'mpi_prefix': "srun -n 384",
        'impurity_problem':[[2, 'd']],
        'impurity_problem_equivalence':[1],
        }

wan_hmat={
       'kgrid': [15, 15, 15],
       'froz_win_min': -15.0,
       'froz_win_max': 10.0,
                  }

imp={'temperature'          : 300,
    '1':
    {
    'impurity_matrix': [
        [1,0,0,0,0],
        [0,1,0,0,0],
        [0,0,2,0,0],
        [0,0,0,1,0],
        [0,0,0,0,2]
        ],
    'thermalization_time': 1,
    'measurement_time': 10,
    'green_cutoff':  80,
    'coulomb': 'full',
    }
    }
```

**■ In Control**

These fields contain basic parameter which control LQSGW+DMFT run.

- 'initial_lattice_dir' : '../lqsgw'
  Enter the path which contains LQSGW output such as quasi particle eigenvalue and eigenfunctions. It is the lqsgw prerun folder.

- 'method' : 'lqsgw+dmft'
  Either lda+dmft or lqsgw+dmft. Currently COMSUITE has these two options. Choose 'lqsgw+dmft' for present work (LQSGW+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 384'
  MPI prefix used for ComCoulomb, ComDC, ComLowH, ComWann, and ComCTQMC. If a different MPI prefixs from this prefix is necessary for individual program, use 'mpi_prefix_coulomb', 'mpi_prefix_lowh', 'mpi_prefix_dc', 'mpi_prefix_wannier', and

'mpi_prefix_impurity'. Note that 384 is the number of total MPI processes we want to use for the present case.
You can set any number you want. Here we note that, for ComCoulomb, comdmft.py will redistribute the number of processes on two dimensional MPI grid using MPI_COMM_SPLIT.

- 'impurity_problem': [[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 "../lqsgw/coord.xsf"
  Shell index is either "d" or "f". Here, Ni-d shell is treated as an impurity problem.

- 'impurity_problem_equivalence': [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 LQSGW+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'].

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

- 'mpi_prefix_dc':
  MPI prefix for ComDC. 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': [15,15,15]
  Crystal momentum grid for the Wannier interpolation of LQSGW band structure.

- 'froz_win_min': -15.0 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

- For each distinct impurity problem indexed by the value in control ["impurity_problem_equivalence"],
  - 'impurity_matrix': [
    [1,0,0,0,0],
    [0,1,0,0,0], 1:$t_{2g}$
    [0,0,2,0,0], 2:$e_g$
    [0,0,0,1,0],
    [0,0,0,0,2]
    ],
    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 $|xy\rangle, |yz\rangle, |z^2\rangle, |xz\rangle, |x^2\text{-}y^2\rangle$ 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': 80,
    Cutoff-energy in eV to sample green's function and self-energy. The values beyond this energy will be provided by analytical equations.

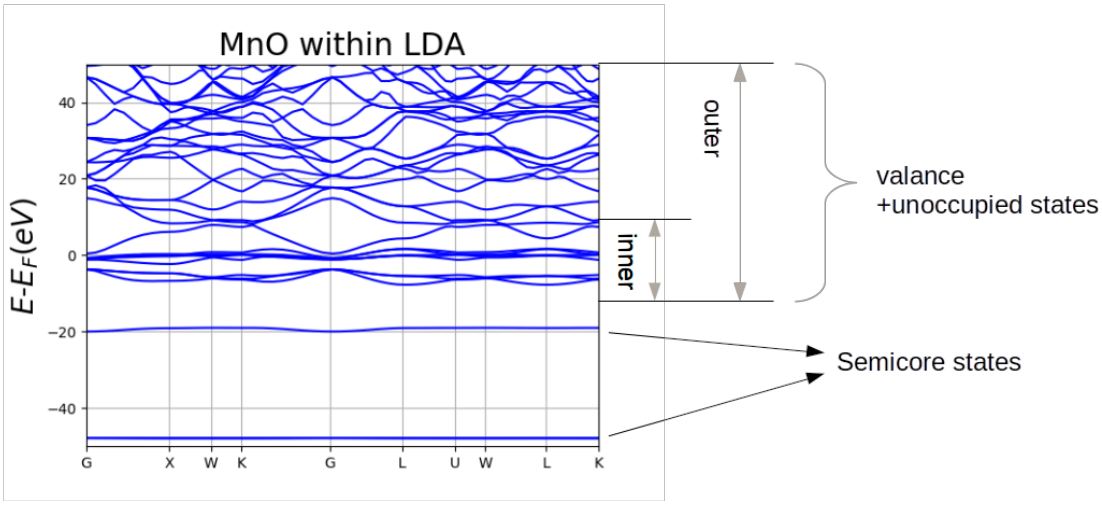
  - 'Coulomb': 'full',
    'full' or 'ising' are available. We construct Coulomb matrix in the following way.
    $$U_{m_1,m_2,m_3,m_4} = \sum_{k=0}^{2l,even} \frac{4\pi}{2k+1} F_l^k \sum_{q=-k}^{k} \langle Y_l^{m_1} | Y_k^q Y_l^{m_4} \rangle \langle Y_l^{m_2} Y_k^q | Y_l^{m_3} \rangle$$
    If 'full',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

  - 'susceptibility_cutoff':

Cutoff-energy to sample susceptibility. The default value is 300 eV.

**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 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 LDA band of MnO as an example to illustrate these concepts).

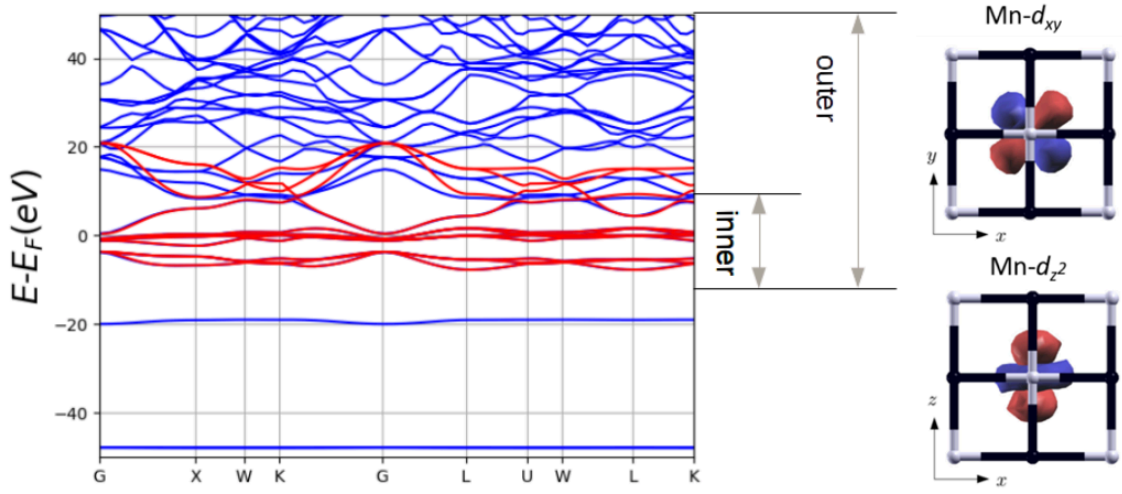



We choose initial trial orbitals $|\tau\mathbf{R}=0\rangle_t$ using MT orbitals with desired angular momentum character. The radial functions of $|\tau\mathbf{R}=0\rangle_t$ are chosen in such a way to maximize

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

, 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 (lqsgw_dmft in this example). The list of files is

cmd.log
convergence.log : convergence log file
delta.dat : hybridization function
sig.dat : impurity self-energy
sig_dc.dat : double-counting self-energy
sig_dc_hf.dat : the high-frequency limit of double-counting self-energy
u_slater.dat : Slater-Condon parameterization of bosonic Weiss-field
v_slater.dat : Slater-Condon parameterization of bare coulomb interaction ($V_{loc}$)
w_slater.dat : Slater-Condon parameterization of screened coulomb interaction ($W_{loc}$)

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

■ **convergence.log**

| step | i_imp | causality | static_f0 | w_sp_min | w_sp_max | mu | std_sig | n_imp | histo_1 | histo_2 |
|---|---|---|---|---|---|---|---|---|---|---|
| wannier | | | | 0.28543421 | 1.7773025 | | | | | |
| coulomb_1 | | | 6.97943595685 | | | | | | | |
| dc_1 | | good | | | | | | | | |
| delta | 1 | good | | | | 0.019644259897 | | | | |
| impurity_1 | 1 | good | | | | | 3.37592293015 | 8.13892 | 104.203172231 | 113.442465644 |
| delta | 2 | good | | | | 0.227452938024 | | | | |
| impurity_1 | 2 | good | | | | | 1.76039597987 | 8.12925 | 95.5346308627 | 93.4049387127 |
| delta | 3 | good | | | | 0.360584306439 | | | | |
| impurity_1 | 3 | good | | | | | 0.873900782988 | 8.12575 | 93.8121360239 | 90.1533755051 |
| delta | 4 | good | | | | 0.438313820721 | | | | |

- keeping track of convergence of some quantities at each iteration
- i_imp: The number of solving impurity problem through ComLowH + ComCTQMC + ComDC
- causality: causality of hybridization function / self-energy
- w_sp_min: minimum spreading of the Wannier functions
- w_sp_max: maximum spreading of the Wannier functions
- mu: LQSGW+DMFT chemical potential w.r.t. LQSGW 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 in the impurity orbitals
- histo_1: the first moment of the perturbation order histogram
- histo_2: the second moment of the perturbation order histogram
- ctqmc_sign: CTQMC sign

■ **u_slater.dat** and **w_slater.dat**

Data format in u_slater.dat (also in w_slater.dat):

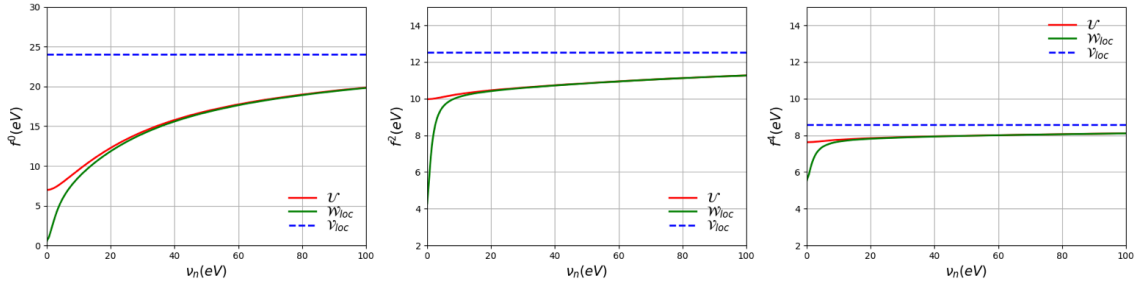
| # nu(eV) | 1:f0(eV) | 1:f2(eV) | 1:f4(eV) |
|---|---|---|---|
| 0.000000000000 | 6.979435956849 | 9.972684910682 | 7.626659183780 |
| 0.162432849384 | 6.991563460566 | 9.974254718886 | 7.627439680636 |
| 0.324865698768 | 6.995381415918 | 9.974733912820 | 7.627681553000 |
| 0.487298548153 | 6.996249914058 | 9.974825995447 | 7.627732241701 |
| 0.649731397537 | 7.003719509740 | 9.975764279332 | 7.628170672937 |
| 0.812164246921 | 7.017060208047 | 9.977474094269 | 7.628991575522 |
| 0.974597096305 | 7.033267110201 | 9.979588473166 | 7.630054710525 |
| 1.137029945690 | 7.051862355810 | 9.982051407717 | 7.631340778350 |
| 1.299462795074 | 7.072740247508 | 9.984834431675 | 7.632809228323 |
| 1.461895644458 | 7.095434905356 | 9.987858550026 | 7.634389875835 |

The first column is the bosonic matsubara frequencies and the second, third, and fourth column is Slater's integral F0, F2, and F4, respectively.

Data format of Bare Coulomb interaction in v_slater.dat:

| # 1:f0(eV) | 1:f2(eV) | 1:f4(eV) |
|---|---|---|
| 24.073782938928 | 12.539899507718 | 8.587692445309 |

Plots of dynamical U using u(v,w)_slater.dat files :




Slater's integrals of partially-screened Coulomb interactions associated with Ni-*d* orbitals are marked by red lines. For comparison, Slater's integrals of bare Coulomb interactions and fully-screened Coulomb interaction are shown by blue dashed lines and green full lines respectively.

**■ sig_dc.dat**

'sig_dc.dat' contains impurity self-energies within local GW approximation. The first column lists matsubara frequencies and the next columns are real and imaginary parts of self-energies of "$t_{2g}$" (Sig_{1,1}) and "$e_g$" (Sig_{1,2}) of Ni d-orbital.

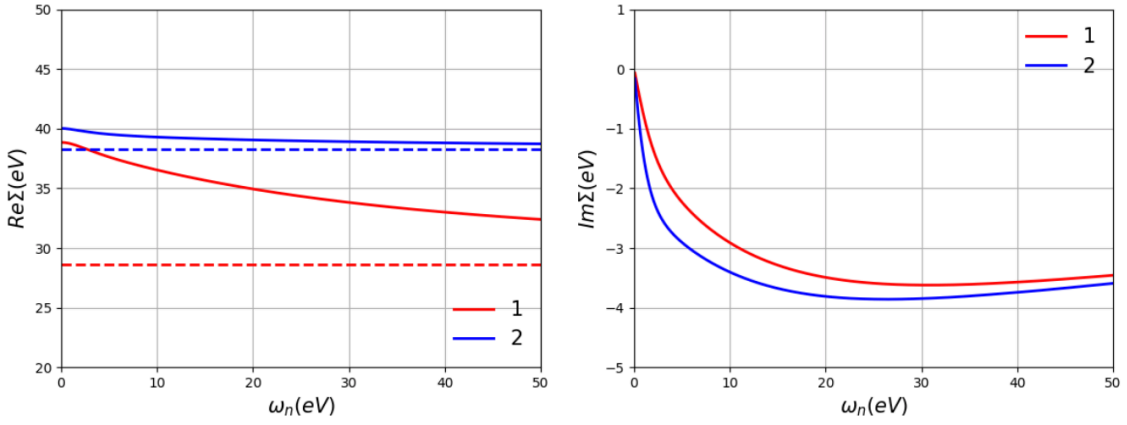
| # omega(eV) | Re Sig_{1,1}(eV) | Im Sig_{1,1}(eV) | Re Sig_{1,2}(eV) | Im Sig_{1,2}(eV) |
|---|---|---|---|---|
| 0.081216424692 | 38.849812100573 | -0.068546031041 | 40.025499346945 | -0.160998380353 |
| 0.243649274076 | 38.843310837938 | -0.204087668350 | 40.019531368126 | -0.455870104979 |
| 0.406082123461 | 38.830545145097 | -0.336860987958 | 40.009263582673 | -0.722950190529 |
| 0.568514972845 | 38.811894580413 | -0.465736619491 | 39.995967618274 | -0.963008760085 |
| 0.730947822229 | 38.787842093861 | -0.589783429676 | 39.980391178088 | -1.177371783712 |
| 0.893380671613 | 38.758942274676 | -0.708323505805 | 39.963076754013 | -1.367777823309 |
| 1.055813520997 | 38.725785079856 | -0.820931932399 | 39.944463348607 | -1.536278967301 |
| 1.218246370382 | 38.688965464350 | -0.927405312935 | 39.924917597311 | -1.685077961169 |
| 1.380679219766 | 38.649060962829 | -1.027719550394 | 39.904746666450 | -1.816380015196 |
| 1.543112069150 | 38.606616266484 | -1.121987778606 | 39.884206853383 | -1.932293825430 |

**■ sig_dc_hf.dat**

'sig_dc_hf.dat' contains real and imaginary part of the Hartree-Fock contribution to the impurity self-energy within local GW approximation

| # Re Sig_{1,1}(eV) | Im Sig_{1,1}(eV) | Re Sig_{1,2}(eV) | Im Sig_{1,2}(eV) |
|---|---|---|---|
| 28.641291666667 | 0.000000000000 | 38.254424000000 | 0.000000000000 |

Plots of the local-GW impurity self-energy using sig_dc.dat and sig_hf_dc.dat files:



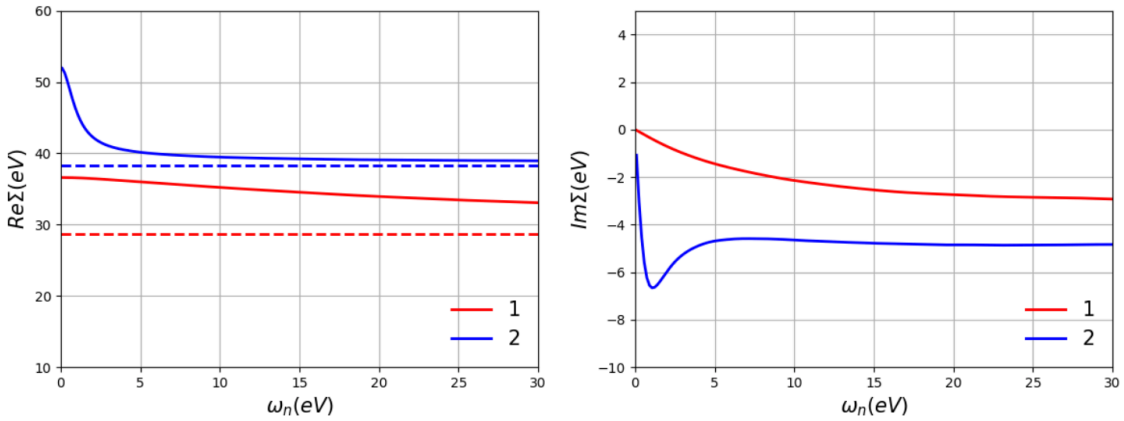

The double-counted electronic self-energy within the local GW approximation associated with the five Ni-*d* orbitals on the imaginary frequency axis. Red and blue lines represent the Mn-$t_{2g}$ ($d_{xy}$, $d_{yz}$, and $d_{zx}$) and Mn-$e_g$ ($d_{z2}$, and $d_{x2-y2}$) orbitals, respectively. Both the real and imaginary parts of self-energy do not show divergent behaviors near the Fermi energy, and the imaginary part is even linear along the imaginary frequency axis. However, if all the Feynman diagrams associated with the five Ni-*d* orbitals are summed, then, as we will see below, the self-energy shows a qualitatively different behavior.

■ **sig.dat**

'sig.dat' contains impurity self-energies obtained from ComCTQMC. The first column lists matsubara frequencies and the next columns are real and imaginary parts of self-energies of "$t_{2g}$" (Sig_{1,1}) and "$e_g$" (Sig_{1,2}) of Ni d-orbital.

| # omega(eV) | Re Sig_{1,1}(eV) | Im Sig_{1,1}(eV) | Re Sig_{1,2}(eV) | Im Sig_{1,2}(eV) |
|---|---|---|---|---|
| 0.081216424692 | 36.610282294250 | -0.030906819896 | 51.930572149778 | -1.075505707898 |
| 0.243649274076 | 36.608094121367 | -0.092632462786 | 51.279742152238 | -3.057365812488 |
| 0.406082123461 | 36.603410911625 | -0.154027532835 | 50.145981734417 | -4.544110991264 |
| 0.568514972845 | 36.596806252338 | -0.215002870849 | 48.878763596073 | -5.599141408326 |
| 0.730947822229 | 36.588122611708 | -0.275358271107 | 47.620334896420 | -6.233197777557 |
| 0.893380671613 | 36.577434855578 | -0.334930772818 | 46.478704946169 | -6.551743060755 |
| 1.055813520997 | 36.564829935732 | -0.393573837945 | 45.494569205726 | -6.658606053485 |
| 1.218246370382 | 36.550421988095 | -0.451152109101 | 44.668866498608 | -6.635019420261 |
| 1.380679219766 | 36.534362029772 | -0.507544937681 | 43.984489853395 | -6.537213188402 |
| 1.543112069150 | 36.516782259693 | -0.562657032187 | 43.419023193729 | -6.401224708965 |
| 1.705544918534 | 36.497812819435 | -0.616416442505 | 42.950717559202 | -6.248932600612 |

Plots of impurity self-energy using the sig.dat file:

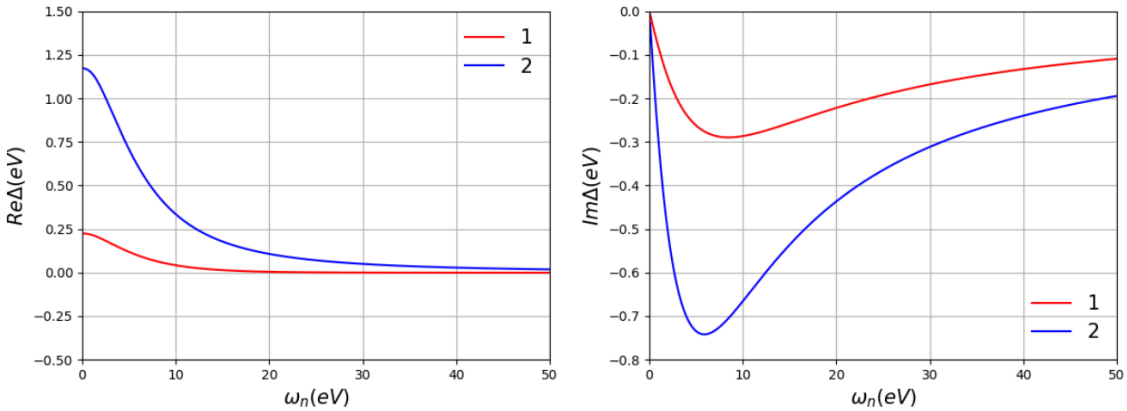



The impurity self-energy from ComCTQMC on the imaginary axis. In contrast to the electronic self-energy within the local GW approximation, both real and imaginary part of self-energy of Ni-$e_g$ on the imaginary frequency axis show divergent behaviors near the Fermi level.

■ **delta.dat**

'delta.dat' is in the same format with 'sig.dat'

Plots of the real and imaginary parts of the hybridization function using the delta.dat file:




The hybridization function associated with Ni-d orbitals on the imaginary frequency axis. The red and blue lines represent Ni-$t_{2g}$ and Ni-$e_g$ 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 "lqsgw_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

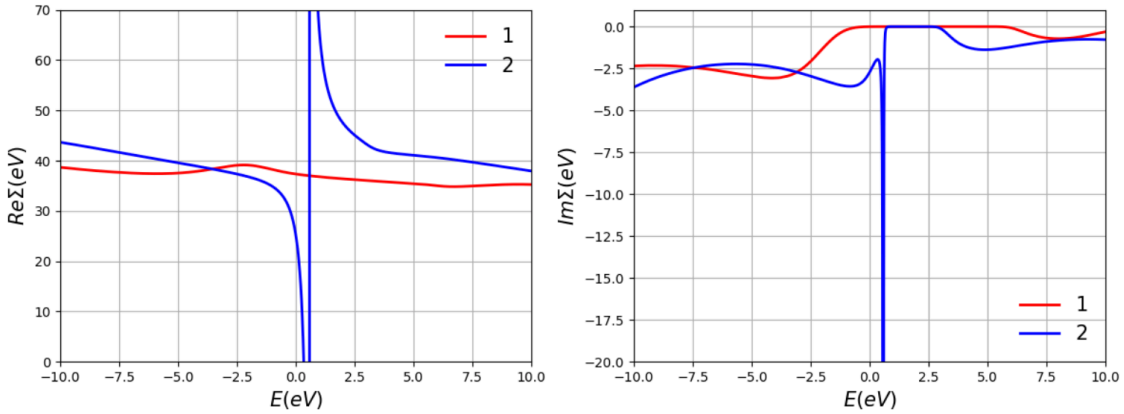
```
usage: maxent_wrapper.py [-h] sig [error]

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 cutfoff
        '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 using the maximum entropy method. Electronic self-energy of Ni-$e_g$ has a pole near the Fermi level indicative of the paramagnetic Mott gap in NiO.

## LQSGW+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 "lqsgw_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

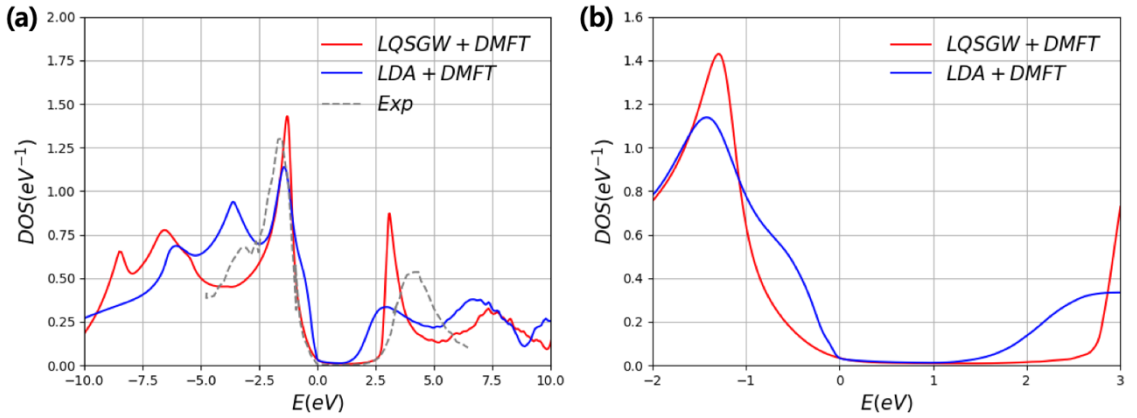
```
#!/bin/bash -l
#SBATCH -J temp
#SBATCH -q debug
#SBATCH -N 1
#SBATCH -e temp.%j.err
#SBATCH -o temp.%j.out
#SBATCH -L SCRATCH
#SBATCH -C haswell
#SBATCH -t 00:30:00
srun -n 30 $COMSUITE_BIN/ComLowH
```

Doing so, you will obtain tdos.dat and pdos.dat.

The format of tdos.dat file is:

```
#       omega (eV)          DOS (1/eV)
    -70.000000000000      0.000091808791
    -65.733023713200      0.000108452955
    -61.955278682000      0.000138301530
    -58.587128546700      0.000227798485
    -55.565331497900      0.000516350837
    -52.839027896300      0.001299313019
    -50.366851286200      0.003019398128
    -48.114812211200      0.006138514245
    -46.054723948000      0.010868081246
    -44.163014879300      0.016848714930
```

Plot of tdos.dat:



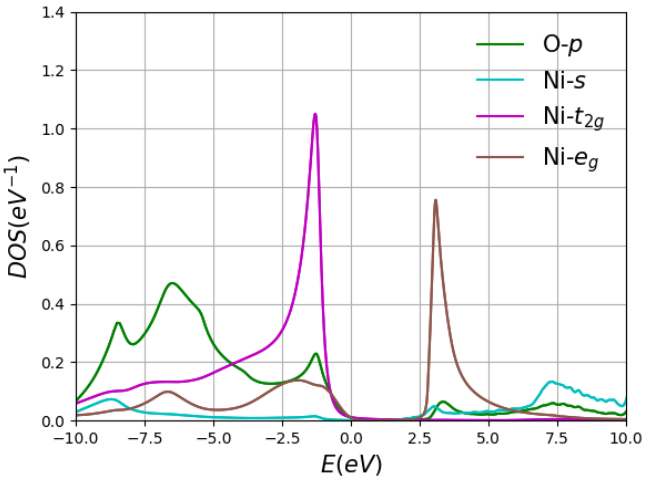

(a)NiO density of states and (b) its zoom-in view. Red and blue lines show the total density of states within *ab initio* LQSGW+DMFT and charge self-consistent LDA+DMFT. Gray dashed lines are from photoemission spectroscopy and Bremsstrahlung Isochromat spectroscopy[1].

The format of pdos.dat file is :

```
#     omega (eV)          (1,1,-1)            (1,1,0)             (1,1,1)             (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)
   -70.000000000000       0.000007506048      0.000007506046      0.000007506050      0.000006114846      0.000005018605      0.000005018609      0.000005018602      0.000010927273
0.000010927264      0.000007669090      0.000010927268      0.000007669090
   -65.733023713200       0.000008615621      0.000008615619      0.000008615624      0.000006929192      0.000005621753      0.000005621757      0.000005621748      0.000013659821
0.000013659808      0.000008916099      0.000013659814      0.000008916099
   -61.955278682000       0.000009821212      0.000009821208      0.000009821216      0.000007800185      0.000006257663      0.000006257668      0.000006257657      0.000020560307
0.000020560286      0.000010291916      0.000020560296      0.000010291916
   -58.587128546700       0.000011134876      0.000011134871      0.000011134881      0.000008742243      0.000006941787      0.000006941794      0.000006941780      0.000046979894
0.000046979842      0.000011943325      0.000046979866      0.000011943325
   -55.565331497900       0.000012589013      0.000012589006      0.000012589020      0.000009803351      0.000007727704      0.000007727715      0.000007727692      0.000139012572
0.000139012401      0.000014279941      0.000139012481      0.000014279941
```

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

Plot of pdos.dat:




The projected density of states of O-p, Ni-s, Ni-$t_{2g}$, and Ni-$e_g$ orbitals within LQSGW+DMFT, marked by green, cyan, purple, and brown colors, respectively.

## LGSGW+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 and move to the directory. For instance:

```
$ 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
```

[1] G. A. Sawatzky, J. W. Allen, Phys. Rev. Lett. **53**, 2339 (1984)

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.

```
186 # The number of k points
  0.00000000   0.00000000   0.00000000
  0.01666667   0.00000000   0.01666667
  0.03333333   0.00000000   0.03333333
  0.05000000   0.00000000   0.05000000
  0.06666667   0.00000000   0.06666667
  0.08333333   0.00000000   0.08333333
  0.10000000   0.00000000   0.10000000
  0.11666667   0.00000000   0.11666667
  0.13333333   0.00000000   0.13333333
```

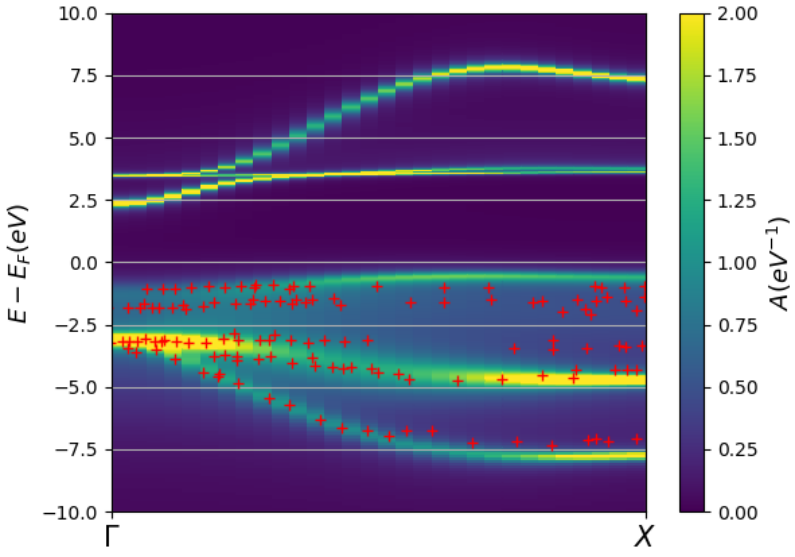
Run ComLowH with job submission script. An example of job script using SLURM is

```
#!/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 spectral.dat file. The format of spectral.dat file is

```
#  kpoint        E (eV)              A (1/eV)
       1    -70.000000000000        0.000089559143
       2    -70.000000000000        0.000089568795
       3    -70.000000000000        0.000089597475
       4    -70.000000000000        0.000089644404
       5    -70.000000000000        0.000089708419
       6    -70.000000000000        0.000089788138
       7    -70.000000000000        0.000089882106
       8    -70.000000000000        0.000089988881
       9    -70.000000000000        0.000090107016
      10    -70.000000000000        0.000090234933
```

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




Spectral function along Γ − X in the first Brillouin zone within *ab initio* LQSGW+DMFT. Red plus symbols in figure are from angle-resolved photoemission spectroscopy data[2].

[2] Z.-X. Shen, R. S. List, D. S. Dessau, B. O. Wells, O. Jepsen, A. J. Arko, R. Barttlet, C. K. Shih, F. Parmigiani, J. C. Huang, P. A. P. Lindberg, Phys. Rev. B **44**, 3604 (1991)