Hands-on Training

In this tutorial, commands you should run in terminal are marked by red colors

Special thanks to Vincent Sacksteder
for installing and testing Comsuite
in the virtual machine

Special thanks to
Moïse Rousseau and Michel Barrette
for installing the virtual machine
in the cluster

https://github.com/comscope/comsuite

1. COMSUITE

A computational materials physics code for simulating correlated quantum materials using Dynamic Mean Field Theory (DMFT) and its extension. It can calculate the electronic structure within three different mathods:

- charge self-consistent LDA+Gutzwiller,
- charge self-consistent LDA+DMFT,
- and ab initio LQSGW+DMFT

For the copyright and license information, please see Copyright.txt and license.txt.

2. New version release announcement

2021. 2. 26

- Updated interface to Flapwmbpt. Now Comsuite requires single input file for FlapwMBPT, Comsuite, and its postprocess.
- Now Comsuite provides an option to calculate quasiparticle bandstructures within LDA+DMFT as well as LQSGW+DMFT.
- Now Comsuite provides options to choose "s"- or "p"-type corrlated orbitals.

2020. 1. 6

- Now Comsuite can calculate antiferromagnetically ordered phase. Please go to tutorial directories (install_directory/tutorials/lda_dmft/NiO_afm and install_directory/tutorials/lqsgw_dmft/NiO_afm). Read pdf f to learn how to calculate the electronic structures of antiferromagnetically ordered NiO. You have two choice of charge self-consistent LDA+DMFT and LQSGW+DMFT.

master comsuite / tutorials /

sangkookchoi version 1.2

..

dft	version 1.2
lda_dmft	version 1.2
lda_risb/MnO	first commit
lqsgw	version 1.2
lqsgw_dmft	version 1.2

Compile COMSUITE package.

- First, define the installation directory in the shell. For example in bash shell, use the following command adds $COMSUITE_BIN to your system $PATH

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

- Then, the compilers, libraries, and flags should be defined in the arch.mk file. An example to install COMSUITE in Cori at NERSC is as follows.

```
##### fortran
F90 = ifort
PF90 = ftn
compfl = -O3

##### f2py
fortran2python = f2py -c --fcompiler=intelem --compiler=intelem

### phdf5
USE_HDF5 = defined  ### comment out this line if you don't want to compile with hdf5 (for LDA+DM
```

[1] S. Choi, P. Semon, B. Kang, A. Kutepov, and G. Kotliar,, Computer Physics Communications 244, 277 (2019).

Rationale of ComDMFT development (as a part of Comsuite)

- **Open source package** under GPL
  (the CPC paper on ComDMFT under review and in arxiv)

- **Multiple methodologies**
  - ab initio LQSGW+DMFT (a simplified version of GW+EDMFT)
  - charge self-consistent LDA+DMFT
  - charge self-consistent LDA+RISB (AKA ComRISB in collaboration with Yongxin)

- **The first open-source package supporting ab initio GW+DMFT**,
  - ab initio LQSGW+DMFT: **a parameter free method**

- **The first open-source package supporting multiple methodology based on first principles+DMFT**

- **GPU-ported impurity solver** by Kwangmin, Patrick and Corey,
  - Asynchronous CPU-GPU algorithm
  - 5X speed-up @TITAN, OLCF, **12.5X speed-up @SUMMIT, OLCF**

[1]S. Choi, P. Semon, B. Kang, A. Kutepov, and G. Kotliar, ArXiv181001679 Cond-Mat (2018).

ComDMFT (as a part of Comsuite)

- Physical observables
  - single particle Green's function
  - local quantities to correlated orbitals
    Impurity self-energy
    Hybridization function
    Double-counting self-energy (for LQSGW+DMFT)
    Bosonic Weiss field within cRPA (for LQSGW+DMFT)

- Paramagnetic phase and AFM phase

- Quasiparticle band within LDA+DMFT and LQSGW+DFMT

- For the LQSGW/LDA part of the LQSGW+DMFT/LDA+DMFT scheme, the code FlapwMBPT was used.

[1]A. L. Kutepov, V. S. Oudovenko, and G. Kotliar, Computer Physics Communications 219, 407 (2017).
[2]A. Kutepov, S. Y. Savrasov, and G. Kotliar, Phys. Rev. B 80, 041103 (2009).
[3]A. Kutepov, K. Haule, S. Y. Savrasov, and G. Kotliar, Phys. Rev. B 85, 155129 (2012).

Source code directory

Located at
/home/max/codes/Compiled_ComsuiteCode/ComsuiteV2/source_code

`ComCTQMC`	: CTQMC impurity solver
`ComCoulomb`	: program to calculate bosonic Weiss field within cRPA
`ComDC`	: program for double counting self-energy
`ComLowH`	: program to calculate fermionic Weiss field, DOS, spectral functions
`ComRISB`	: program for Gutzwiller calculation
`ComWann`	: program to construct Wannier functions
`Copyright.txt`	
`GNUmakefile`	
`README.md`	
`arch.mk`	
`bin`	
`gw`	: FlapwMBPT code by Andrey Kutepov
`license.txt`	
`tutorials`	: tutorials (NiO and FeSe)
`wannier90_2.1`	: Wannier90 package

Environmental variable check

- Check if COMSUITE_BIN has been defined

    echo $COMSUITE_BIN

-If you get "/home/max/codes/Compiled_ComsuiteCode/ComsuiteV2/source_code/bin", you are good. Otherwise,

1) Add the following line in the ~/.bashrc

    export COMSUITE_BIN=/home/max/codes/Compiled_ComsuiteCode/ComsuiteV2/source_code/bin

2) Execute the bash setup file

    source ~/.bashrc

3) Check if COMSUITE_BIN has been defined in your shell, again.

    echo $COMSUITE_BIN

Copy directories and input files

- Copy the directory with input files
  cp –r ~/codes/Compiled_ComsuiteCode/ComsuiteV2/tutorials_input ~/

- Move into the directory
  cd ~/tutorials_input

LDA+DMFT tutorial on Na

Warning: parameters in input files are set to run on two cpu cores in an hour.
This means that the results are not fully converged w.r.t. the number of k points,
CTQMC measurements, and LDA+DMFT iteration.

Converged calculation results are located at
“/home/max/codes/Compiled_ComsuiteCode/ComsuiteV2/tutorials_converged”

Simple metal including Na is not the best materials for local self-energy assumption

Goal

1. LDA+DMFT self-consistent calculation
2. Quasiparticle bandstructure calculation

DFT-LDA prerun

- Go to the DFT directory
  cd dft

- Check input files
  ls –al

`Na.cif`	: Crystallographic information file
`comdmft.ini`	: DFT calculation input file

- Run Comsuite
  $COMSUITE_BIN/comdmft.py

comdmft.ini

```
control ={
        'method':'dft',
        'mpi_prefix':'mpirun -np 2',
        'nproc_k_flapwmbpt':2,
        'nproc_tau_flapwmbpt':1,
        }

flapwmbpt={
        'cif':'./Na.cif',
        'iter_dft':50,
        'dft_mix':0.1,
        'rel':1,
        'magn':False,
        'kmesh':[5, 5, 5]
                }
```

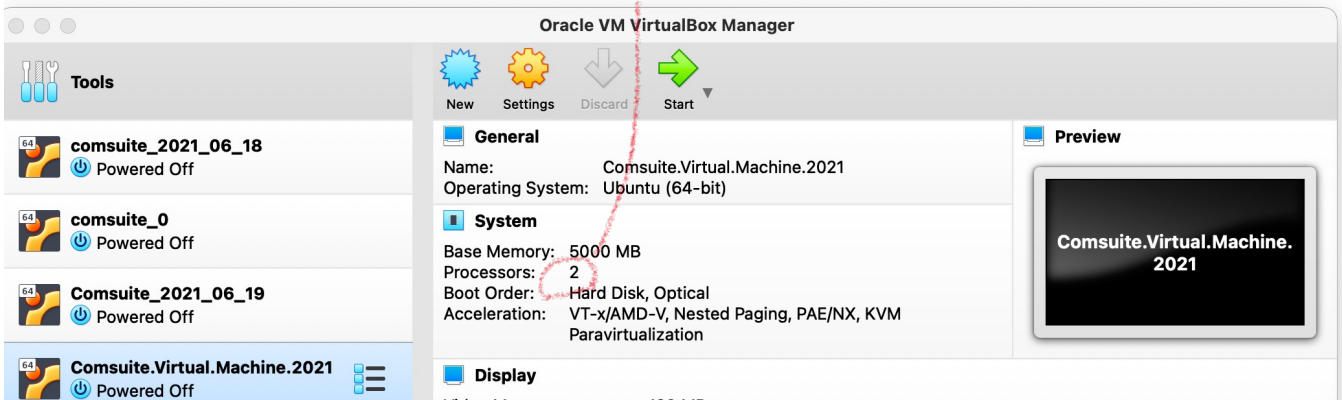
control in comdmft.ini

- method: ‘dft’
  ab initio methodology. Choose among “dft”, “lqsgw”, “lda+dmft”, or “lqsgw+dmft”.

- mpi_prefix: ‘mpirun –np 2’
  MPI prefix used for FlapwMBPT dft run.

- nproc_k_flapwmbpt: ‘2’
  The number of MPI processes for k parallelization

- restart:’false’
  option to resume dft calculation from a checkpoint. Default: False



flapwmbpt in comdmft.ini

- cif: ‘./Na.cif’

  the path to the cif file which contains crystal structure information

- iter_dft: ’50’

  the number of dft iteration

- dft_mix: ‘0.1’

  linear density mixing coefficient.

- rel: 1

  relativisity option (0: nonrelativistic, 1: scalar relativistic, 2: fully relativistic)

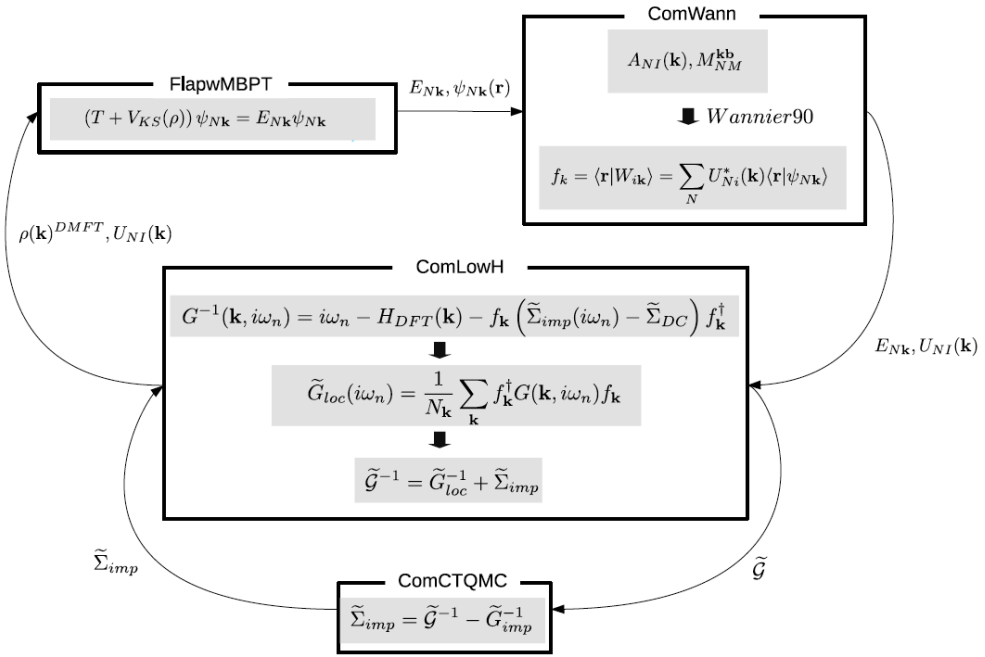
- magn: ‘false’

  spin polarization. ‘true’ or ‘false’

- kmesh: [5, 5, 5]

  k point grid

LDA+DMFT calculation



U and $\widetilde{\Sigma}_{DC}$ as external parameters

LDA+DMFT calculation

- Go to the LDA+DMFT directory
  cd ../lda_dmft

- Check input files
  ls –al

`analysis`	: directory containing python script for the data plots
`band`	: directory for the band plot postprocessing step
`comdmft.ini`	LDA+DMFT input file

- Run Comsuite
  $COMSUITE_BIN/comdmft.py

comdmft.ini for LDA+DMFT calculation

```
control={'initial_lattice_dir'          : '../dft',
         'method'                 : 'lda+dmft',
         'spin_orbit'             : False,
         'mpi_prefix': "mpirun -np 2",
         'impurity_problem':[[1, 's']],
         'impurity_problem_equivalence':[1],
         'restart': False,
         'max_iter_num_outer': 1
         }

wan_hmat={
        'kgrid': [5, 5, 5],
        'froz_win_min': -15.0,
        'froz_win_max': 10.0,
                    }

imp={'temperature'            : 900, # temperature (in K)
     '1':
     {
      'f0': 5.0,
      'nominal_n': 1.0,
     'impurity_matrix': [ # equivalent orbital index matrix. starting from 1.
         [1]
         ],
     'thermalization_time': 1,
     'measurement_time': 2,
     'green_cutoff':  10,
     'coulomb': 'full',
     }
     }
```

In control

- 'methods': 'lda+dmft'
- 'initial_lattice_dir': '../dft'
  - the path to DFT prerun directory
- 'impurity_problem': [[1,'s']]
  - a python list to specify correlated orbitals. The first and second indices are for the atom index and shell type.
  - atom index: in the order listed in the "../dft/crystal_structure.xsf"
  - shell index: "s", "p", "d" or "f"
- 'impurity_problem_equivalence': [1]
  - equivalence of each impurity problem.
  - identified by an integer starting from 1. If this value is the same, they are equivalent.
  - If this value is negative, it is the time-reversal symmetry pair to the one with the same absolute value.
- 'max_iter_num_outer': 1
  - maximum iteration for the charge self-consistent loop.
  - default value: 50
- 'spin_orbit': True or False
  - if False, correlated orbitals correspond to cubic spherical harmonics

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

where Y_l^m is a spherical harmonics.

In control

- if True, correlated orbitals chosen at each correlated atom correspond spin-angular functions |l,i,m>

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

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

- 'mpi_prefix': : 'mpirun -np 2'
  - MPI prefix commonly used for ComLowH, ComWann, and ComCTQMC.
  - If a different MPI prefixs from this prefix is necessary for a program, use 'mpi_prefix_lowh', 'mpi_prefix_wannier', and 'mpi_prefix_impurity',
- 'restart': : False
  - True or False. If True, It will resume the calculation from the prerun.
  - default value: False
- 'mpi_prefix_lowh':
  - MPI prefix for ComLowH
  - default value: control['mpi_prefix']
- 'mpi_prefix_impurity':
  - MPI prefix for the impurity solver
  - default value: control['mpi_prefix']
- 'mpi_prefix_wannier'
  - MPI prefix for ComWann
  - default value: control['mpi_prefix']

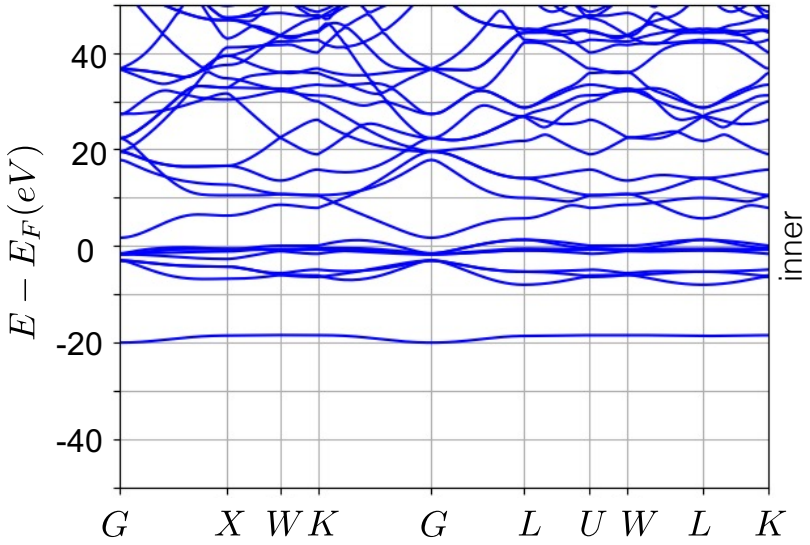
In control

- 'sigma_mix_ratio'
  - impurity self-energy linear mixing ratio.
  - default value: 0.5
- 'proj_win_min':
  - low-energy cutoff to renormalize the projectors
  - default value: wan_hmat['dis_win_min']
- 'proj_win_max':
  - high-energy cutoff to renormalize the projectors
  - default value: wan_hmat['dis_win_max']

Important concepts for wan_hmat

- For Wannier function construction
  - Choice of the inner (frozen) energy window: large energy window in the E_F±10eV
  - Choice of the outer (disentanglement) energy window: from E_F-10eV to E_F+50eV

NiO within LDA



outer

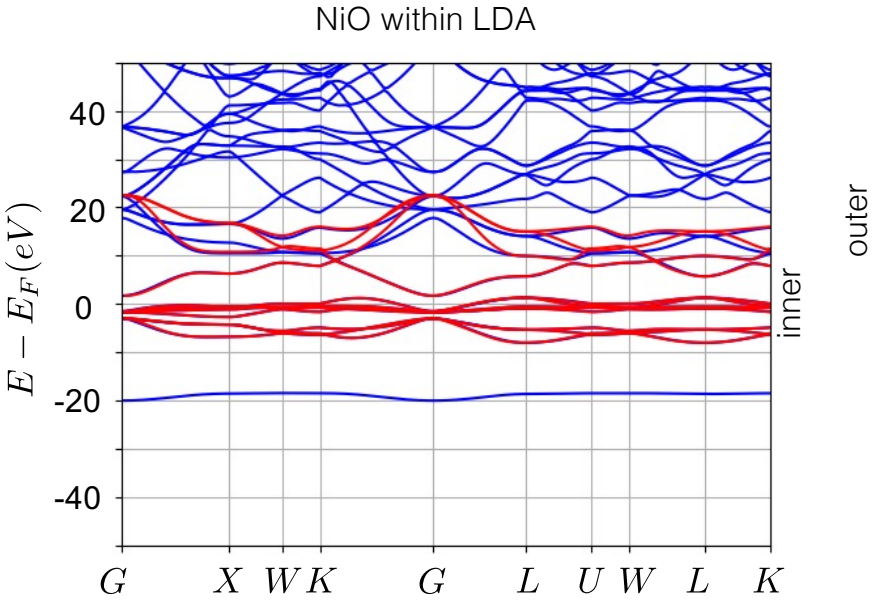
inner

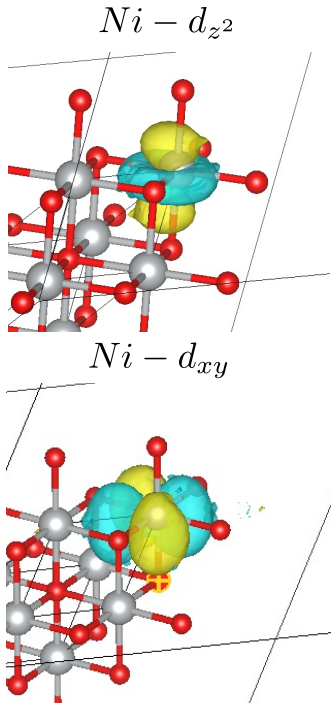
valence
+unoccupied states

Semicore states

Wannier functions and interpolated bandstructure of NiO

- The number of bands in the inner window: 10
- The number of bands in the outer window: 25
- The number of trial orbitals: 12 orbitals (Ni-s, Ni-p, Ni-d, O-p)





In wan_hmat

- 'kgrid': [5,5,5],
  - crystal momentum grid for the wannier interpolation of LDA bandstructure
- 'froz_win_min': -15 eV,
  - lower boundary of the inner (frozen) window in eV
- 'froz_win_max': 10 eV,
  - upper boundary of the inner (frozen) window in eV
- 'dis_win_min':
  - lower boundary of the outer (disentanglement) window in eV.
  - defaule value: froz_win_min
- 'dis_win_max':
  - upper boundary of the outer (disentanglement) window in eV.
  - defaule value: froz_win_max +40.0
- 'num_iter':
  - the number of minization step for the wannierization process. (gauge dependent part of total spreading)
  - default value: 0
- 'dis_num_iter':
  - the number of minization step for the disentanglement process. (gauge independent part of total spreading)
  - defaule value: 100

In imp

- **'temperature': 900**

  - simulation temperature in K

- for each distinct impurity problem indexed by the value in control ["impurity_problem_equivalence"]

  - 'impurity_matrix': [[1]],

    --equivalence of the matrix element of the fermionic Weiss field and impurity self-energy. Starting from "1"

    --if these values are the same, the values of the elements will be assumed to be identical.

    --if the element in the matrix is zero, then it will not be sampled by the impurity solver.

    --each column and row corresponds to the Wannier orbitals in the following order.

    --If control['spin_orbit']==False, "m" is sorted in ascending order.

    To illustrate for "d" orbitals, in this order: $|xy\rangle$,$|yz\rangle$,$|z^2\rangle$,$|xz\rangle$, $|x^2\text{-}y^2\rangle$

    --if control['spin_orbit']==True, the most rapidly changing index is "m" and the next one is "i". They are sorted in ascending order,

    To illustrate for "f" orbitals, in this order: |3,-0.5, -2.5>,|3,-0.5, -1.5>,|3,-0.5, -0.5>,
    |3,-0.5, 0.5>,|3,-0.5, 1.5>,|3,-0.5, 2.5>, |3,0.5, -3.5>,|3,0.5, -2.5>,|3,0.5, -1.5>,
    |3,0.5, -0.5>,|3,0.5, 0.5>,|3,0.5, 1.5>,|3,0.5, 2.5>, |3,0.5, 3.5>,

In imp

- '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.
- ‘f0’: 5
  the monopole term of bosonic Weiss field.
- ‘nominal_n’: 1
  electron occupation in the impurity orbital for the nominal double counting energy $U(N-\frac{1}{2}) - J/2(N-1)$
- 'thermalization_time': 1,
  » wall time for the thermalization in minutes
- 'measurement_time’: 2,
  » wall time for the measurement in minutes
- 'green_cutoff’: 20,
  » cutoff-energy in eV to sample green’s function and self-energy.
  » values beyond this energy will be provided by analytical equations.

Output directory

- in lda_dmft directory

```
analysis
band
cmd.log                 : command log file
comdmft.ini             : input file
convergence.log         : convergence log
dc                      : directory for the double counting calculation
delta.dat               : hybridization function
impurity                : directory for the quantum impurity problem
lattice                 : directory for DFT calculation with updated charge density
lowh                    : directory for fermionic Weiss field calculation
sig.dat                 : impurity self-energy
trans_basis.dat
wannier                 : directory for Wannier function calculation
```

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	ctqmc_sign
wannier	1					2.83903403	3.16936125						
delta	1		1	good				-0.01645111621					
impurity_1	1		1	good					0.32635444719831463	0.7453301851	165.20786445892114	167.94632639486187	1
dft	2	1			0.003981117								
wannier	2					2.83903413	3.16935564						
delta	2		1	good				-0.157048587494					
impurity_1	2		1	good					0.20118722456537202	0.7152362616	159.4363906949742	166.62052643305128	1
dft	3	1			0.002464323								
wannier	3					2.84203035	3.16923542						
delta	3		1	good				-0.252597980239					
impurity_1	3		1	good					0.12672167809183085	0.6945175952	155.78643805195514	169.74120450338341	1
dft	4	1			0.001383939								
wannier	4					2.8452773	3.17114223						
delta	4		1	good				-0.315051432465					

- keeping track of convergence of some quantities at each iteration
- causality: causality of hybridization function / self-energy
- delta_rho: density changes from previous iteration
- w_sp_min: minimum spreading of the Wannier functions
- w_sp_max: maximum spreading 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 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

Impurity self-energy

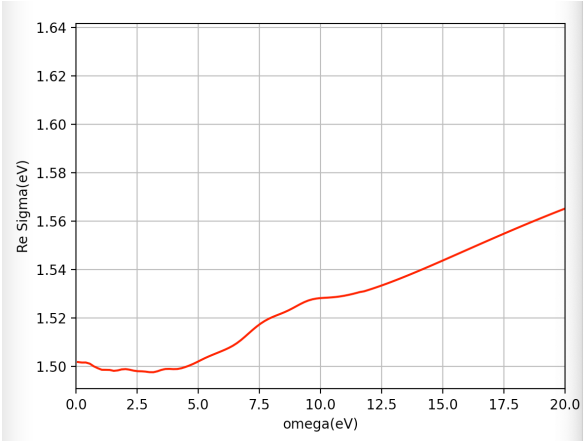
- “sig.dat”
  » Real and imaginary part of impurity self-energy

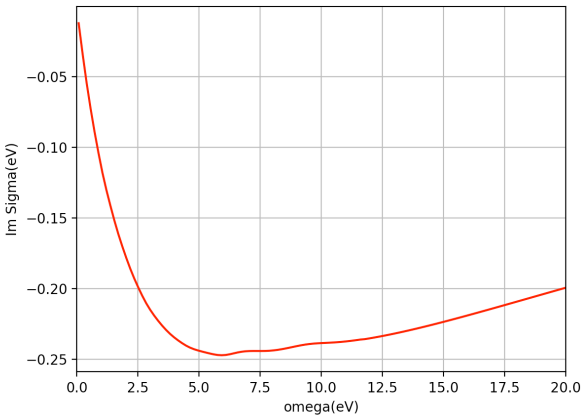
# omega(eV)	Re Sig_{1,1}(eV)	Im Sig_{1,1}(eV)
0.081216424692	1.501800431626	-0.012268251317
0.243649274076	1.501588177463	-0.034063609310
0.406082123461	1.501601337665	-0.054366239901
0.568514972845	1.501110822638	-0.072508424919
0.730947822229	1.500027409077	-0.089041707011
0.893380671613	1.499250948871	-0.104164319516
1.055813520997	1.498605056075	-0.118189374120
1.218246370382	1.498588018057	-0.130392007481
1.380679219766	1.498537768366	-0.141387853780
1.543112069150	1.498168137125	-0.151863364836
1.705544918534	1.498330599474	-0.161486104294

- Let’s plot it
  cd analysis
  python sig.py

Impurity self-energy

For the visualization, I used data at “/home/max/codes/ComsuiteV2/tutorials_converged”





- No divergent self-energy near Fermi-level.
- Up to 2eV, the impurity self-energy shows linear energy dependence.

Hybridization function

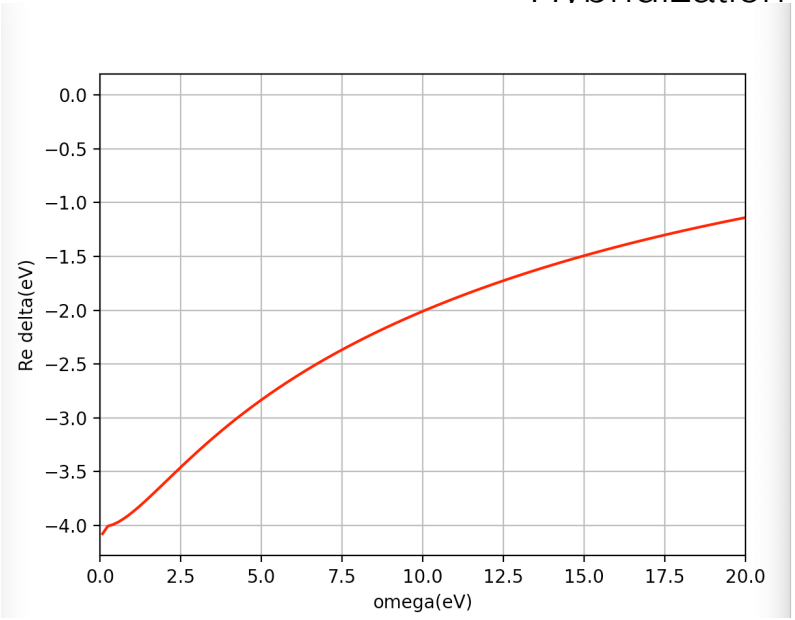
- “delta.dat”
  » Real and imaginary part of hybridization function

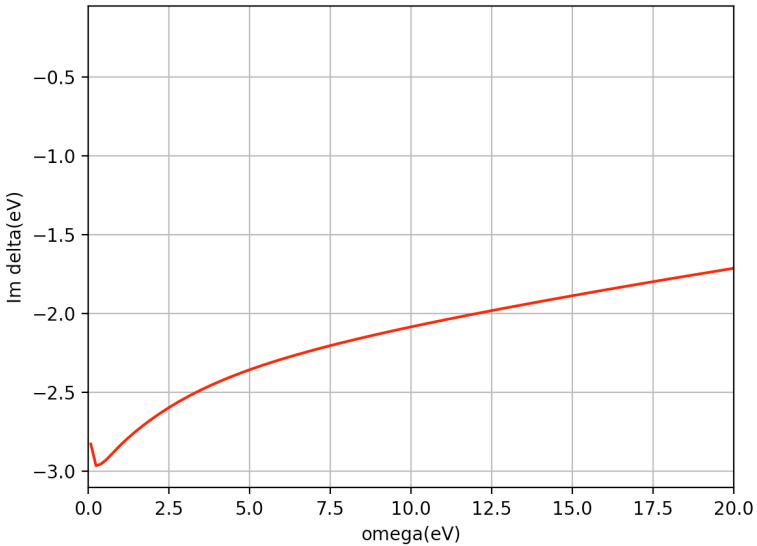
```
0.081216424692     -4.077402095983     -2.828521433978
0.243649274076     -4.006144819843     -2.966827164573
0.406082123461     -3.991149773784     -2.953881842766
0.568514972845     -3.968126243833     -2.926582297915
0.730947822229     -3.938154963765     -2.892171692592
0.893380671613     -3.903350147782     -2.857399777300
1.055813520997     -3.864792500134     -2.824214718055
1.218246370382     -3.823426294363     -2.793440776542
1.380679219766     -3.779812922422     -2.764457834912
1.543112069150     -3.734606699404     -2.736752971151
1.705544918534     -3.688584198508     -2.710484210705
1.867977767919     -3.642016615893     -2.685508905212
2.030410617303     -3.595109067127     -2.661525905159
```

- Let’s plot it

  python delta.py

Hvbridization function





- It shows metallic behavior (imaginary part of delta is nonzero at zero frequency)

LDA+DMFT quasiparticle bandstructure

- Go to the band directory
  cd ../band

- Check input files
  ls –al

`comdmft.ini`	Bandstructure calculation input file

- Run Comsuite
  $COMSUITE_BIN/comdmft.py

comdmft.ini

```
control ={
        'method':'band',
        'mpi_prefix':'mpirun -np 2',
        }

postprocessing={
        'comsuite_dir':'../',
        }
```

- in control
  - ‘method’: ‘band’
    postprocessing calculation. Choose among “band”, “dos”, and “spectral”

  - ‘mpi_prefix’: ‘mpirun –np 2’
    MPI prefix used for bandstructure calculation.

- in postprocessing
  - ‘comsuite_dir’: ‘../’
    The directory where comsuite calculation has been done.
  - ‘kpoints’:
    k point path along which spectral functions are calculated. If not provided, comsuite follow the path defined in Ref[1]

[1] W. Setyawan and S. Curtarolo, Computational Materials Science 49, 299 (2010).

comdmft.ini

“kpoints” format

- w.r.t. reciprocal lattice vectors

```
frac
  650
    1    0.00000000   0.00000000   0.00000000   G
    2    0.00423729  -0.00423729   0.00423729
    3    0.00847458  -0.00847458   0.00847458
    4    0.01271186  -0.01271186   0.01271186
    5    0.01694915  -0.01694915   0.01694915
    6    0.02118644  -0.02118644   0.02118644
    7    0.02542373  -0.02542373   0.02542373
    8    0.02966102  -0.02966102   0.02966102
    9    0.03389831  -0.03389831   0.03389831
```

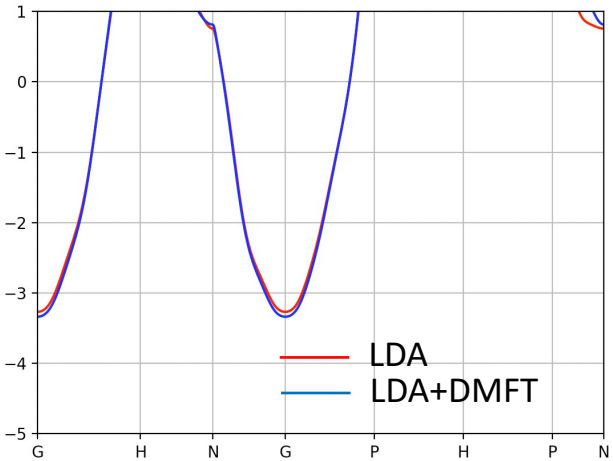
LDA+DMFT bandstructure

Let's plot it

cd ../analysis

python ./band.py

LDA	mBJ	B3LYP	eDMFT	G_0W_0	Expt
3.30	3.29	4.09	2.84	3.15	2.65



[1] S. Mandal, K. Haule, K. M. Rabe, and D. Vanderbilt, ArXiv:2101.03262 [Cond-Mat] (2021).

LQSGW+DMFT tutorial on Na

Warning: parameters in input files are set to run on two cpu cores in an hour.
This means that the results are not fully converged w.r.t. the number of k points,
CTQMC measurements, and DMFT iteration.

Converged calculation results are located at
“/home/max/codes/Compiled_ComsuiteCode/ComsuiteV2/tutorials_converged”

Simple metal including Na is not the best materials for local self-energy assumption

Goal

1. LQSGW+DMFT self-consistent calculation
2. Spectral function calculation

LQSGW prerun

Go to the DFT directory

cd ~/tutorials_input/lqsgw

Check input files

ls –al

`Na.cif`	: Crystallographic information file
`comdmft.ini`	: DFT calculation input file

- Run Comsuite

$COMSUITE_BIN/comdmft.py

comdmft.ini

```
control ={
        'method':'lqsgw',
        'mpi_prefix':'mpirun -np 2',
        'nproc_k_flapwmbpt':1,
        'nproc_tau_flapwmbpt':2,
        }

flapwmbpt={
        'cif':'./Na.cif',
        'iter_dft':50,
        'iter_lqsgw':1,
        'dft_mix':0.1,
        'rel':1,
        'magn':False,
        'kmesh':[5, 5, 5]
                }
```

control in comdmft.ini

- method: ‘lqsgw’
  ab initio methodology. Choose among “dft”, “lqsgw”, “lda+dmft”, or “lqsgw+dmft”.

- mpi_prefix: ‘mpirun –np 2’
  MPI prefix used for FlapwMBPT lqsgw run.

- nproc_k_flapwmbpt: ‘1’
  The number of MPI processes for k parallization

- nproc_tau_flapwmbpt: ‘2’
  The number of MPI processes for τ parallization

- restart:’false’
  option to resume lqsgw calculation from a checkpoint. Default: False

flapwmbpt in comdmft.ini

- cif: ‘./Na.cif’
  the path to the cif file which contains crystal structure information

- iter_dft: ’50’
  the number of dft iteration

- iter_lqsgw: ’1’
  the number of lqsgw iteration

- dft_mix: ‘0.1’
  linear density mixing coefficient.

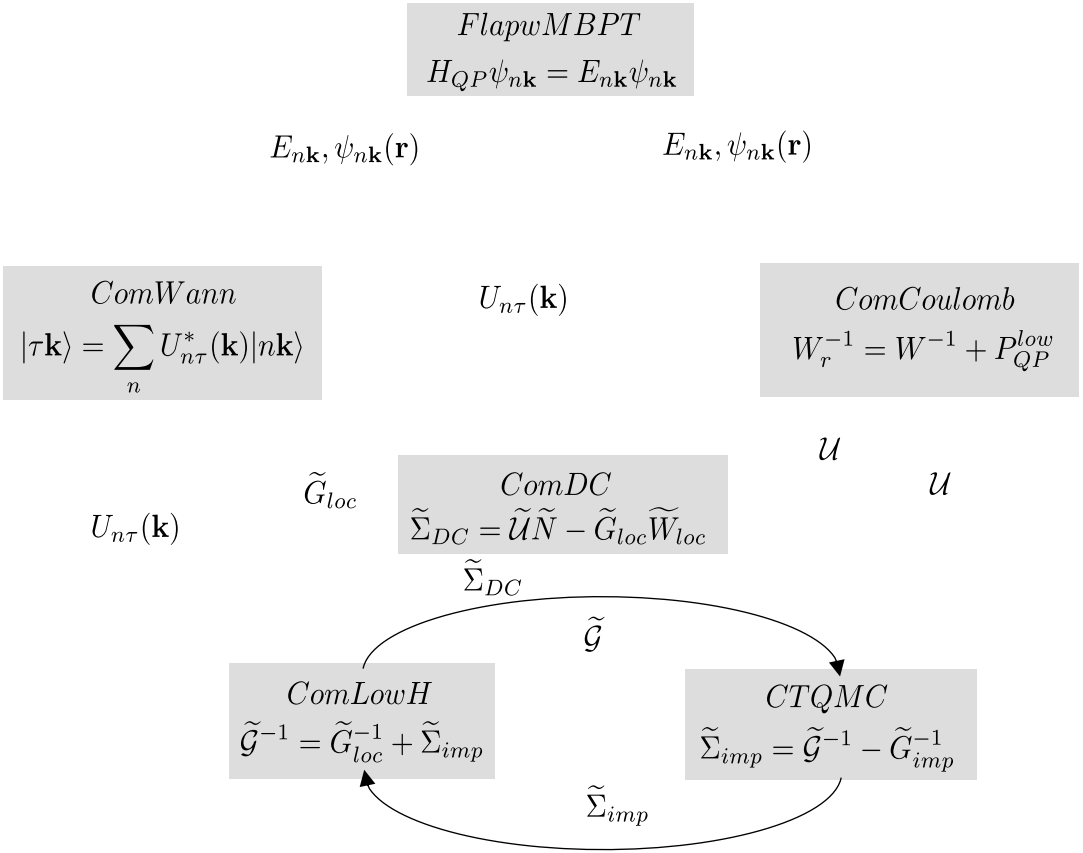
- rel: 1
  relativisity option (0: nonrelativistic, 1: scalar relativistic, 2: fully relativistic)

- magn: ‘false’
  spin polarization. ‘true’ or ‘false’

- kmesh: [5, 5, 5]
  k point grid

- gw_mix: ‘0.1’
  linear self-energy mixing coefficient

LQSGW+DMFT calculation



LQSGW+DMFT calculation

- Go to the LQSGW+DMFT directory
  cd ../lqsgw_dmft

- Check input files
  ls –al

analysis	: directory containing python script for the data plots
comdmft.ini	LQSGW+DMFT input file
realaxis	: directory for the spectral function plot postprocessing step

- Run Comsuite
  $COMSUITE_BIN/comdmft.py

comdmft.ini for LQSGW+DMFT calculation

```
control={'initial_lattice_dir'          : '../lqsgw',
         'method'                 : 'lqsgw+dmft',
         'spin_orbit'             : False,
         'mpi_prefix': "mpirun -np 2",
         'impurity_problem':[[1, 's']],
         'impurity_problem_equivalence':[1],
         'restart': False,
         'max_iter_num_impurity': 1
         }

wan_hmat={
        'kgrid': [5, 5, 5],
        'froz_win_min': -15.0,
        'froz_win_max': 10.0,
                      }

imp={'temperature'            : 900, # temperature (in K)
     '1':
     {
     'impurity_matrix': [ # equivalent orbital index matrix. starting from 1.
         [1]
         ],
     'thermalization_time': 1,
     'measurement_time': 2,
     'green_cutoff':  20,
     'coulomb': 'full',
     }
     }
```

In control

- 'methods': ‘lqsgw+dmft'
- 'initial_lattice_dir’: ‘../lqsgw’
  - the path to LQSGW output directory
- 'impurity_problem': [[1,’s’]]
  - a python list to specify correlated orbitals. The first and second indices are for the atom index and shell type.
  - atom index: in the order listed in the “../dft/crystal_structure.xsf”
  - shell index: “s”, “p”, “d” or “f”
- 'impurity_problem_equivalence': [1]
  - equivalence of each impurity problem.
  - identified by an integer starting from 1. If this value is the same, they are equivalent.
  - If this value is negative, it is the time-reversal symmetry pair to the one with the same absolute value.
- ‘max_iter_num_impurity’: 1
  - total number of DMFT self-consistent loop
- 'spin_orbit': True or False
  - if False, correlated orbitals correspond to cubic spherical harmonics

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

where Y_l^m is a spherical harmonics.

In control

- if True, correlated orbitals chosen at each correlated atom correspond spin-angular functions |l,i,m>

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

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

- 'mpi_prefix': : 'mpirun -np 2'
  - MPI prefix commonly used for ComLowH, ComWann, and ComCTQMC.
  - If a different MPI prefixs from this prefix is necessary for a program, use 'mpi_prefix_lowh', 'mpi_prefix_wannier', and 'mpi_prefix_impurity',
- 'restart': : False
  - True or False. If True, It will resume the calculation from the prerun.
  - default value: False
- 'mpi_prefix_lowh':
  - MPI prefix for ComLowH
  - default value: control['mpi_prefix']
- 'mpi_prefix_impurity':
  - MPI prefix for the impurity solver
  - default value: control['mpi_prefix']
- 'mpi_prefix_wannier'
  - MPI prefix for ComWann
  - default value: control['mpi_prefix']

In control

- 'sigma_mix_ratio'
  - impurity self-energy linear mixing ratio.
  - default value: 0.5
- 'max_iter_num_outer':
  - maximum iteration for the charge self-consistent loop.
  - default value: 50
- 'proj_win_min':
  - low-energy cutoff to renormalize the projectors
  - default value: wan_hmat[‘dis_win_min’]
- 'proj_win_max':
  - high-energy cutoff to renormalize the projectors
  - default value: wan_hmat[‘dis_win_max’]

In wan_hmat

- 'kgrid': [5,5,5],
  - crystal momentum grid for the wannier interpolation of LDA bandstructure
- 'froz_win_min': -15 eV,
  - lower boundary of the inner (frozen) window in eV
- 'froz_win_max': 10 eV,
  - upper boundary of the inner (frozen) window in eV
- 'dis_win_min':
  - lower boundary of the outer (disentanglement) window in eV.
  - defaule value: froz_win_min
- 'dis_win_max':
  - upper boundary of the outer (disentanglement) window in eV.
  - defaule value: froz_win_max +40.0
- 'num_iter':
  - the number of minization step for the wannierization process. (gauge dependent part of total spreading)
  - default value: 0
- 'dis_num_iter':
  - the number of minization step for the disentanglement process. (gauge independent part of total spreading)
  - defaule value: 100

In imp

- **'temperature': 900**

  - simulation temperature in K

- for each distinct impurity problem indexed by the value in control["impurity_problem_equivalence"]

  - 'impurity_matrix': [[1]],

    --equivalence of the matrix element of the fermionic Weiss field and impurity self-energy. Starting from "1"

    --if these values are the same, the values of the elements will be assumed to be identical.

    --if the element in the matrix is zero, then it will not be sampled by the impurity solver.

    --each column and row corresponds to the Wannier orbitals in the following order.

    --If control['spin_orbit']==False, "m" is sorted in ascending order.

    To illustrate for "d" orbitals, in this order: $|xy\rangle$,$|yz\rangle$,$|z^2\rangle$,$|xz\rangle$, $|x^2\text{-}y^2\rangle$

    --if control['spin_orbit']==True, the most rapidly changing index is "m" and the next one is "i". They are sorted in ascending order,

    To illustrate for "f" orbitals, in this order: |3,-0.5, -2.5>,|3,-0.5, -1.5>,|3,-0.5, -0.5>,
    |3,-0.5, 0.5>,|3,-0.5, 1.5>,|3,-0.5, 2.5>, |3,0.5, -3.5>,|3,0.5, -2.5>,|3,0.5, -1.5>,
    |3,0.5, -0.5>,|3,0.5, 0.5>,|3,0.5, 1.5>,|3,0.5, 2.5>, |3,0.5, 3.5>,

In imp

- '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.
- 'thermalization_time': 1,
  » wall time for the thermalization in minutes
- 'measurement_time’: 2,
  » wall time for the measurement in minutes
- 'green_cutoff’: 20,
  » cutoff-energy in eV to sample green’s function and self-energy.
  » values beyond this energy will be provided by analytical equations.
- 'susceptibility_cutoff':
  » cutoff-energy to sample susceptibility.
  » Default value: 300 eV

Output directory

- in lqsgw_dmft directory

```
analysis
band
cmd.log                 : command log file
comdmft.ini             : input file
convergence.log         : convergence log
coulomb                 : directory for the bosonic Weiss field within cRPA
dc                      : directory for the double counting calculation
delta.dat               : hybridization function
impurity                : directory for the quantum impurity problem
lowh                    : directory for fermionic Weiss field calculation
sig.dat                 : impurity self-energy
sig_dc.dat              : double counting self-energy
sig_dc_hf.dat           : HF contribution in double counting self-energy
trans_basis.dat
u_slater.dat            : bosonic Weiss field within cRPA
v_slater.dat            : local screened Coulomb interaction
w_slater.dat            : local bare Coulomb interaction
wannier                 : directory for Wannier function calculation
```

convergence.log

step	i_imp	causality	static_f0	w_sp_min	w_sp_max	mu	std_sig	n_imp	histo_1	histo_2	ctqmc_sign
wannier				2.47087035	3.9065202						
coulomb_1			2.48540688534606								
dc_1		good									
delta	1	good				0.009788133749					
impurity_1	1	good					0.2237649690574862	0.5721617043	48.63501107725202	63.61860388300722	1
delta	2	good				0.015149694009					
impurity_1	2	good					0.11295662631020237	0.5756367493	48.72429348779647	64.82274549948158	1
delta	3	good				0.020317629267					
impurity_1	3	good					0.05509831723450446	0.5800384964	48.91087647734551	65.05737585460773	1
delta	4	good				0.023045781482					
impurity_1	4	good					0.02796692374404145	0.5759111688	48.480377296698926	66.23955144614358	1
delta	5	good				0.022763114314					

- keeping track of convergence of some quantities at each iteration
- causality: causality of hybridization function / self-energy
- static_f0: static value of bosonic Weiss field
- w_sp_min: minimum spreading of the Wannier functions
- w_sp_max: maximum spreading 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 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

Dynamical U

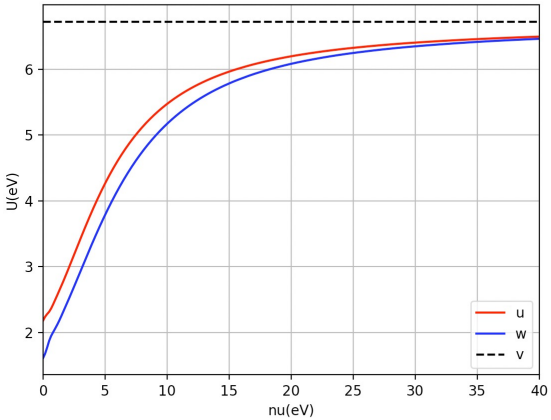
```
      # nu(eV)        1:f0(eV)
0.000000000000  2.178325249978
0.162432849384  2.237485235575
0.324865698768  2.278462848603
0.487298548153  2.312986665643
0.649731397537  2.363690070133
0.812164246921  2.427157767991
0.974597096305  2.494456594169
1.137029945690  2.563385246819
1.299462795074  2.633348723611
1.461895644458  2.703308925822
1.624328493842  2.774400841373
1.786761343226  2.847649955031
1.949194192611  2.922569601886
2.111627041995  2.998565106935
2.274059891379  3.075089392286
```

- Bare Coulomb interaction in v_slater.dat

```
   # 1:f0(eV)
6.725307308007
```

Dynamical U

- Let's plot it
  cd analysis
  python u_omega.py



- At high frequency, U and W_{loc} converge to V_{loc}
- U is larger than W but smaller than V

Impurity self-energy

- “sig.dat”
  » Real and imaginary part of impurity self-energy

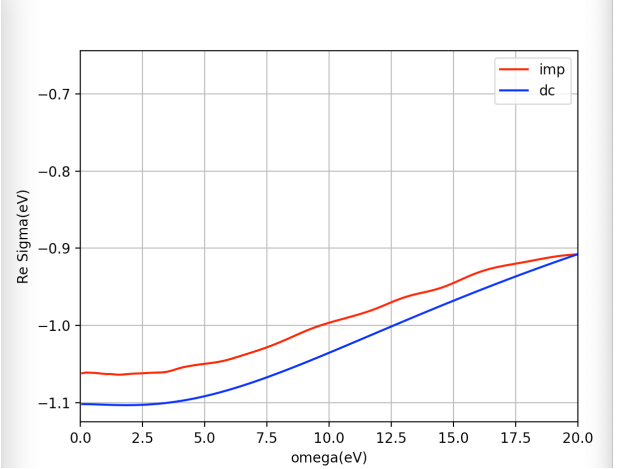
```
   # omega(eV)     Re Sig_{1,1}(eV)     Im Sig_{1,1}(eV)
0.081216424692      1.501800431626      -0.012268251317
0.243649274076      1.501588177463      -0.034063609310
0.406082123461      1.501601337665      -0.054366239901
0.568514972845      1.501110822638      -0.072508424919
0.730947822229      1.500027409077      -0.089041707011
0.893380671613      1.499250948871      -0.104164319516
1.055813520997      1.498605056075      -0.118189374120
1.218246370382      1.498588018057      -0.130392007481
1.380679219766      1.498537768366      -0.141387853780
1.543112069150      1.498168137125      -0.151863364836
1.705544918534      1.498330599474      -0.161486104294
```

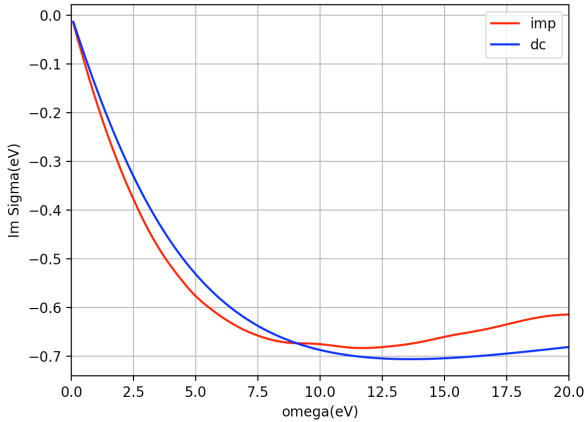
- Let’s plot it

  python sig.py

Local-GW impurity self-energy

For the visualization, I used data at “/home/max/codes/ComsuiteV2/tutorials_converged”





- No divergent self-energy near Fermi-level.
- Up to 5eV, the impurity self-energy shows linear energy dependence.
- smaller z factor within DMFT than GW

Hybridization function

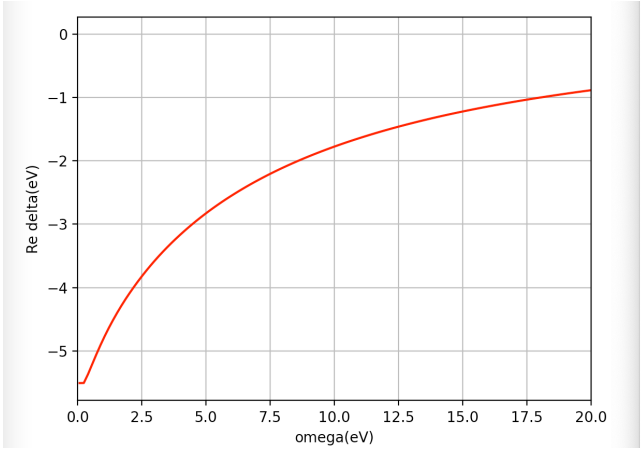
- “delta.dat”
  » Real and imaginary part of hybridization function

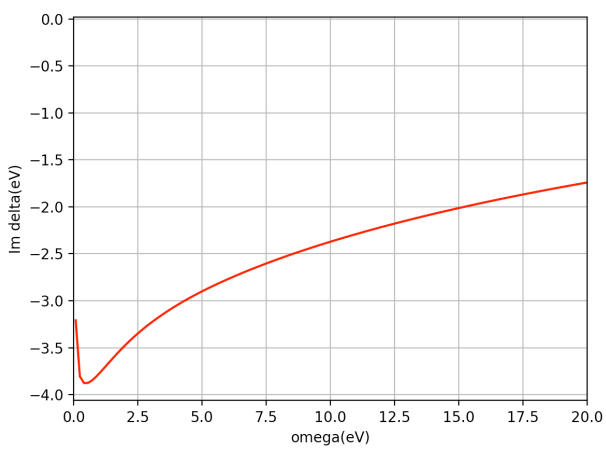
```
0.081216424692     -4.077402095983     -2.828521433978
0.243649274076     -4.006144819843     -2.966827164573
0.406082123461     -3.991149773784     -2.953881842766
0.568514972845     -3.968126243833     -2.926582297915
0.730947822229     -3.938154963765     -2.892171692592
0.893380671613     -3.903350147782     -2.857399777300
1.055813520997     -3.864792500134     -2.824214718055
1.218246370382     -3.823426294363     -2.793440776542
1.380679219766     -3.779812922422     -2.764457834912
1.543112069150     -3.734606699404     -2.736752971151
1.705544918534     -3.688584198508     -2.710484210705
1.867977767919     -3.642016615893     -2.685508905212
2.030410617303     -3.595109067127     -2.661525905159
```

- Let’s plot it

  python delta.py

Hybridization function

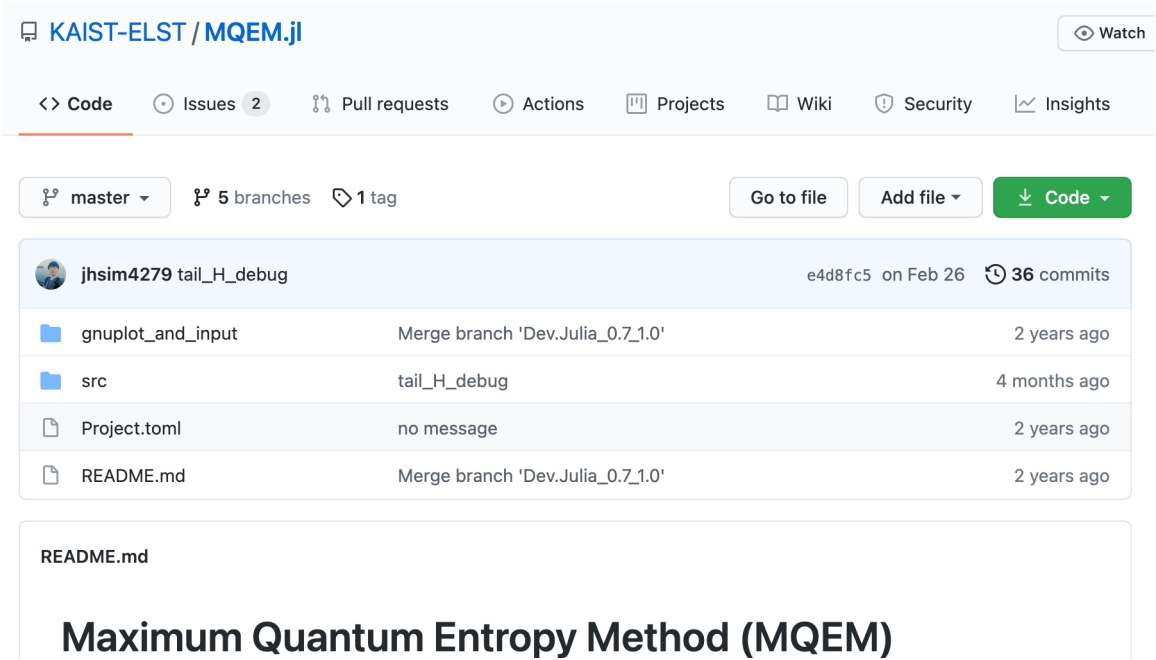




- It shows metallic behavior (imaginary part of delta is nonzero at zero frequency)

Analytical continuation

We will use the maximum entropy (maxent) method for the analytical continuation. For the purposes of this tutorial, we will use MQEM package (https://github.com/KAIST-ELST/MQEM.jl)



Analytical continuation

- To run the maxent code, create the maxent directory and then move to it

  $ cd ../

  $ mkdir maxent

  $ cd maxent

- To run the maxent code (~10 minutes)

  $ COMSUITE_BIN/mqem_wrapper ../sig.dat

  => We will skip this step due to time limit . We will use the self-energy file I provided instead (located at /home/max/codes/ComsuiteV2/Compiled_ComsuiteCode/tutorials_converged/lqsgw_dmft/maxent/sig_realaxis.dat)

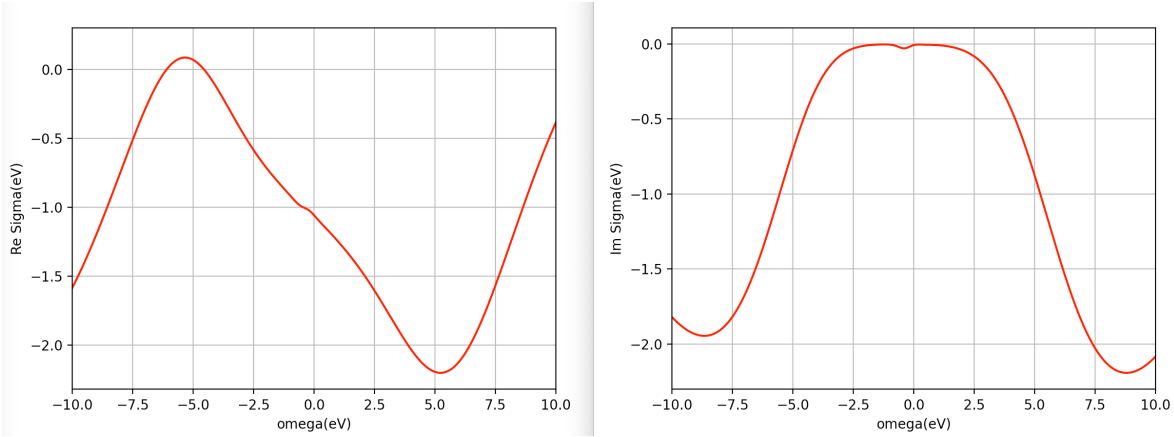
  You may try it as a homework:)

Analytical continuation

Let's plot it

cd ../analysis

python ./sig_realaxis.py



- Linear self-energy within $\mathrm{E_F} \pm 5\mathrm{eV}$
- Small pole near zero energy

LQSGW+DMFT spectral function calculation

- Go to the spectral function directory
  cd ../realaxis

- Check input files
  ls –al

`comdmft.ini`	Bandstructure calculation input file

- Run Comsuite
  $COMSUITE_BIN/comdmft.py

comdmft.ini

```
control ={
        'method':'spectral',
        'mpi_prefix':'mpirun -np 2',
        }

postprocessing={
        'comsuite_dir':'../',
        'self energy':'/home/max/codes/ComsuiteV2/tutorials_converged/lqsgw_dmft/maxent/sig_realaxis.dat',
        'broadening': 0.01,
        'kpoints': './kpoints'
        }
```

- in control
  - method: ‘spectral’
    postprocessing calculation. Choose among “band”, “dos”, and “spectral”

  - mpi_prefix: ‘mpirun –np 2’
    MPI prefix used for bandstructure calculation.

- in postprocessing
  - comsuite_dir: ‘../’
    The directory where comsuite calculation has been done.
  - self-energy: ‘/home/max/codes/ComsuiteV2/tutorials_converged/lqsgw_dmft/maxent/sig_realaxis.dat’
    real-axis self-energy file.
  - broadening: ‘0.01’
    broadening for the mean-field band
  - kpoints: ‘./kpoints’
    k-path file. If not provided, comsuite follow the path defined in Ref[1]

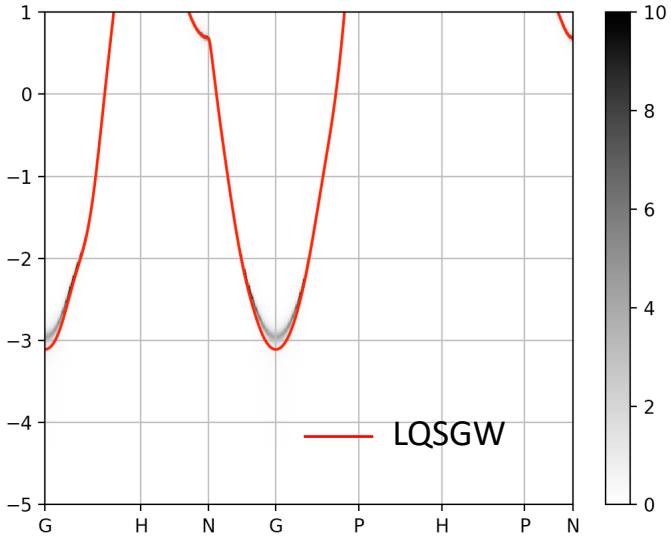
[1] W. Setyawan and S. Curtarolo, Computational Materials Science 49, 299 (2010).

LQSGW+DMFT bandstructure

Let's plot it

cd ../analysis

python band_spectra.py



LDA	mBJ	B3LYP	eDMFT	G_0W_0	Expt
3.30	3.29	4.09	2.84	3.15	2.65

[1] S. Mandal, K. Haule, K. M. Rabe, and D. Vanderbilt, ArXiv:2101.03262 [Cond-Mat] (2021).