

We provide the input data/files, and the commandlines for launching LDA, QSGW and DMFT calculations.

Input data for QSGW

Here we provide the ctrl and basp files required for launching a LDA and QSGW calculations.

The ctrl.sr2ruo4 file contains:

```
# Autogenerated from init.sr2ruo4 using:
# blm --gw --express=1 --nk=12 --nkgw=6 --gmax=11.0 --nit=100 sr2ruo4
% const nit=100
% const met=5
% const so=0 nsp=so?2:1
% const lxcf=2 lxcf1=0 lxcf2=0
% const pwmode=0 pwemax=3
% const sig=12 gwemax=2.46 gcutb=3.1 gcutx=2.5
% const nkabc=12 nkgw=6 gmax=11 beta=.3
```

```
VERS  LM:7 FP:7 # ASA:7
IO     SHOW=f HELP=f IACTIV=f VERBOS=35,35  OUTPUT=*
EXPRESS
  file=  site
  nit=    {nit}
  mix=    B2,b={beta},k=7
  conv=   1e-5
  convc=  3e-5
  nkabc=  {nkabc}
  metal=  {met}
  nspin=  {nsp}
  so=     {so}
  xcfun=  {lxcf},{lxcf1},{lxcf2}

#SYMGRP i r4z mx
HAM    GMAX={gmax}
      AUTOBAS[PNU=1 LOC=1 MTO=4 LMTO=5 GW=1 PFLOAT=2,1]
      PWMODE={pwmode} PWEMIN=0 PWEMAX={pwemax} OVEPS=0
      XCFUN={lxcf},{lxcf1},{lxcf2}
      FORCES={so==0} ELIND=-0.7 NSPIN={nsp} SO={so}
      RDSIG={sig} SIGP[EMAX={gwemax}]
ITER   MIX=B2,b={beta},k=7  NIT={nit}  CONV=1e-5
BZ     METAL={met}  NKABC={nkabc}
GW     NKABC={nkgw} GCUTB={gcutb} GCUTX={gcutx} DELRE=.01 .1
      GSMEAR=0.003 PBTOL=3e-4,3e-4,1e-3
STRUC
      SHEAR=1 0 0 1.0
      NL=5  NBAS=7  NSPEC=3
      ALAT= 7.30111097
      PLAT= -0.5  0.5  1.6455593
              0.5  -0.5  1.6455593
              0.5  0.5  -1.6455593
```

```

SPEC
  ATOM=Sr      Z= 38  R= 2.985910  LMX=3  LMXA=4
  ATOM=Ru      Z= 44  R= 2.068587  LMX=3  LMXA=4  PZ=0,0,5.4
  ATOM=O       Z=  8  R= 1.581969  LMX=3  LMXA=4
SITE
  ATOM=Sr      POS=  0.5000000  0.5000000 -0.4851109
  ATOM=Sr      POS= -0.5000000 -0.5000000  0.4851109
  ATOM=Ru      POS=  0.0000000  0.0000000  0.0000000
  ATOM=O       POS=  0.0000000  0.5000000  0.0000000
  ATOM=O       POS=  0.0000000  0.0000000  0.5348068
  ATOM=O       POS= -0.5000000  0.0000000  0.0000000
  ATOM=O       POS=  0.0000000  0.0000000 -0.5348068

```

The basp.sr2ruo4 file contains:

```

BASIS:
Sr RSMH= 1.991 1.991 1.91 1.991 EH= -0.3 -0.3 -0.3 -0.3 RSMH2= 1.991 1.991 1.91
EH2= -1.1 -1.1 -1.1 P= 5.55 5.35 4.808 4.184 5.102 PZ= 14.9431 14.9266
Ru RSMH= 1.379 1.379 1.053 1.379 EH= -0.3 -0.3 -0.3 -0.3 RSMH2= 1.379 1.379 1.053
EH2= -1.1 -1.1 -1.1 P= 5.5 5.35 4.865 4.187 5.102 PZ= 0 14.9275 5.4
O RSMH= 0.852 0.82 1.055 1.055 EH= -0.464 -0.4 -0.4 -0.4 RSMH2= 0.852 0.82 1.055
EH2= -1.264 -1.2 -1.2 P= 2.878 2.852 3.3 4.148 5.102

```

With these input files it is possible to launch a LDA calculation using the commandline (check the tutorial on the Questaal website for launching the job in parallel mode using mpi),

```
lmf sr2ruo4
```

and a QSGW calculation using the commandline (check the tutorial on the Questaal website for launching the job in parallel mode using mpi):

```
lmgwsc --wt --tol=2e-5 --maxit=20 -vnit=100 sr2ruo4
```

Once a QSGW calculation converges it produces the new charge density (rst.sr2ruo4) and self energy (sigm.sr2ruo4). With these files it is now possible to set up a CT-QMC-DMFT calculation (see our Questaal website for the tutorial). To build the atomic Hamiltonian use the atom_d.py from Kristjan Haule's CT-QMC implementation available on his webpage.

The most important input file is a PARAMS file which contains the input parameters for CTQMC-DMFT calculation.

A PARAMS file contains:

```

OffDiagonal real
Sig Sig.out
Gf Gf.out
Delta Delta.inp
cix actqmc.cix
mode GM
SampleVertex 100 # switch for vertex calculation
nOm 1 # switch for vertex calculation
nomv 60 # switch for vertex calculation

```

```

Nmax 3000          # Maximum perturbation order allowed
nom 120            # Number of Matsubara frequency points sampled
exe ctqmc          # Name of the executable
tsample 20         # How often to record measurements
Ed [ ] # Ed: Eimp-Edc for PARAMS, copy from the Eimp.in file
M 150000000        # Total number of Monte Carlo steps per core
Ncout 5000000      # How often to print out info
PChangeOrder 0.9
mu      # mu = -Eimp[0] for PARAMS, copy from the Eimp.in file
warmup 20000000    # Warmup number of QMC steps
sderiv 0.02
aom 10
U 4.5
J 1.0
nf0 4.0
beta 30.0

```

Follow the tutorial provided on the Questaal website to run a QSGW+DMFT calculations and also to launch the susceptibility calculations.