QSGW calculation for Gd. T.kotani 1dec2018

Key setting: IDMOD=1 for f orbitals. Probably, together with PWMODE=1

/home/usr2/h70252a/SWJ/GdTEST/15p5f_pwmode1_66_r33_idmod

ctrl.gd ----------

- **ITER MIX=A2,b=.2, (smaller b, b=0.2 may give slow but stable convergence for lmf)**
- **APW setting**

  PWMODE=1

  G vectors of APW basis sets is given at the energy cutoff at q=0.

  The set of G vectors are q-independent for PWMODE=1

  This gives smoother interpolation in BZ. Stable convergence.
- **SPEC settings**

  ATOM=Gd Z=64 R=3.3 # we enlarge R (ctrlgen use R=3.0 as upper limit.)-->use lmchk to know MT overlaps

  EH=-1 -1 -1 -1 RSMH=1.65 1.65 1.65 1.65

  EH2=-2 -2 -2 -2 RSMH2=1.65 1.65 1.65 1.65 # we use 2-MTO's for f channel.

  KMXA={kmxa} LMX=3 LMXA=6 NMCORE=1 # LMXA (charge expanded in MT is up to l=6)

  PZ=0,15.9,0,5.5 we add LO for 5p and 5f --- +10.0 for 5p means extended lo (for cores).

  MMOM=0 0 0 7 #Initial condition for magnetic moment for s,p,d,f

  IDMOD=0 0 0 1 #This fix radial basis for f orbitals. —> you can use FRZWF=T instead (this means all IDMOD=1).

  Takao found IDMOD is needed to make calculation stable→ too many MTO basis for 4f. Roles of MTO basis can switches-->seesaw like instability).

  Type *lmfa|grep conf*. It shows what MTO basis we use for

  6s6p5f4d \times 2 basis + 5p5f as local orbital

  (10+5.9=15.9 for 5p is better setting for semicore.15.9 is 'extended local orbital'--it is similar with MTO.)

  16X2+ 3+7= 40 MTO for each spin.

  It is better to treat 5p (spilt core)-->grep spill llmf
- **SO setting and nk**

  % const pwemax=3 nk1=13 nk2=13 nk3=9 nit=150 gmax=15 nspin=2 metal=3 so=2 xcfun=1 ssig=1.0

  so=2 is for LdotS case. Not needed for Gd.
- **Crystal symmetry setting**

  SYMGRP r4z

  Tthis may be needed to have finite orbital moment. (If we set 'find, it means that we use alll the lattice symmetry---we use 'find' for Gd).

  We may need

  IDU= 0 0 0 2 UH= 0 0 0 0 JH= 0 0 0 0

  in order to to show density matrix for 4f channel (two representations shown-- real harmonics and spherical harmonics).

  (occunum.gd is needed for initial condition of "LDA+U" setting. But it is dummy).

GWinput ----------

- **Product basis setting 1**

<PRODUCT_BASIS>
tolerance to remove products due to poor linear-independency
1.0E-02
lcutmx(atom) = maximum l-cutoff for the product basis. =4 is required for atoms with valence d, like Ni Ga
6 6

This gives product basis at atomic sites up to l=6. l=6 is required for 4f systems.
Proabably because 4fx4f gives l up to l=6.

The numbers
1.0E-02
is a cutoff numbers for linear dependency cutoff for all l=0,1,2,3,4,5,6.

>grep nb lbas
shows number of product basis for each l of atomic sites as

```
 *** lx  *** Used nb =          0         6 <--(for each l we show  numbers of radial functions)
 *** lx  *** Used nb =          1         5
 *** lx  *** Used nb =          2         5
 *** lx  *** Used nb =          3         5
 *** lx  *** Used nb =          4         4
 *** lx  *** Used nb =          5         3
 *** lx  *** Used nb =          6         3
basnfp: BASFP... kmx nblocha=   31  189
```

189 is total numbers of PB at a site.

- **Product basis setting 2**

Mixed product basis (caution. we have two atomic sites!)

```
2  3  1  1  1  ! 4f_p
2  3  2  0  1  ! 4f_d
2  3  3  0  1  ! 5f_l
```

This is for MixedProductBasis to expand 4fx4f orbitals.

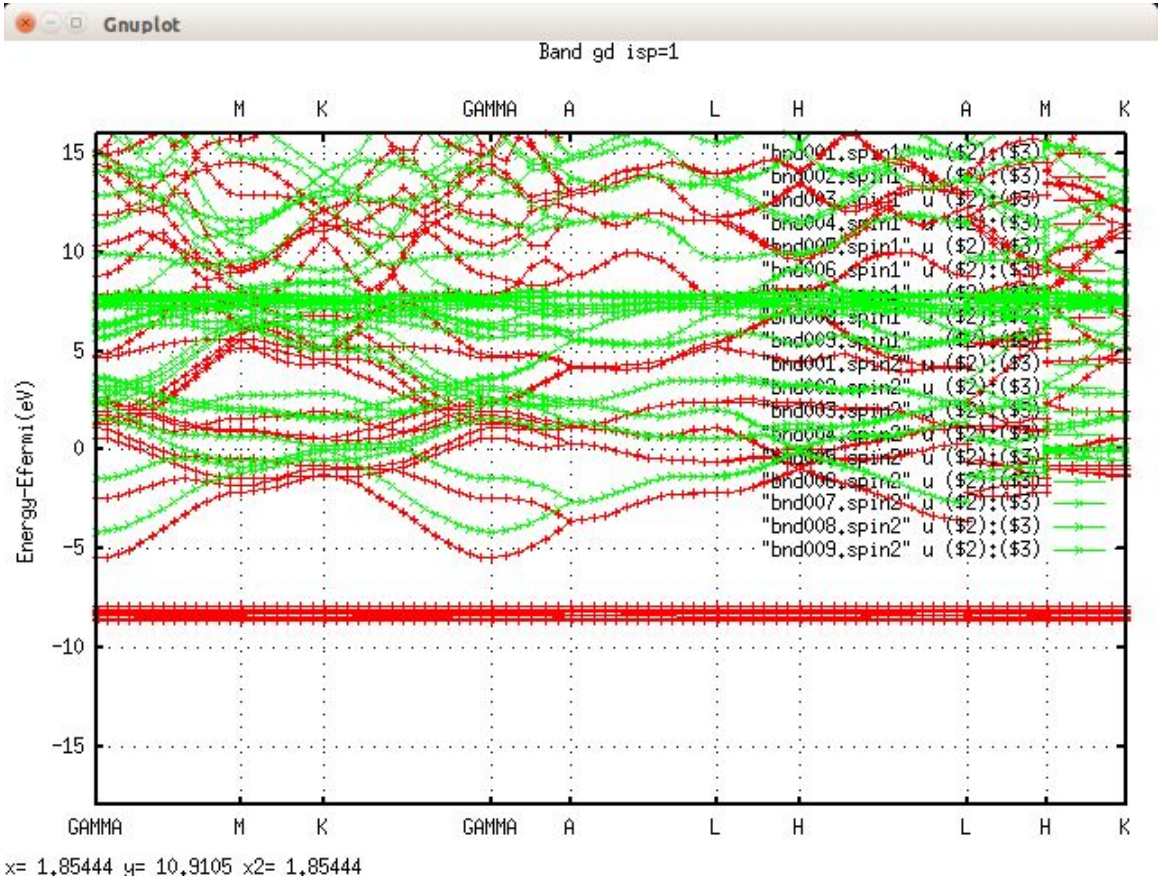
- k points

n1n2n3 6 6 4

(probably reasonable.
I recommend 6x6x6 for ZB. for 0.1 eV
level of convergence for band gaps)

- Reduce computational efforts.

niw 6
emax_sigm 2
QpGcut_psi 3.0
QpGcut_cou 2.5



RESULT

/home/usr2/h70252a/SWJ/GdTEST/15p5f_pwmode1_66_r33_idmod
45 minutes per iteration with 24core.
mmom=15.60 -8eV,8eV.

/home/usr2/h70252a/SWJ/GdTEST/15p5f_pwmode1_66_r33_idmod_3
is for

```
 QpGcut_psi 4.0  !(See unit_2pioa for unit) |q+G| cutoff for eigenfunction.
 QpGcut_cou 3.0  !(See unit_2pioa for unit) |q+G| cutoff for Coulomb and W.
 emax_sigm  3  !(Ry)  emax cutoff for Sigma
 niw      10  ! Number of frequencies along Im axis. Used for integration to get Sigma_c
```

4f level is 0.1eV shallower.

Use attatched datta for plotting (bandplot.isp. bandplot.isp.comp).

A different settings (large cutoff) at 15p5f_pwmode1_66_r33_idmod_lc

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Changes from 15p5f_pwmode1_66_r33_idmod

- **Larger setting for**
  QpGcut_psi 4.0 !(See unit_2pioa for unit) |q+G| cutoff for eigenfunction.
  QpGcut_cou 3.0 !(See unit_2pioa for unit) |q+G| cutoff for Coulomb and W.
  emax_sigm 3 !(Ry) emax cutoff for Sigma
  niw 10 ! Number of frequencies along Im axis. Used for integration to get Sigma_c

- **lcutmx**
  1.0E-03 1.0E-03 1.0E-03 1.0E-03 1.0E-02 3.0E-02 3.0E-02

  These numbers are cutoff numbers for linear dependency cutoff. Each for l=0,1,2,3,4,5,6.

- product basis

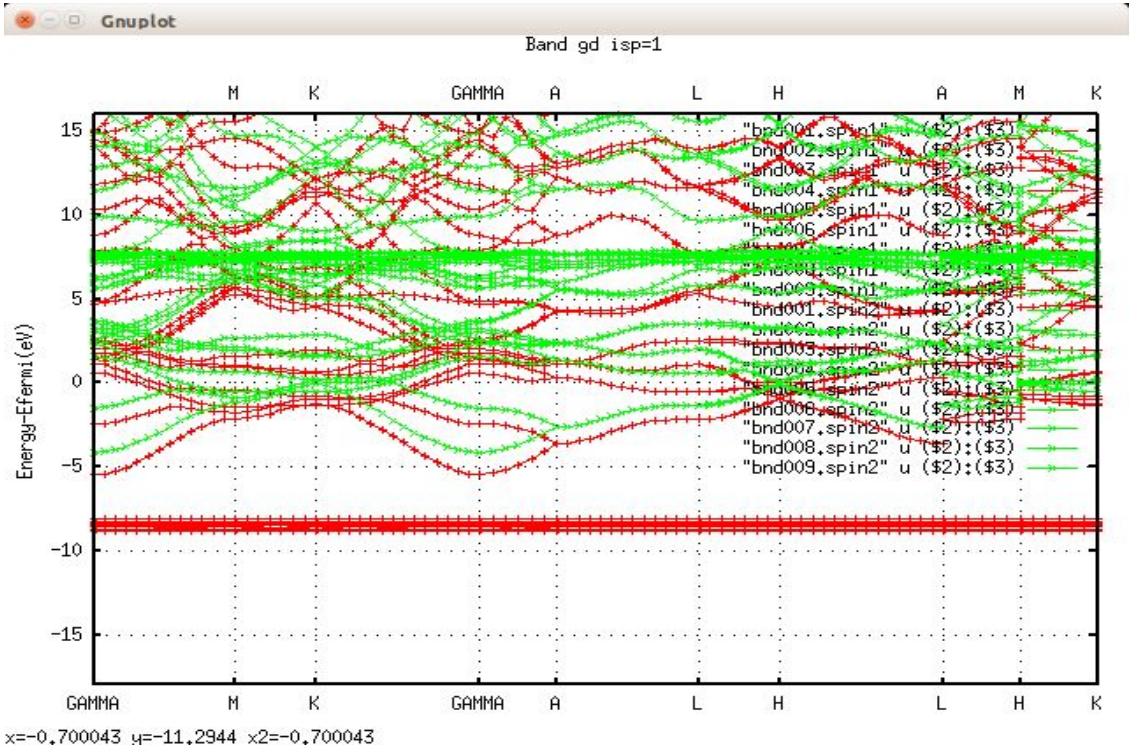
Mixed product basis (caution. we have two atomic sites)

```
3  1  1  1  ! 4f_p
3  2  1  1  ! 4f_d
```

This is for MixedProductBasis to expand 4fx4f orbitals.

```
> grep nb lbas
 *** lx  *** Used nb =      0      8
 *** lx  *** Used nb =      1      7
 *** lx  *** Used nb =      2      8
 *** lx  *** Used nb =      3      6
 *** lx  *** Used nb =      4      6
 *** lx  *** Used nb =      5      3
 *** lx  *** Used nb =      6      3
 basnfp: BASFP... kmx nblocha=   41  237
```

- **pwemax=3 in ctrl file**



RESULT

65 minutes per iteration with 24core.
mmom=15.58 -8eV,8eV. (~0.15eV deeper 4f level).

We see good agreement with
15p5f_pwmode1_66_r33_idmod.

A different settings (large MTO basis) at 7s15p6d5f_pwmode1_pz7555_66

Changes from 15p5f_pwmode1_66_r33_idmod

- **mixbeta 0.2**
  mixing parameter of self-energy → not effective.
- **Larger setting for**
  QpGcut_psi 4.0 !(See unit_2pioa for unit) |q+G| cutoff for eigenfunction.
  QpGcut_cou 3.0 !(See unit_2pioa for unit) |q+G| cutoff for Coulomb and W.
  emax_sigm 2 !(Ry) emax cutoff for Sigma
  niw 10 ! Number of frequencies along Im axis. Used for integration to get Sigma_c
- **lcutmx**
  1.0E-03 1.0E-03 1.0E-03 1.0E-03 1.0E-02 3.0E-02 3.0E-02
- product basis

Mixed product basis (caution. we have two atomic sites)

3 1 1 1 ! 4f_p
3 2 1 1 ! 4f_d

This is for MixedProductBasis to expand 4fx4f orbitals.

> grep nb lbas
***** lx *** Used nb = 0 9**
***** lx *** Used nb = 1 8**
***** lx *** Used nb = 2 10**
***** lx *** Used nb = 3 8**
***** lx *** Used nb = 4 7**
***** lx *** Used nb = 5 3**
***** lx *** Used nb = 6 3**
basnfp: BASFP... kmx nblocha= 48 274

- **pwemax=3, PZ=7.5,15.9,6.5,5.5, and FRZWF=T (instead of IDMOD).**
  Thus we tread 7s, 5p, 6d, 5f as local orbitals.

RESULT

65 minutes per iteration with 24core.
mmom=15.56 -8eV,8eV. (~0.01ejV agreement for 4f level).

We see good agreement with 15p5f_pwmode1_66_r33_idmod.
Energy bands can be slightly diffrent for higher energy above >10 eV or so.