

TOMBO 2019 tutorial

How to use all-electron mixed basis program TOMBO 2019

2019. 7. 23

TOMBO Group

<http://www.ohno.ynu.ac.jp/tombo>

Basic usage

Install TOMBO 2019 executable file on your Windows PC by installer.

Open DOS prompt from “ACCESSORY” in “START” menu.

cd Documents

cd TOMBO

cd Examples

cd => one of the Li2_GW, Li2_X, Si, and Si_GW directories.

(These are the same as the Li2_GW, Li2_X, Si, and Si_GW folders in Examples in USB)

Type TOMBO and press the “ENTER” key.

For multicore PC (e.g. 4 cores), type TOMBO -np 4 or TOMBO /np 4

After the job finished, look at *.out files by using “more” or “word pad.”

Tutorial 1.

Calculation of GW quasiparticle energy spectra and Bethe-Salpeter photoabsorption energy spectra of Li dimer

Purpose:

Electron excitation spectra cannot be calculated by LDA or GGA in density functional theory (DFT).

Here we calculate quasiparticle spectra corresponding photoemission or inverse photoemission spectroscopy measurements by using the GW approximation, and then calculate photoabsorption spectra by solving the Bethe-Salpeter equation. For simplicity, isolated Li₂ cluster is selected as a target system.

Method:

By beginning with LDA, TOMBO calculate quasiparticle spectra by the one-shot GW approximation and then the photoabsorption spectra by solving the Bethe-Salpeter equation.

How to set COORDINATES.inp

```
Li2          ← name of the target system (arbitrary)
12.000000000 ← length of lattice vector  $\mathbf{a}_1$  in [Å].  $\mathbf{a}_1$  should be normalized to 1:  $|\mathbf{a}_1| = 1$ 
    0.000000000000000    0.7071067811865    0.7071067811865 ←  $\mathbf{a}_1$ 
    0.7071067811865    0.000000000000000    0.7071067811865 ←  $\mathbf{a}_2$ 
    0.7071067811865    0.7071067811865    0.000000000000000 ←  $\mathbf{a}_3$ 
2            ← number of atoms
Direct      ← give fractional coordinates of atomic positions (coefficients for  $\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3$ )
            (Cartesian : give Cartesian coordinates of atomic positions in units of [Å])
Li  0.5378444  0.5378444  0.5378444 ← 1st atomic species and coordinates
Li  0.4621556  0.4621556  0.4621556 ← 2nd atomic species and coordinates
mesh = 48   ← if not set, default value is used for the unit-cell mesh
END_PARA    ← Always necessary at the end
```

How to set INPUT.inp

```
SYSTEM=Li2          ← name of the target system (arbitrary)
iApp=LDWN          ! G for GW, B for Bethe-Salpeter, D for both of them
  1st character indicates the method of the SCF Loop:
    L or N (None): the default, LDA.  M: molecular dynamics (MD) is available only for LDA.
    H: Hartree-Fock (available only for very limited  $\Gamma$ -point calculations in this  $\beta$  version).
    G: Self-consistent GW (available only for very limited  $\Gamma$ -point calculations).
  2nd to 4th characters indicate the method after the SCF Loop:
    G: one-shot GW calculation.
    B: Bethe-Salpeter calculation.
    D: one-shot GW + Bethe-Salpeter calculation.
```

T: T-matrix calculation.
S: Second-order Møller–Plesset calculation.
A: Adiabatic LDA, electron dynamics calculation by solving the TD Kohn-Sham equation.
W: Wave-Function output.

```

iAlg=D          ! D for Matrix Diagonalization
               D: Matrix Diagonalization (recommended for small target systems)
               S: Steepest Descent
               C: Block Davidson
nod    =    6    ! number of nodes in PW in each direction
               Max number of  $|n_1|,|n_2|,|n_3|$  of reciprocal lattice vector  $\mathbf{G}=n_1\mathbf{b}_1+n_2\mathbf{b}_2+n_3\mathbf{b}_3$  for PWs.
#Ecutoff = 2.7d0 ! comment=> PW cut-off energy in Ry (1Ry=13.6eV)
               Cutoff Energy (Maximum Kinetic Energy) for Plane Waves (PWs) #Comment
               Set either nod or Ecutoff. (necessary item for all calculations)
               3Ry for alkaline metals, 7Ry for carbon, 18Ry for hydrogen, 24Ry for transition metals
nog    =   12    ! number of nodes in G (Fock exchange)
               Max number of  $|n_1|,|n_2|,|n_3|$  of reciprocal lattice vector  $\mathbf{G}=n_1\mathbf{b}_1+n_2\mathbf{b}_2+n_3\mathbf{b}_3$  for Exchange.
               Set double of nod. (necessary item for HF and GW calculations).
ncut   =    6    ! number of nodes in G (correlation)
               Max number of  $|n_1|,|n_2|,|n_3|$  of reciprocal lattice vector  $\mathbf{G}=n_1\mathbf{b}_1+n_2\mathbf{b}_2+n_3\mathbf{b}_3$  for Correlation.
               Set same number as nod. (necessary item for GW calculations).
noz    =   24    ! number of Fourier mesh for Nuclear Coulomb Tail
               Mesh number used for Fourier decomposition of AO-screened nuclear Coulomb tail.
               Usually set at 16-32, but 64 is recommended for a very accurate calculation.
ncs    =    2    ! number of core states fixed in correlation/TDDFT
               Number of core states to be eliminated from Correlation or Adiabatic LDA calculations.
nol    =   300   ! number of levels
               Number of states to be included in Correlation calculations (Polarization and Self-Energy).
iTotale = 1     ! frag for Total Energy calculation : ON
               Flag to calculate LDA Total Energy (1 for ON, 0 for OFF).
iCHG   = 1     ! frag for Total Charge Density output : ON
               Flag to output Total Charge Density (1 for ON, 0 for OFF).
ippmG  = 0     ! 0 or 3 for GPP, 1 for Engel-Farid, 2 for von der
               ! Linden-Forsch, 4 for  $\omega$  integration
               Selection of plasmon pole models or numerical  $\omega$  integration for the GW self-energy.
jmax   = 0     ! positive (real & imaginary) points for  $\omega$  integration
               Number of points for  $\omega$  integration. Set 0 for ippmG=0-3 and typically 200 for ippmG=4.
lpri   = 0     ! frag for detail list print : OFF
               Flag to output detailed information in calculations in ISYS.out (1 for ON, 0 for OFF).
nspin  = 0     ! spin magnetic moment in  $\mu_B$  (= N_up - N_down)
               spin magnetic moment [ $\mu_B$ ] (spin multiplicity is equal to S = nspin + 1).
nband  = 10    ! number of output level (band)
               Number of states in valence and conduction levels to be displayed in GW (GWA.out).
smixSCF = 0.20 ! Charge Mixing Rate for LoopTD = 1
               Rate of mixing (MAX) previous Charge Density for the 1st MD step (LoopTD = 1).
smixTD  = 0.10 ! Charge Mixing Rate for LoopTD > 1
               Rate of mixing (MAX) previous Charge Density after the 1st MD step (LoopTD > 1).
iMIX   = 3     ! 0: Linear, 1: Optimized Linear, 2: RMM-DIIS Charge Mixing
               ! 3: Broyden Charge Mixing
               Method of SCF Charge Density Mixing (Usually set 1 (or 2), if not converged, set 0).
icontinue = 0  ! 0 for new calc. or 1 to skip LDA SCF Loop.

```

Flag to continue to the previous calculation (0 for new calc., 1 to skip LDA SCF Loop).
 isphcut = 1 ! Coulomb spherical cut (only for isolated systems)
 Flag to truncate Coulomb potential tail at half of the lattice constant. (0 is not to truncate.)
 iSblp = 999 ! Max SCF Loop for LoopTD = 1
 Number of max SCF Loops (for the 1st step in the dynamics Loop).
 iCry = 0 ! Cluster Calculation (Crystal OFF)
 Flag to calculate crystal calculation (0 for cluster calculation, 1 for crystal calculation).
 iasym = 0 ! asymmetric potential inside atomic sphere : OFF
 Flag to treat asymmetric AO charge inside atomic spheres (1 for ON, 0 for OFF).
 icalAO = 0 ! AO redetermination at each SCF loop : OFF
 Flag to update Atomic Orbitals (AOs) at each SCF step (1 for ON, 0 for OFF).
 iFTapp = 0 ! approximation for 3D > 1D Fourier Transformation
 Flag to approximate 3D to 1D Fourier Transformation
 iCheb = 0 ! Chebyshev fitting for atomic potential
 Flag to fit AO potential in atomic spheres to Chebyshev polynomial (1 for ON, 0 for OFF),
 in order to reduce the time required for the computation of $\langle PW|V|AO \rangle$ matrix elements.
 Mcheb = 30 ! number of Chebyshev polynomials
 Highest power of Chebyshev polynomial for potential fitting (effective only for iCheb = 1).
 precLDA = 0.0001d0 ! convergence criterion for Total Energy in eV
 Criterion of Total Energy convergence (SCF loop ends when ΔE becomes less than this).
 END_PARA ← Always necessary at the end

How to look at OUTPUT files:

GWA.out

```

Loopk_q = 0 Loopk_k = 1
Na_2: mesh= 48 size= 2.117 nod= 6 nog=12 nol= 300 ncut= 6 nspin= 0
q=0 only, iDiag= 0

```

	$\langle \mu_{xc} \rangle$	LDA eigenvalue	$\langle \Sigma_x \rangle$	Correlation $\langle \Sigma_c \rangle$	QP energy QP (GWA)	Renormalized QP energy RQP (GWA)
Na 2	exc (LDA)	eps (LDA)	xg (Fock)	slf (GWA)	QP (GWA)	RQP (GWA)
* 3	-5.5682	-3.5408	-7.3972	-0.8465	-6.2163	-5.6038
4	-3.5836	-1.7990	-1.3020	-0.9539	-0.4713	-0.7052
5	-3.8425	-1.5722	-1.2141	-1.0514	0.0048	-0.2900
6	-3.8425	-1.5722	-1.2141	-1.0513	0.0049	-0.2899
7	-3.0842	-1.0258	-0.9242	-1.0423	0.0920	-0.1084
8	-1.7537	-0.0763	-0.2596	-0.8076	0.6102	0.4784
9	-2.0835	-0.0312	-0.2372	-1.0481	0.7669	0.5806
10	-2.0835	-0.0312	-0.2372	-1.0482	0.7669	0.5806
11	-1.6420	0.4796	-0.1403	-0.8559	1.1254	0.9919
12	-1.6420	0.4796	-0.1403	-0.8559	1.1254	0.9919
13	-1.0370	1.0156	-0.0488	-0.5180	1.4857	1.4327
Eg (LDA) :	1.742	Eg (GWA) :	5.745			
IP (LDA) :	3.541	IP (GWA) :	6.216			

PhotoAbsorptionSpectra.out

Photo Absorption Spectra

singlet =	0.000000000 (eV),	triplet =	0.000000000 (eV)
multiplicity =	0		1
0.000000000	0.002468937		0.185138621
0.005440000	0.002480351		0.192629777
0.010880000	0.002491845		0.200584522
0.016320000	0.002503421		0.209041862
0.021760000	0.002515078		0.218044985
0.027200000	0.002526818		0.227641812
0.032640000	0.002538641		0.237885633
0.038080000	0.002550548		0.248835838
0.043520000	0.002562540		0.260558778
0.048960000	0.002574617		0.273128761
0.054400000	0.002586781		0.286629224
energy (eV)	singlet exciton		triplet exciton

ChargeDensity.cube ... for GaussView
 ChargeDensity.vasp ... for VASP VESTA
 ChargeDensity.grd ... for Materials Studio

← Total Charge Density Distribution

WaveF_HOMO.*** ... similar
 WaveF_LUMO.***

← Kohn-Sham wave functions

Tutorial 2.

Structural relaxation of Li2 within LDA

Purpose:

Here we perform a standard structural relaxation of Li2.

Method:

Force acting on each atom is calculated within LDA of density functional theory (DFT). According to Born-Oppenheimer's adiabatic approximation, Broyden algorithm is used to update nuclear positions. (When the number of atoms is equal to or greater than 4, damped MD algorithm is used.)

How to set COORDINATES.inp

```
Li2
8.0000000000
      0.0000000000      0.7071067812      0.7071067812
      0.7071067812      0.0000000000      0.7071067812
      0.7071067812      0.7071067812      0.0000000000
2
Cartesian ← give Cartesian coordinates of atomic positions in units of [Å]
Li  0.000000000000  0.000000000000  0.000000000000
    ← 1st atomic species and coordinates
Li  1.38560652110  1.38560652110  1.38560652110
    ← 2nd atomic species and coordinates
modify_rct = 0 ← Set rct (radius of atomic sphere) at half of bond length (0: NO, 1: YES)
dTime      = 1  ! Time interval (Delta t) in fs (femto second)
             Time step Δt in units of [fs] for MD.
END_PARA    ← Always necessary at the end
```

How to set INPUT.inp

```
SYSTEM=Li2          ← name of the target system (arbitrary)
iApp=LXNN          ! M for MD, X for Relax, W for Wave Function output
  1st character indicates the method of the SCF Loop:
    L or N (None): the default, LDA. X: structural relaxation, M: molecular dynamics (MD).
  2nd to 4th characters indicate the method after the SCF Loop:
    A: Adiabatic LDA, electron dynamics calculation by solving the TD Kohn-Sham equation.
    W: Wave-Function output.
iAlg=D            ! D for Matrix Diagonalization
  D: Matrix Diagonalization (recommended for small target systems)
  S: Steepest Descent
```

C: Conjugate Gradient, etc. (now under test, coming soon!)

```

#nod      = 11      ! number of nodes in PW in each direction
            Max number of  $|n_1|, |n_2|, |n_3|$  of reciprocal lattice vector  $\mathbf{G} = n_1\mathbf{b}_1 + n_2\mathbf{b}_2 + n_3\mathbf{b}_3$  for PWs.
            #Comment
Ecutoff   = 5.d0    ! comment=> PW cut-off energy in Ry (1Ry=13.6eV)
            Cutoff Energy (Maximum Kinetic Energy) for Plane Waves (PWs)
            Set either nod or Ecutoff. (necessary item for all calculations)
            3Ry for alkaline metals, 7Ry for carbon, 18Ry for hydrogen, 24Ry for transition metals
ncs       = 2       ! number of core states fixed in correlation/TDDFT
            Number of core states to be eliminated from Correlation or Adiabatic LDA calculations.
noz       = 32      ! number of Fourier mesh for Nuclear Coulomb Tail
            Mesh number used for Fourier decomposition of AO-screened nuclear Coulomb tail.
            Usually set 16-32, but 64 is recommended for a very accurate calculation.
nol       = 80      ! number of levels
            Number of states to be included in Correlation calculations (Polarization and Self-Energy).
#identify = 1       ! 0 to distinguish atoms, or 1 to identify atoms
#q_min_mod = 0.01d0 ! criterion to truncate AOs (ratio in norm)
FORCE_TOLERANCE = 1.5d-2 ! Force tolerance for Structural Relax
icontinue = 0       ! 0 for new calc. or 1 to skip LDA SCF Loop.
            Flag to continue to the previous calculation (0 for new calc., 1 to skip LDA SCF Loop).
ispkcut   = 0       ! Coulomb spherical cut (only for isolated systems)
            Flag to truncate Coulomb potential tail at half of the lattice constant. (0 is not to truncate.)
nspin     = 0       ! spin magnetic moment in  $\mu_B$  (=  $N_{up} - N_{down}$ )
            spin magnetic moment [ $\mu_B$ ] (spin multiplicity is equal to  $S = nspin + 1$ ).
iTotale   = 1       ! frag for Total Energy calculation : ON
            Flag to calculate LDA Total Energy (1 for ON, 0 for OFF)
iCHG      = 0       ! frag for Total Charge Density output : ON
            Flag to output Total Charge Density (1 for ON, 0 for OFF)
lpri      = 1       ! frag for detail list print : OFF
            Flag to output detailed information in calculations in ISYS.out. (1 for ON, 0 for OFF)
#ntran    = 1       ! crystal symmetrization off
            number of symmetry (coordinate transformation) operations.
            Usually set automatically, but, for MD, set ntran = 1.
nband     = 10      ! number of output level (band)
            Number of states in valence and conduction levels to be displayed in GW (GWA.out).
smixSCF   = 0.10    ! Charge Mixing Rate for LoopTD = 1
            Rate of mixing (MAX) previous Charge Density for the 1st MD step (LoopTD = 1).
smixTD    = 0.10    ! Charge Mixing Rate for LoopTD > 1
            Rate of mixing (MAX) previous Charge Density after the 1st MD step (LoopTD > 1).
iMIX      = 3       ! 0: Linear, 1: Optimized Linear, 2: RMM-DIIS Charge Mixing
            ! 3: Broyden Charge Mixing
            Method of SCF Charge Density Mixing (Usually set 1 (or 2), if not converged, set 0).
nSDCG     = 1       ! Number of Steepest Descent Loops
            number of Steepest-Descent (SD) or Conjugate-Gradient (CG) iterations at time step..
iSblp     = 999     ! Max SCF Loop for LoopTD = 1
            Number of max SCF Loops for the 1st step in the dynamics Loop (LoopTD = 1).
mSblp     = 888     ! Max SCF Loop for LoopTD > 1
            Number of max SCF Loops after the 1st step in the dynamics Loop (LoopTD > 1).
iCry      = 0       ! Cluster Calculation (Crystal OFF)
            Frag to calculate crystal calculation (0 for cluster calculation, 1 for crystal calculation)

```

```

iasym  =  0    ! asymmetric potential inside atomic sphere : OFF
      Frag to treat asymmetric AO charge inside atomic spheres (1 for ON, 0 for OFF).
icalAO =  0    ! AO redetermination at each SCF loop : OFF
      Frag to update Atomic Orbitals (AOs) at each SCF step (1 for ON, 0 for OFF).
iFTapp =  0    ! approximation for 3D > 1D Fourier Transformation
      Frag to approximate 3D to 1D Fourier Transformation
iCheb  =  0    ! Chebyshev fitting for atomic potential
      Frag to fit AO potential in atomic spheres to Chebyshev polynomial (1 for ON, 0 for OFF),
      in order to reduce the time required for the computation of <PW|V|AO> matrix elements.
Mcheb  =  30    ! number of Chebyshev polynomials
      Highest power of Chebyshev polynomial for potential fitting (effective only for iCheb = 1).
precLDA = 0.0001d0 ! convergence criterion for Total Energy in eV
      Criterion of Total Energy convergence (SCF loop ends when  $\Delta E$  becomes less than this).
nStep  =  500  ! Max Dynamics Loop (Max LoopTD)
      number of MD steps.
END_PARA

```

How to look at OUTPUT files:

```

MD_Coordinates.xyz    ... for VMD
MD_Coordinates.arc    ... for Materials Studio

```


Tutorial 3.

LDA calculation for Si crystal

Purpose:

Here we perform a standard band structure calculation of Si crystal.

Method:

Self-consistent field (SCF) loop with special-point sampling and band structure calculations at the k-points (KPOINT.inp) are performed within standard local density approximation (LDA) of density functional theory (DFT).

How to set COORDINATES.inp

```
Si          ← name of the target system (arbitrary)
 3.83959000000 ← length of lattice vector  $a_1$  in [Å].  $a_1$  should be normalized to 1:  $|a_1| = 1$ 
 0.000000000000000000 0.7071067811865475 0.7071067811865475 ←  $a_1$ 
 0.7071067811865475 0.000000000000000000 0.7071067811865475 ←  $a_2$ 
 0.7071067811865475 0.7071067811865475 0.000000000000000000 ←  $a_3$ 
2          ← number of atoms
Direct     ← give fractional coordinates of atomic positions (coefficients for  $a_1, a_2, a_3$ )
           (Cartesian : give Cartesian coordinates of atomic positions in units of [Å])
Si 0.3750000000 0.3750000000 0.3750000000 ← 1st atomic species and coordinates
Si 0.6250000000 0.6250000000 0.6250000000 ← 2nd atomic species and coordinates
modify_rct = 0 ← Set rct (radius of atomic sphere) at half of bond length (0: NO, 1: YES)
mesh = 16     ← mesh division of unit cell (same for all directions)
qmesh=2 2 2   ← Monkhorst Pack special point division in the irreducible 1st Brillouin zone
END_PARA     ← Always necessary at the end
```

How to set INPUT.inp

```
SYSTEM=Si2          ← name of the target system (arbitrary)
iApp=LNNN          ! (L for LDA is default) N for non
 1st character indicates the method of the SCF Loop. L or N (None): the default, LDA.
 2nd to 4th characters indicate the method after the SCF Loop: N is None.
iAlg=D            ! D for Matrix Diagonalization
  D: Matrix Diagonalization (recommended for crystal calculations)
#nod = 3          ! number of nodes in PW in each direction
  Max number of  $|n_1|, |n_2|, |n_3|$  of reciprocal lattice vector  $G=n_1b_1+n_2b_2+n_3b_3$  for PWs.
#Comment
Ecutoff = 6.d0    ! comment=> PW cut-off energy in Ry (1Ry=13.6eV)
  Cutoff Energy (Maximum Kinetic Energy) for Plane Waves (PWs)
```

Set either `nod` or `Ecutoff`. (necessary item for all calculations)
3Ry for alkaline metals, 7Ry for carbon, 18Ry for hydrogen, 24Ry for transition metals

```

noz      = 12      ! number of Fourier mesh for Nuclear Coulomb Tail
Mesh number used for Fourier decomposition of AO-screened nuclear Coulomb tail.
Usually set 16-32, but 64 is recommended for a very accurate calculation.
ncs      = 0       ! number of core states fixed in correlation/TDDFT
Number of core states to be eliminated from Correlation or Adiabatic LDA calculations.
nol      = 60      ! number of levels
Number of states to be included in Correlation calculations (Polarization and Self-Energy).
nband    = 10      ! number of output level (band)
Number of states in valence and conduction levels to be displayed in GW (GWA.out).
nspin    = 0       ! spin magnetic moment in mu_B (= N_up - N_down)
spin magnetic moment [ $\mu_B$ ] (spin multiplicity is equal to  $S = nspin + 1$ ).
icontinue = 0      ! 0 for new calc. or 1 to skip LDA SCF Loop.
Flag to continue to the previous calculation (0 for new calc., 1 to skip LDA SCF Loop).
ispicut  = 0       ! Coulomb spherical cut (only for isolated systems)
Flag to truncate Coulomb potential tail at half of the lattice constant. (0 is not to truncate.)
iTotale  = 1       ! frag for Total Energy calculation : ON
Flag to calculate LDA Total Energy (1 for ON, 0 for OFF).
lpri     = 0       ! frag for detail list print : OFF
Flag to output detailed information in calculations in ISYS.out (1 for ON, 0 for OFF).
smixSCF  = 0.80    ! Charge Mixing Rate for LoopTD = 1
Rate of mixing (MAX) previous Charge Density for the 1st MD step (LoopTD = 1).
smixTD   = 0.90    ! Charge Mixing Rate for LoopTD > 1
Rate of mixing (MAX) previous Charge Density after the 1st MD step (LoopTD > 1).
iMIX     = 0       ! 0: Linear, 1: Optimized Linear, 2: RMM-DIIS Charge Mixing
! 3: Broyden Mixing
Method of SCF Charge Density Mixing (Usually set 1 (or 2), if not converged, set 0).
iSblp    = 999    ! Max SCF Loop for LoopTD = 1
Number of max SCF Loops (for the 1st step in the dynamics Loop).
iSblp2   = 15     ! Max SCF Loop with only Gamma point
! LoopSCF > iSblp2 : special point loop using SPOINT
Number of max SCF Loops only for  $\Gamma$  point (special-point loop starts after this cycle).
iCry     = 1       ! Cluster Calculation (Crystal OFF)
Flag to calculate crystal calculation (0 for cluster calculation, 1 for crystal calculation).
iasym    = 0       ! asymmetric potential inside atomic sphere : OFF
Flag to treat asymmetric AO charge inside atomic spheres (1 for ON, 0 for OFF).
icalAO   = 0       ! AO redetermination at each SCF loop : OFF
Flag to update Atomic Orbitals (AOs) at each SCF step (1 for ON, 0 for OFF).
iFTapp   = 0       ! approximation for 3D > 1D Fourier Transformation
Flag to approximate 3D to 1D Fourier Transformation
iCheb    = 0       ! Chebyshev fitting for atomic potential
Flag to fit AO potential in atomic spheres to Chebyshev polynomial (1 for ON, 0 for OFF),
in order to reduce the time required for the computation of  $\langle PW|V|AO \rangle$  matrix elements.
Mcheb    = 30      ! number of Chebyshev polynomials
Highest power of Chebyshev polynomial for potential fitting (effective only for iCheb = 1).
precLDA  = 0.0001d0 ! convergence criterion for Total Energy in eV
Criterion of Total Energy convergence (SCF loop ends when  $\Delta E$  becomes less than this).
END_PARA      ← Always necessary at the end

```

How to set KPOINT.inp

Give k points (on symmetry lines) for energy-band outputs: “band_0001.out”, “band_0002.out”, ...

Direct ← give k points in the fractional coordinates (coefficients for b_1, b_2, b_3)
(Cartesian : give coefficients for $2\pi/a$ in Cartesian coordinates)
(FCC : give coefficients for $2\pi/A$ ($A=\sqrt{2}a$) in Cartesian coordinates)
(BCC : give coefficients for $2\pi/A$ ($A=2a/\sqrt{3}$) in Cartesian coordinates)
(a is the lattice constant of rhombohedral unit cell; A is the length of the cubic Bravais lattice)

16 ← numbers of k points

0.500000000	0.250000000	0.750000000	0.1176470588	← 1 st k point and weight
0.500000000	0.333333333	0.666666666	0.0588235294	← 2 nd k point and weight
0.500000000	0.416666666	0.583333333	0.0588235294	← 3 rd k point and weight
0.500000000	0.500000000	0.500000000	0.0588235294	← 4 th k point and weight
0.375000000	0.375000000	0.375000000	0.0588235294	← 5 th k point and weight
0.250000000	0.250000000	0.250000000	0.0588235294	← 6 th k point and weight
0.125000000	0.125000000	0.125000000	0.0588235294	← 7 th k point and weight
0.000000000	0.000000000	0.000000000	0.0588235294	← 8 th k point and weight
0.100000000	0.000000000	0.100000000	0.0588235294	← 9 th k point and weight
0.200000000	0.000000000	0.200000000	0.0588235294	← 10 th k point and weight
0.300000000	0.000000000	0.300000000	0.0588235294	← 11 th k point and weight
0.400000000	0.000000000	0.400000000	0.0588235294	← 12 th k point and weight
0.500000000	0.125000000	0.500000000	0.0588235294	← 13 th k point and weight
0.500000000	0.312500000	0.625000000	0.0588235294	← 14 th k point and weight
0.437500000	0.375000000	0.750000000	0.0588235294	← 15 th k point and weight
0.375000000	0.375000000	0.750000000	0.0588235294	← 16 th k point and weight

(weight is meaningless but should not be all zero)

How to look at output data

band_0001.out energy eigenvalues (at sequential k points) in the 1st band

band_0001.out energy eigenvalues (at sequential k points) in the 2nd band

band.out energy eigenvalues (at sequential k points) in all bands for EXCEL (line graph plots)

Tutorial 4.

Calculation of GW quasiparticle energy spectra of Si crystal

Purpose:

Here we perform a standard band structure calculation of Si crystal.

Method:

Self-consistent field (SCF) loop with special-point sampling (SPOINT.inp) is performed within LDA and then one-shot GW crystal calculation is performed. To calculate the polarization function $P_{GG}(\mathbf{q}, \omega=0)$, \mathbf{k} -point sampling is performed for the points in the whole BZ assigned as “sum” in KPOINT.inp. Then the correlation part of the self-energy, Σ_c is calculated within the generalized plasmon pole (GPP) model by taking \mathbf{q} -point sampling in the irreducible BZ by using QPOINT.inp. Finally, the expectation values of the exchange (Σ_x) and correlation (Σ_c) parts of the self-energy are evaluated for the \mathbf{k} points (typically at symmetry points in the irreducible BZ) assigned as “out” in KPOINT.inp. If the \mathbf{k} -points assigned for “out” and “sum” are the same, they should be assigned as “out+sum”, not individually as “out” or “sum”.

How to set COORDINATES.inp (This is identical to that of Tutorial 2.)

```
Si2          ← name of the target system (arbitrary)
 3.83959000000 ← length of lattice vector  $\mathbf{a}_1$  in [Å].  $\mathbf{a}_1$  should be normalized to 1:  $|\mathbf{a}_1| = 1$ 
 0.000000000000000000 0.7071067811865475 0.7071067811865475 ←  $\mathbf{a}_1$ 
 0.7071067811865475 0.000000000000000000 0.7071067811865475 ←  $\mathbf{a}_2$ 
 0.7071067811865475 0.7071067811865475 0.000000000000000000 ←  $\mathbf{a}_3$ 
2           ← number of atoms
Direct      ← give fractional coordinates of atomic positions (coefficients for  $\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3$ )
            (Cartesian : give Cartesian coordinates of atomic positions in units of [Å])
Si 0.3750000000 0.3750000000 0.3750000000 ← 1st atomic species and coordinates
Si 0.6250000000 0.6250000000 0.6250000000 ← 2nd atomic species and coordinates
modify_rct = 0 ← Set rct (radius of atomic sphere) at half of bond length (0: NO, 1: YES)
mesh=16     ← mesh division of unit cell (same for all directions)
nion=0      ← excess electron number measured from the charge neutrality
qmesh=2 2 2 ← Monkhorst Pack special point division and  $\Gamma$  point  $\mathbf{q}$  point division in the
            irreducible 1st Brillouin zone, and  $\Gamma$  point  $\mathbf{k}$  point division in the whole zone
Si_ns=2     ← 1s & 2s AOs are used but 3s AO is not used in the overcompleteness problem
Si_np=1     ← 2p AO is used but 3p AO is not used to avoid the overcompleteness problem
END_PARA    ← Always necessary at the end
```

How to set INPUT.inp

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SYSTEM=Si2          ← name of the target system (arbitrary)
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iApp=LGNN      ! (L for LDA is default) N for non
  1st character indicates the method of the SCF Loop. L or N (None): the default, LDA.
  2nd to 4th characters indicate the method after the SCF Loop: G: one-shot GW calculation.
iAlg=D        ! D for Matrix Diagonalization
  D: Matrix Diagonalization (recommended for crystal calculations)
#nod   =   4    ! number of nodes in PW in each direction
  Max number of  $|n_1|,|n_2|,|n_3|$  of reciprocal lattice vector  $\mathbf{G}=n_1\mathbf{b}_1+n_2\mathbf{b}_2+n_3\mathbf{b}_3$  for PWs.
  #Comment
Ecutoff = 11.d0 ! comment=> PW cut-off energy in Ry (1Ry=13.6eV)
  Cutoff Energy (Maximum Kinetic Energy) for Plane Waves (PWs)
  Set either nod or Ecutoff. (necessary item for all calculations)
  3Ry for alkaline metals, 7Ry for carbon, 18Ry for hydrogen, 24Ry for transition metals
nog    =  10    ! number of nodes in G (Fock exchange)
  Max number of  $|n_1|,|n_2|,|n_3|$  of reciprocal lattice vector  $\mathbf{G}=n_1\mathbf{b}_1+n_2\mathbf{b}_2+n_3\mathbf{b}_3$  for Exchange.
  Set double of nod. (necessary item for HF and GW calculations).
ncut   =   4    ! number of nodes in G (correlation)
  Max number of  $|n_1|,|n_2|,|n_3|$  of reciprocal lattice vector  $\mathbf{G}=n_1\mathbf{b}_1+n_2\mathbf{b}_2+n_3\mathbf{b}_3$  for Correlation.
  Set same number as nod. (necessary item for GW calculations).
noz    =  16    ! number of Fourier mesh for Nuclear Coulomb Tail
  Mesh number used for Fourier decomposition of AO-screened nuclear Coulomb tail.
  Usually set 16-32, but 64 is recommended for a very accurate calculation.
ncs    =  10    ! number of core states fixed in correlation/TDDFT
  Number of core states to be eliminated from Correlation or Adiabatic LDA calculations.
nol    =  150    ! number of levels
  Number of states to be included in Correlation calculations (Polarization and Self-Energy).
iTotalE =  0    ! frag for Total Energy calculation : OFF
  Flag to calculate LDA Total Energy (1 for ON, 0 for OFF).
iCHG   =  0    ! frag for Total Charge Density output : ON
  Flag to output Total Charge Density (1 for ON, 0 for OFF)
lpri   =  0    ! frag for detail list print : OFF
  Flag to output detailed information in calculations in ISYS.out (1 for ON, 0 for OFF).
nspin  =  0    ! spin magnetic moment in  $\mu_B$  (=  $N_{up} - N_{down}$ )
  spin magnetic moment [ $\mu_B$ ] (spin multiplicity is equal to  $S = nspin + 1$ ).
nband  =  10    ! number of output level (band)
  Number of states in valence and conduction levels to be displayed in GW (GWA.out).
iMIX   =   3    ! 0: Linear, 1: Optimized Linear, 2: RMM-DIIS Charge Mixing
  ! 3: Broyden Mixing
  Method of SCF Charge Density Mixing (Usually set 1 (or 2), if not converged, set 0).
smixSCF = 0.20 ! Charge Mixing Rate for LoopTD = 1
  Rate of mixing (MAX) previous Charge Density for the 1st MD step (LoopTD = 1).
icontinue = 0 ! 0 for new calc. or 1 to skip LDA SCF Loop.
  Flag to continue to the previous calculation (0 for new calc., 1 to skip LDA SCF Loop).
#isphcut = -1 ! Coulomb spherical cut (only for isolated systems)
  Flag to truncate Coulomb potential tail at half of the lattice constant. (0 is not to truncate.)
iSblp  =  999 ! Max SCF Loop for LoopTD = 1
  Number of max SCF Loops (for the 1st step in the dynamics Loop).
iSblp2 =  15 ! Max SCF Loop with only Gamma point
  ! LoopSCF > iSblp2 : special point loop using SPOINT
  Number of max SCF Loops only for  $\Gamma$  point (special-point loop starts after this cycle).
iCry   =   1    ! Cluster Calculation (Crystal OFF)

```

Frag to calculate crystal calculation (0 for cluster calculation, 1 for crystal calculation).
nEX = 0 ! 0 for normal or -n (n is e.g. 10) for save memory GW calc.
Fock exchange calculation is divided to n times if nEX is set greater than or smaller than 0.
nBSE = 1 ! 1 for normal or n (n is e.g. 10) for save memory BSE calc.
BSE calculation is divided to n times if nBSE is set greater than 0.
iCheb = 0 ! Chebyshev fitting for atomic potential
Frag to fit AO potential in atomic spheres to Chebyshev polynomial (1 for ON, 0 for OFF),
in order to reduce the time required for the computation of $\langle PW|V|AO \rangle$ matrix elements.
Mcheb = 30 ! number of Chebyshev polynomials
Highest power of Chebyshev polynomial for potential fitting (effective only for iCheb = 1).
irelativ = 0 ! semi-relativistic correction, = 1 : ON, = 0 : OFF
iFTapp = 0 ! approximation for 3D > 1D Fourier Transformation
Frag to approximate 3D to 1D Fourier Transformation
iasym = 0 ! asymmetric potential inside atomic sphere : OFF
Frag to treat asymmetric AO charge inside atomic spheres (1 for ON, 0 for OFF).
ippmG = 0 ! 0 or 3 for GPP, 1 for Engel-Farid, 2 for von der
! Linden-Forsch, 4 for ω integration
Selection of plasmon pole models or numerical ω integration for the GW self-energy.
jmax = 0 ! positive (real & imaginary) points for ω integration
Number of points for ω integration. Set 0 for ippmG=0-3 and typically 200 for ippmG=4.
deltaE = 0.5d0 ! delta E for numerical derivative of the self-energy
 ΔE in units of eV. Default value is deltaE = 0.5d0 [eV].
precLDA = 0.0001d0 ! convergence criterion for Total Energy in eV
Criterion of Total Energy convergence (SCF loop ends when ΔE becomes less than this).
nStep = 1 ! Max Dynamics Loop (Max LoopTD)
number of MD steps.
END_PARA ← Always necessary at the end

How to set SPOINT.inp

Give special k points used for the SCF iteration loop in a crystal calculation.

Direct ← give k points in the fractional coordinates (coefficients for b_1, b_2, b_3)
(Cartesian : give coefficients for $2\pi/a$ in Cartesian coordinates)
(FCC : give coefficients for $2\pi/A$ ($A=\sqrt{2}a$) in Cartesian coordinates)
(BCC : give coefficients for $2\pi/A$ ($A=2a/\sqrt{3}$) in Cartesian coordinates)
(a is the lattice constant of rhombohedral unit cell; A is the length of the cubic Bravais lattice)
2 ← number of k points
0.2500000 0.2500000 0.2500000 1.00 ← 1st k point and weight
0.2500000 0.2500000 -0.2500000 3.00 ← 2nd k point and weight

How to set KPOINT.inp

Give k points (on symmetry lines) for energy-band outputs: “band_0001.out”, “band_0002.out”, ...

FCC ←coefficients for $2\pi/A$ ($A=\sqrt{2}a$) in Cratesian cooredinates
 (Cartesian : give coefficients for $2\pi/a$ in Cratesian cooredinates)
 (BCC : give coefficients for $2\pi/A$ ($A=2a/\sqrt{3}$) in Cratesian cooredinates)
 (Direct : give k points in the fractional coordinates (coefficients for b_1, b_2, b_3))
 (a is the lattice constant of rhombohedral unit cell; A is the length of the cubic Bravais lattice)
 16 0 0 ← numbers of k points for “out+sum”, “out”, and “sum”,
 where “out” is for output and “sum” is for Correlation and Self-Energy (GW) calculation.
 (k points in “out” are inside the irreducible BZ, but “sum” should be given in the whole BZ.)
 0.500000000 0.000000000 0.000000000 1.00 ← 1st k point and weight
 1.000000000 0.000000000 0.000000000 1.00 ← 2nd k point and weight
 0.000000000 1.000000000 0.000000000 1.00 ← 3rd k point and weight
 0.000000000 0.000000000 1.000000000 1.00 ← 4th k point and weight
 (weight for “out+sum” and “sum” k points is meaningful in the calc. of polarization function.)

How to set QPOINT.inp

Give momentum transfer, q points, inside the irreducible BZ required in GW calculation only.

Direct ←coefficients for $2\pi/A$ ($A=\sqrt{2}a$) in Cratesian cooredinates
 (Cartesian : give coefficients for $2\pi/a$ in Cratesian cooredinates)
 (BCC : give coefficients for $2\pi/A$ ($A=2a/\sqrt{3}$) in Cratesian cooredinates)
 (Direct : give k points in the fractional coordinates (coefficients for b_1, b_2, b_3))
 (a is the lattice constant of rhombohedral unit cell; A is the length of the cubic Bravais lattice)
 3 32 ← number of q points, and ratio of BZ volume / (Γ point) microzone volume:
 see: M. S. Hybertsen and S. G. Louie, Phys. Rev. B 34, 5390-5413 (1986), Appendix B, Eq.(B4).
 0.0000001 0.0000000 0.0000000 2.00 ← 1st q point and weight
 1.0000000 0.0000000 0.0000000 5.00 ← 2nd q point and weight
 1.0000000 1.0000000 0.0000000 1.00 ← 3rd q point and weight

How to look at OUTPUT files:

GWA.out

```

Loopk_q = 1 Loopk_k = 1
Na_2: mesh= 32 size= 4.410 nod= 3 nog= 8 nol= 60 ncut= 3 nspin= 0
q=0 only, iDiag= 0 Correlation Renormalized
< $\mu_{xc}$ > LDA eigenvalue < $\Sigma_x$ > < $\Sigma_c$ > QP energy QP energy
Na 2 exc(LDA) eps(LDA) xg(Fock) slf(GWA) QP(GWA) RQP(GWA)

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...

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Loopk_q = 3 Loopk_k = 4

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Na_2: mesh= 32 size= 4.410 nod= 3 nog= 8 nol= 60 ncut= 3 nspin= 0
q=0 only, iDiag= 0

Na 2	exc (LDA)	eps (LDA)	xg (Fock)	slf (GWA)	QP (GWA)	RQP (GWA)
11	-13.0183	-0.1540	-11.0681	0.7477	2.5439	4.4345
12	-12.8860	-0.1222	-10.5709	0.9717	3.1646	4.4549
13	-12.0066	4.8609	-8.8399	0.1028	8.1305	8.0167
* 14	-12.0066	4.8609	-8.8901	-0.0295	7.9480	7.4317
15	-9.8662	8.3105	-3.8791	-1.8455	12.4521	12.1179
16	-9.7821	8.4394	-3.8831	-1.8203	12.5181	12.1886
17	-12.7190	18.1271	-5.1363	-1.7893	23.9205	22.2985
18	-12.7190	18.1271	-5.1636	-1.8215	23.8610	22.0834
19	-10.6056	20.0307	-5.0769	-1.5417	24.0177	23.6240
20	-10.6056	20.0307	-5.2065	-1.3089	24.1209	22.5848
21	-12.8435	20.8238	-5.1120	-2.1672	26.3881	26.0637

...
Eg (LDA): 3.450 Eg (GWA): 4.504
IP (LDA): -4.861 IP (GWA): -7.948

← These are intermediate results and not the final result. The final result is below.

The Result of q-point sum

Loopk_k =	1 ← 1 st k point			Correlation	Renormalized	
	<μ _{xc} >	LDA eigenvalue	<Σ _x >	<Σ _c >	QP energy	QP energy
Level	exc (LDA)	eps (LDA)	xg (Fock)	slf (GWA)	QP (GWA)	RQP (GWA)
11	-12.2990	-4.3792	-11.7865	0.9095	-2.9572	-2.8079
12	-13.1112	7.8915	-9.2389	-0.7487	11.0150	10.7929
13	-13.1112	7.8915	-9.0366	-0.8446	11.1214	10.8920
* 14	-13.1111	7.8915	-9.1532	-0.8109	11.0385	10.8140
15	-11.2881	10.3212	-5.6455	-1.2759	14.6879	14.4144
16	-11.2881	10.3212	-5.9197	-1.2334	14.4561	14.1452
17	-11.2881	10.3212	-5.3777	-1.2643	14.9673	14.6864
18	-15.0350	11.1751	-7.4796	-1.5890	17.1415	17.0960
19	-9.3636	15.2080	-3.0094	-1.7034	19.8587	19.7567
20	-10.0478	16.1870	-4.2285	-1.3469	20.6594	20.4667
21	-10.0478	16.1870	-3.8528	-1.8014	20.5806	20.3230
22	-8.6114	18.8405	-2.2575	-2.2444	22.9500	25.4778
23	-8.6114	18.8405	-2.2680	-2.0640	23.1199	23.4978
24	-8.6114	18.8405	-2.2497	-2.1289	23.0733	22.9509

Loopk_k =	2 ← 2 nd k point					
Level	exc (LDA)	eps (LDA)	xg (Fock)	slf (GWA)	QP (GWA)	RQP (GWA)
11	-13.0183	-0.1540	-10.6793	-0.1316	2.0534	1.9483
12	-12.8860	-0.1222	-10.6104	0.3196	2.4730	2.2270
13	-12.0066	4.8609	-8.7334	-0.4609	7.6733	7.3523
* 14	-12.0066	4.8609	-8.7334	-0.4505	7.6836	7.3407
15	-9.8662	8.3105	-3.9148	-1.2613	13.0006	12.7146
16	-9.7821	8.4394	-3.8677	-1.3823	12.9714	12.6919
17	-12.7190	18.1271	-5.0681	-2.5965	23.1815	22.4702
18	-12.7190	18.1271	-5.0681	-2.5712	23.2068	22.2454
19	-10.6056	20.0307	-4.7897	-1.3743	24.4723	25.5046
20	-10.6056	20.0307	-4.7897	-1.3959	24.4507	25.0999
21	-12.8435	20.8238	-4.9520	-2.0276	26.6877	26.2378

22	-10.1033	21.1819	-3.3278	-2.8844	25.0731	24.5887
23	-13.1408	21.1994	-5.1505	-2.2295	26.9601	29.4824
24	-9.9001	21.4392	-3.2032	-2.2563	25.8799	24.8086
Loopk_k =		3 ← 3 rd k point				
Level	exc (LDA)	eps (LDA)	xg (Fock)	slf (GWA)	QP (GWA)	
RQP (GWA)						
11	-13.0183	-0.1540	-11.0691	0.2827	2.0778	1.8428
12	-12.8860	-0.1222	-10.8682	0.3149	2.2105	1.9860
13	-12.0066	4.8609	-8.3610	-0.7003	7.8062	7.5890
* 14	-12.0066	4.8609	-8.3610	-0.7051	7.8014	7.5844
15	-9.8662	8.3105	-4.9854	-1.0784	12.1128	11.8668
16	-9.7821	8.4394	-4.8688	-1.1035	12.2492	12.0050
17	-12.7190	18.1271	-5.1236	-1.9281	23.7944	23.7970
18	-12.7190	18.1271	-5.1236	-1.9236	23.7989	23.1645
19	-10.6056	20.0307	-4.0752	-1.4995	25.0616	24.9026
20	-10.6056	20.0307	-4.0752	-1.4963	25.0648	24.8110
21	-12.8435	20.8238	-4.9406	-1.7614	26.9653	27.3762
22	-10.1033	21.1819	-3.5327	-2.0631	25.6894	25.4481
23	-13.1408	21.1994	-5.1295	-2.0765	27.1342	31.6701
24	-9.9001	21.4392	-3.3770	-1.7854	26.1769	25.8927
Loopk_k =		4 ← 4 th k point				
Level	exc (LDA)	eps (LDA)	xg (Fock)	slf (GWA)	QP (GWA)	
RQP (GWA)						
11	-13.0183	-0.1540	-11.0104	0.2411	2.0950	2.0010
12	-12.8860	-0.1222	-10.7549	0.2705	2.2794	2.1564
13	-12.0066	4.8609	-8.4205	-0.6393	7.8077	7.6061
* 14	-12.0066	4.8609	-8.4268	-0.6721	7.7687	7.5192
15	-9.8662	8.3105	-4.7862	-1.1606	12.2298	11.9727
16	-9.7821	8.4394	-4.6809	-1.1840	12.3566	12.1026
17	-12.7190	18.1271	-5.1187	-1.8360	23.8914	23.8229
18	-12.7190	18.1271	-5.1221	-1.8381	23.8860	23.0833
19	-10.6056	20.0307	-4.1844	-1.4100	25.0419	24.3069
20	-10.6056	20.0307	-4.2006	-1.3917	25.0440	24.0893
21	-12.8435	20.8238	-4.9326	-1.7149	27.0198	27.6593
22	-10.1033	21.1819	-3.5299	-2.0408	25.7145	25.3951
23	-13.1408	21.1994	-5.1098	-2.0905	27.1399	31.9630
24	-9.9001	21.4392	-3.3351	-1.8902	26.1140	27.5615