

# TOMBO Ver.2 tutorial

## How to use all-electron mixed basis program TOMBO Ver.2

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TOMBO Group

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

### Basic usage

Install TOMBO Ver.2 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+BSE, Si\_LDA, CO2+2H\_MD, Si\_GW directories.  
(These are the same as Li2\_GW, Si, CO2+2H, Si\_GW in Tutorial INPUT files Download)

Type TOMBO and press the “ENTER” key.

For multicore PC (e.g. 2 cores), type TOMBO -np 2 or TOMBO /np 2

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 Li<sub>2</sub> cluster is selected as a target system.

Method:

By beginning with LDA, TOMBO calculate quasiparticle spectra by the on-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  $a_1$  in [Å].  $a_1$  should be normalized to 1:  $|a_1| = 1$ 
    0.000000000000000    0.7071067811865    0.7071067811865 ←  $a_1$ 
    0.7071067811865    0.000000000000000    0.7071067811865 ←  $a_2$ 
    0.7071067811865    0.7071067811865    0.000000000000000 ←  $a_3$ 
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])
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: Conjugate Gradient, etc. (now under test, coming soon!)
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   =  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   =   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).
iMIX  =  2     ! 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).
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 1<sup>st</sup> step in the dynamics Loop).  
iCry = 0 ! Cluster Calculation (Crystal OFF)  
Frag to calculate crystal calculation (0 for cluster calculation, 1 for crystal calculation).  
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 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	Renormalized QP energy
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
<b>energy (eV)</b>	<b>singlet exciton</b>	<b>triplet exciton</b>

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.

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 (SPOINT.inp) and band structure calculations at the k-points (KPOINT.inp) on symmetry lines 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)
 3.8395900000 ← 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)
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).
isphcut  = 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).
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)
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).
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).
iFTapp   = 0       ! approximation for 3D > 1D Fourier Transformation
Frag to approximate 3D to 1D Fourier Transformation
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 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	← 1 <sup>st</sup> $k$ point and weight
0.2500000	0.2500000	-0.2500000	3.00	← 2 <sup>nd</sup> $k$ point and weight

## How to set KPOINT.inp

Give  $k$  points (on symmetry lines) for energy-band outputs: “band\_0001.out”, “band\_0002.out”, ...

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 0 0 ← numbers of  $k$  points (the first number) is meaningful within LDA band structure calculation, but the second and third numbers( ,0 ,0 ) is anyway required.

0.500000000	0.250000000	0.750000000	0.1176470588	← 1 <sup>st</sup> $k$ point and weight
0.500000000	0.333333333	0.666666666	0.0588235294	← 2 <sup>nd</sup> $k$ point and weight

...

(weight is meaningless in the LDA calculation and “out”-only  $k$  points, but should be given.)

## How to look at output data

band\_0001.out energy eigenvalues (at sequential  $k$  points) in the 1<sup>st</sup> band  
band\_0001.out energy eigenvalues (at sequential  $k$  points) in the 2<sup>nd</sup> band

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

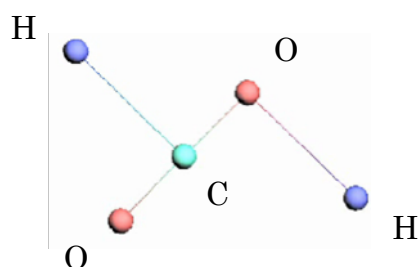


### Tutorial 3.

#### First-principles molecular dynamics (MD) simulation

Purpose:

Here we perform a standard first-principles MD simulation to produce formic acid from carbon dioxide by introducing two hydrogen atoms;  $\text{CO}_2 + 2\text{H} \rightarrow \text{HCOOH}$ .



Method:

Force acting on each atom is calculated within LDA of density functional theory (DFT). According to Born-Oppenheimer's adiabatic approximation, Newtonian equation of motion is discretized in time by using Verlet algorithm to update nuclear positions.

#### How to set COORDINATES.inp

```
P3HT_monomer
  5.500000000000000
  1.0000000000000000  0.0000000000000000  0.0000000000000000
  0.0000000000000000  1.0000000000000000  0.0000000000000000
  0.0000000000000000  0.0000000000000000  1.0000000000000000
  5
Cartesian ← give Cartesian coordinates of atomic positions in units of [Å]
C      -0.0288675  -0.0288675  -0.0288675 ← 1st atomic species and coordinates
O       0.6639528   0.6639528   0.6639528 ← 2nd atomic species and coordinates
O      -0.7216878  -0.7216878  -0.7216878 ← 3rd atomic species and coordinates
H       1.7246130   0.6639528   0.3967074 ← 4th atomic species and coordinates
H      -1.0895277  -0.0288675   1.1183952 ← 5th atomic species and coordinates
modify_rct = 0 ← Set rct (radius of atomic sphere) at half of bond length (0: NO, 1: YES)
dTime      = 0.1 ! 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=CO2+2H          ← name of the target system (arbitrary)
iApp=MWNN              ! M for MD (Force Calculation ON)
  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.
  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   =   8           ! 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 = 13.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    =   0           ! number of core states fixed in correlation/TDDFT
  Number of core states to be eliminated from Correlation or Adiabatic LDA calculations.
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.
nol    =  80           ! number of levels
  Number of states to be included in Correlation calculations (Polarization and Self-Energy).
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 = 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   =  1           ! 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)
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 = 0.80       ! 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      =    2      ! 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).
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     =    1      ! 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).
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).
iFTapp    =    0      ! approximation for 3D > 1D Fourier Transformation
                Frag to approximate 3D to 1D Fourier Transformation
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 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,  $\Sigma_c$  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 ( $\Sigma_x$ ) and correlation ( $\Sigma_c$ ) 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.)

```
Si          ← 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)
END_PARA    ← Always necessary at the end
```

How to set INPUT.inp

```
SYSTEM=Si2          ← name of the target system (arbitrary)
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 = 3          ! 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 = 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  
nog = 8 ! 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 = 3 ! 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 = 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 = 10 ! 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<sub>up</sub> - N<sub>down</sub>)  
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).  
isphcut = 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 = 0 ! frag for Total Energy calculation : OFF  
Flag to calculate LDA Total Energy (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).  
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 1<sup>st</sup> 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).  
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).

```

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).
iFTapp  =   0   ! approximation for 3D > 1D Fourier Transformation
           Frag to approximate 3D to 1D Fourier Transformation
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 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 Cartesian coordinates
              (Cartesian : give coefficients for  $2\pi/a$  in Cartesian coordinates)
              (BCC : give coefficients for  $2\pi/A$  ( $A=2a/\sqrt{3}$ ) in Cartesian coordinates)
              (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 Cartesian coordinates  
(Cartesian : give coefficients for  $2\pi/a$  in Cartesian coordinates)  
(BCC : give coefficients for  $2\pi/A$  ( $A=2a/\sqrt{3}$ ) in Cartesian coordinates)  
(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 / ( $\Gamma$  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	← 1 <sup>st</sup> $q$ point and weight
1.0000000	0.0000000	0.0000000	5.00	← 2 <sup>nd</sup> $q$ point and weight
1.0000000	1.0000000	0.0000000	1.00	← 3 <sup>rd</sup> $q$ 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
      <μxc> LDA eigenvalue <Σx> Correlation <Σc> QP energy Renormalized
Na 2 exc(LDA) eps(LDA) xg(Fock) slf(GWA) QP(GWA) QP energy
      ...
Loopk_q = 3 Loopk_k = 4
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 <sup>st</sup> k point			Correlation	Renormalized	
Level	$\langle \mu_{xc} \rangle$ exc (LDA)	LDA eigenvalue eps (LDA)	$\langle \Sigma_x \rangle$ xg (Fock)	$\langle \Sigma_c \rangle$ slf (GWA)	QP energy QP (GWA)	QP energy 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 <sup>nd</sup> k point				
Level	exc (LDA)	eps (LDA)	xg (Fock)	slf (GWA)	QP (GWA)	
11	-13.0183	-0.1540	-10.6793	-0.1316	2.0534	
12	-12.8860	-0.1222	-10.6104	0.3196	2.4730	
13	-12.0066	4.8609	-8.7334	-0.4609	7.6733	
* 14	-12.0066	4.8609	-8.7334	-0.4505	7.6836	
15	-9.8662	8.3105	-3.9148	-1.2613	13.0006	
16	-9.7821	8.4394	-3.8677	-1.3823	12.9714	
17	-12.7190	18.1271	-5.0681	-2.5965	23.1815	
18	-12.7190	18.1271	-5.0681	-2.5712	23.2068	
19	-10.6056	20.0307	-4.7897	-1.3743	24.4723	
20	-10.6056	20.0307	-4.7897	-1.3959	24.4507	
21	-12.8435	20.8238	-4.9520	-2.0276	26.6877	
22	-10.1033	21.1819	-3.3278	-2.8844	25.0731	
23	-13.1408	21.1994	-5.1505	-2.2295	26.9601	
24	-9.9001	21.4392	-3.2032	-2.2563	25.8799	

Loopk_k =		3 ← 3 <sup>rd</sup> k point				
Level	exc (LDA)	eps (LDA)	xg (Fock)	slf (GWA)	QP (GWA)	
11	-13.0183	-0.1540	-11.0691	0.2827	2.0778	
12	-12.8860	-0.1222	-10.8682	0.3149	2.2105	
13	-12.0066	4.8609	-8.3610	-0.7003	7.8062	
* 14	-12.0066	4.8609	-8.3610	-0.7051	7.8014	
15	-9.8662	8.3105	-4.9854	-1.0784	12.1128	
16	-9.7821	8.4394	-4.8688	-1.1035	12.2492	
17	-12.7190	18.1271	-5.1236	-1.9281	23.7944	
18	-12.7190	18.1271	-5.1236	-1.9236	23.7989	
19	-10.6056	20.0307	-4.0752	-1.4995	25.0616	
20	-10.6056	20.0307	-4.0752	-1.4963	25.0648	
21	-12.8435	20.8238	-4.9406	-1.7614	26.9653	
22	-10.1033	21.1819	-3.5327	-2.0631	25.6894	
23	-13.1408	21.1994	-5.1295	-2.0765	27.1342	



Level	exc (LDA)	eps (LDA)	xg (Fock)	slf (GWA)	QP (GWA)
24	-9.9001	21.4392	-3.3770	-1.7854	25.8927
Loopk_k = 4 ← 4 <sup>th</sup> k point					
RQP (GWA)					
11	-13.0183	-0.1540	-11.0104	0.2411	2.0010
12	-12.8860	-0.1222	-10.7549	0.2705	2.1564
13	-12.0066	4.8609	-8.4205	-0.6393	7.6061
* 14	-12.0066	4.8609	-8.4268	-0.6721	7.5192
15	-9.8662	8.3105	-4.7862	-1.1606	11.9727
16	-9.7821	8.4394	-4.6809	-1.1840	12.1026
17	-12.7190	18.1271	-5.1187	-1.8360	23.8229
18	-12.7190	18.1271	-5.1221	-1.8381	23.0833
19	-10.6056	20.0307	-4.1844	-1.4100	24.3069
20	-10.6056	20.0307	-4.2006	-1.3917	24.0893
21	-12.8435	20.8238	-4.9326	-1.7149	27.6593
22	-10.1033	21.1819	-3.5299	-2.0408	25.3951
23	-13.1408	21.1994	-5.1098	-2.0905	31.9630
24	-9.9001	21.4392	-3.3351	-1.8902	27.5615