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## Alpha-AlF<sub>3</sub>

**Exercise :** Determine the <sup>27</sup>Al C<sub>q</sub> value and the Al and F shieldings.

α-AlF<sub>3</sub> crystallizes in the trigonal R -3c space group.

a = b = 4.9305 Å; c = 12.4462 Å

α = β = 90°; γ = 120°

The unit cell contains two independent atoms (1 Al and 1 F) with 6 formula units (AlF<sub>3</sub>) per unit cell (Z=6). AlF<sub>6</sub> octahedron units are linked together by corner sharing. As the conventional unit cell is non-primitive, the primitive rhombohedral one is used for the calculation. It saves a lot of computational time !

We suggest you to use VESTA for generation the POSCAR file from the AlF<sub>3</sub>.cif file. In the standard export procedure, the POSCAR file is generated with the conventional unit cell (non primitive R-cell with 24 atoms inside). Ask VESTA to reduce to unit cell to the primitive one. You will then have only 8 atoms in the POSCAR file.

In this exercise one wants first to calculate the EFG tensor components of <sup>27</sup>Al. This is very fast task calculated at the end of the first SCF calculation (ground state property). The experimental values for the C<sub>q</sub> is 0.21 MHz. The nuclear quadrupolar momentum used to transform EFG in C<sub>q</sub> is Q = 14.66 10<sup>-30</sup> m<sup>2</sup> (see the paper of Sadoc *et al.* (<http://www.sciencedirect.com/science/article/pii/S0926204014000022>)) (Fluorine has a 1/2 nuclear spin, so Q is zero)

In a second step one wants to calculate the shielding parameters for Al and F. This is done using the linear response using the GIPAW formalism. As the calculation is quite time consuming, only very few k-points and small ENCUT are used with standard PAW data sets. The calculated shielding tensors components can be compared to the ones obtained by Sadoc *et al.*

### ■ INCAR

```
SYSTEM      = Al F3
GGA        = PE
ISTART     = 1
ICHARG    = 0
INIWAV    = 1
LREAL      = AUTO
ISYM       = 2
ISPIN      = 1
```

### Ionic minimisation

```
NSW        = 0
ISIF       = 2
IBRION    = 2
```

1. EDIFFG = -2E-2

```
POTIM     = 0.1
```

### Electronic minimisation

```
IALGO     = 38
LWAVE     = .TRUE.
EMIN      = -20.0
EMAX      = 10.0
NEDOS    = 1601
```

### EFG Calculation

```
LEFG      = .TRUE.
QUAD_EFG = 146.6 0.0
```

### Chemical Shift

```
PREC      = Normal # nice
ENCUT    = 400.0 # typically higher cutoffs than usual are needed
ISMEAR = 0; SIGMA= 0.1 # no fancy smearings, SIGMA sufficiently small
EDIFF    = 1E-9 # you'd need much smaller EDIFFs.
LCHIMAG  = .TRUE. # to switch on linear response for chemical shifts
DQ       = 0.001 # often the default is sufficient
ICHIBARE = 1 # often the default is sufficient
LNMR_SYM_RED = .TRUE. # be on the safe side
NLSPLINE = .TRUE. # only needed if LREAL is NOT set.
LREAL    = A # helps for speed for large systems, not needed
NBANDS   = 25 # to save memory, ??? = NELECT/2
```

## ■ KPOINTS

```
automatic mesh
0
Auto
20
```

## ■ POSCAR

```
AI1 F3
1.0
 4.9305000305    0.0000000000    0.0000000000
 2.4652500153    4.2699382798    0.0000000000
 2.4652650832    1.4233214594    4.1486879977
AI   F
2   6
Direct
 0.0000000000    0.5000000000    0.0000000000
 0.5000000000    0.0000000000    0.5000000000
 0.177499995    0.2500000000    0.7500000000
 0.822499990    0.7500000000    0.2500000000
 0.677500010    0.322499990    0.2500000000
 0.322499990    0.677500010    0.7500000000
 0.2500000000    0.177499995    0.2500000000
 0.7500000000    0.822499990    0.7500000000
```

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## Alpha-SiO<sub>2</sub>

**Exercise :** Determine the <sup>17</sup>O C<sub>q</sub> value and the Si and O shieldings.

α-SiO<sub>2</sub> crystallizes in the trigonal P3<sub>1</sub>2 space group.

a = b = 4.604 Å; c = 5.207 Å

α = β = 90°; γ = 120°

The unit cell contains two independent atoms (1 Si and 1 O) with 3 formula units (SiO<sub>2</sub>) per unit cell (Z=3). SiO<sub>4</sub> tetrahedron units are linked together by corner sharing.

In this exercise one wants first to calculate the EFG tensor components of <sup>17</sup>O. This is very fast task calculated at the end of the first SCF calculation (ground state property). The experimental values for the C<sub>q</sub> is 5.19 MHz. The nuclear quadrupolar momentum used to transform EFG in C<sub>q</sub> is Q = 2.55 10<sup>-30</sup> m<sup>2</sup> (see the paper of Profeta *et al.* (<http://pubs.acs.org/doi/abs/10.1021/ja027124r>) (Silicon has a 1/2 nuclear spin, so Q is zero)

In a second step one wants to calculate the shielding parameters for Si and O. This is done using the linear response using the GIPAW formalism. As the calculation is quite time consuming, only very few k-points and small ENCUT are used with standard PAW data sets. The calculated shielding tensors components can be compared to the ones obtained by Profeta *et al.*

### ■ INCAR

```
SYSTEM      = Si O2
GGA        = PE
ISTART     = 1
ICHARG     = 0
INIWAV     = 1
LREAL       = AUTO
ISYM        = 2
ISPIN       = 1
```

### Ionic minimisation

```
NSW        = 0
ISIF       = 2
IBRION     = 2
```

### 1. EDIFFG = -2E-2

```
POTIM      = 0.1
```

### Electronic minimisation

```
IALGO      = 38
LWAVE      = .TRUE.
EMIN       = -20.0
EMAX       = 10.0
NEDOS      = 1601
```

### EFG Calculation

```
LEFG       = .TRUE.
QUAD_EFG   = 0.0 25.5
```

### Chemical Shift

```
PREC      = Normal # nice
ENCUT    = 400.0 # typically higher cutoffs than usual are needed
ISMEAR = 0; SIGMA= 0.1 # no fancy smearings, SIGMA sufficiently small
EDIFF    = 1E-9 # you'd need much smaller EDIFFs.
LCHIMAG  = .TRUE. # to switch on linear response for chemical shifts
DQ       = 0.001 # often the default is sufficient
ICHIBARE = 1 # often the default is sufficient
LNMR_SYM_RED = .TRUE. # be on the safe side
NLSPLINE = .TRUE. # only needed if LREAL is NOT set.
LREAL    = A # helps for speed for large systems, not needed
NBANDS   = 30 # to save memory, ??? = NELECT/2
```

### ■ KPOINTS

```
automatic mesh
0
Auto
```

■ POSCAR

```
O2 Si1
1.000000000000000
4.6040000915999997 0.000000000000000 0.000000000000000
-2.3020000457999998 3.987181038300001 0.000000000000000
0.000000000000000 0.000000000000000 5.206999778700002
Si O
3 6
Direct
0.4436617824484789 -0.000000000000000 0.333333429999996
-0.000000000000000 0.4436617824484789 0.666666687000029
0.5563382175515210 0.5563382175515210 -0.000000000000000
0.3926661416221499 0.3062177364999842 0.2428214976299141
0.6937822635000156 0.0864484051221655 0.5761548406299137
0.9135515948778347 0.6073338583778505 0.9094881546299145
0.3062177364999842 0.3926661416221499 0.7571785323700884
0.0864484051221655 0.6937822635000156 0.4238451593700863
0.6073338583778505 0.9135515948778347 0.0905118383700884
```

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# At and mol further

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- How does the energy change when one decreases `SIGMA` to 0.001 in the `INCAR` file starting from the `O_atom`? Why?
- Try to copy `CONTCAR` to `POSCAR` after running the example `O_dimer`. Why is the calculation so fast?
- Try to play with the parameter `POTIM` for the example `O_dimer`. What is the optimal value?
- What is the reason for the imaginary frequency in the example `CO_vibration`? Does the behaviour improve when the step width (smaller or larger) is changed? Also try to improve the precision to which the ground state is converged (`EDIFF=1E-5`). What happens if the accuracy of the calculations is improved (`PREC=Accurate`)).
- Try to use the conjugate gradient algorithm to the `H2O` molecule (example `H2O`).
- Calculate the vibrational frequencies of the `H2O` molecule (example `H2O`) after relaxation (example `H2Ovib`). Why does one find 3 modes that have small frequencies? Try `EDIFF=1E-5` instead of `EDIFF=1E-4`.

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# Bandgap of Si in GW

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 > Equilibrium volume of Si in the RPA > List of tutorials

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## Task

Calculation of the bandgap of Si using various flavours of GW.

**Mind:** before you start doing GW calculations it might be beneficial to have a look at the examples on the [description of dielectric properties](#).

To do GW calculations we have to follow a 3-step procedure.

### Step 1: a DFT groundstate calculation

Everything starts with a standard DFT groundstate calculation (in this case PBE).

- [INCAR](#) (see INCAR.DFT)

```
ISMEAR = 0
SIGMA = 0.05
EDIFF = 1E-8
```

- [KPOINTS](#) (see KPOINTS.6)

```
6x6x6
0
G
6 6 6
0 0 0
```

or to save some time use a "quick-and-dirty" setup (take KPOINTS.4):

```
4x4x4
0
G
4 4 4
0 0 0
```

- [POSCAR](#)

```
system Si
5.430
0.5 0.5 0.0
0.0 0.5 0.5
0.5 0.0 0.5
2
cart
0.00 0.00 0.00
0.25 0.25 0.25
```

### Step 2: obtain DFT virtual orbitals

To obtain a [WAVECAR](#) file with a reasonable number of virtual orbitals (50-100 per atom) we need to restart from the previous groundstate calculation with [ALGO=Exact](#), and manually set the number of bands by means of the [NBANDS](#)-tag. To obtain the corresponding [WAVEDER](#) file we additionally specify [LOPTICS=.TRUE..](#)

- [INCAR](#) (see INCAR.DIAG)

```
ALGO = Exact
NBANDS = 64
LOPTICS = .TRUE. ; CSHIFT = 0.1
NEDOS = 2000
# you might try
```

```
#LPEAD = .TRUE.
```

```
ISMEAR = 0  
SIGMA = 0.05  
EDIFF = 1E-8
```

**Mind:** make a copy of your [WAVECAR](#) and [WAVEDER](#) files, as we will repeatedly need them in the following. For instance

```
cp WAVECAR WAVECARLOPTICS  
cp WAVEDER WAVEDERLOPTICS
```

### Step 3: the actual GW calculation

Restart from the [WAVECAR](#) and [WAVEDER](#) files of the previous calculation, with

- [INCAR](#) (see [INCAR.GW](#))

```
# Frequency dependent dielectric tensor including  
# local field effects within the RPA (default) or  
# including changes in the DFT xc-potential (LRPA=.FALSE.).  
# N.B.: beware one first has to have done a  
# calculation with ALGO=Exact, LOPTICS=.TRUE.  
# and a reasonable number of virtual states (see above)  
ALGO = GW0 ; LSPECTRAL = .TRUE. ; NOMEGA = 50  
  
# be sure to take the same number of bands as for  
# the LOPTICS=.TRUE. calculation, otherwise the  
# WAVEDER file is not read correctly  
NBANDS = 64  
  
# Add this to update the quasiparticle energies  
# in the Green's function (GW0)  
#NELM = 4  
  
ISMEAR = 0  
SIGMA = 0.05  
EDIFF = 1E-8
```

At the bottom of the [OUTCAR](#) file you will find the quasi-particle (QP) energies.

```
QP shifts <psi_nk| G(iteration)W_0 |psi_nk>: iteration 1  
for sc-GW calculations column KS-energies equals QP-energies in previous step  
and V_xc(KS)= KS-energies - (<T + V_ion + V_H > + <T+V_H+V_ion>^1 + <V_x>^1)
```

```
k-point 1 : 0.0000 0.0000 0.0000  
band No. KS-energies QP-energies sigma(KS) V_xc(KS) V^pw_x(r,r') Z occupation
```

1	-6.4888	-6.8243	-10.9766	-10.4570	-17.5189	0.6458	2.0000
2	5.4800	5.1162	-11.8859	-11.4060	-12.7290	0.7580	2.0000
3	5.4800	5.1162	-11.8859	-11.4060	-12.7290	0.7580	2.0000
4	5.4800	5.1162	-11.8859	-11.4060	-12.7290	0.7580	2.0000
5	8.0443	8.3296	-9.7235	-10.1038	-5.7364	0.7502	0.0000
6	8.0443	8.3296	-9.7235	-10.1038	-5.7364	0.7502	0.0000
7	8.0443	8.3296	-9.7235	-10.1038	-5.7364	0.7502	0.0000
8	8.8407	9.2475	-10.5130	-11.0594	-6.0662	0.7445	0.0000

```
k-point 2 : 0.1667 0.0000 0.0000  
band No. KS-energies QP-energies sigma(KS) V_xc(KS) V^pw_x(r,r') Z occupation
```

1	-6.1276	-6.4734	-11.0208	-10.4905	-17.3978	0.6521	2.0000
2	3.0946	2.6991	-11.4452	-10.9063	-13.1354	0.7340	2.0000
3	5.0279	4.6595	-11.7159	-11.2282	-12.6625	0.7552	2.0000
4	5.0279	4.6595	-11.7159	-11.2282	-12.6625	0.7552	2.0000
5	7.8309	8.1065	-9.8441	-10.2097	-5.8680	0.7539	0.0000
6	8.6943	8.9816	-9.8669	-10.2533	-5.6768	0.7436	0.0000
7	8.6943	8.9816	-9.8669	-10.2533	-5.6768	0.7436	0.0000
8	10.9341	11.2678	-10.4716	-10.9278	-5.5632	0.7316	0.0000

.. .. .. .. .. .. .. ..  
.. .. .. .. .. .. .. ..  
.. .. .. .. .. .. .. ..  
.. .. .. .. .. .. .. ..

```
k-point 16 : -0.3333 0.5000 0.1667  
band No. KS-energies QP-energies sigma(KS) V_xc(KS) V^pw_x(r,r') Z occupation
```

1	-2.2240	-2.5911	-11.4857	-10.9550	-16.0663	0.6917	2.0000
2	-2.2240	-2.5911	-11.4857	-10.9550	-16.0663	0.6917	2.0000
3	1.8279	1.3698	-10.7735	-10.1380	-12.9637	0.7209	2.0000
4	1.8279	1.3698	-10.7735	-10.1380	-12.9637	0.7209	2.0000
5	8.2346	8.4128	-9.3111	-9.5472	-5.1975	0.7546	0.0000
6	8.2346	8.4128	-9.3111	-9.5472	-5.1975	0.7546	0.0000
7	12.2605	12.5170	-9.7969	-10.1486	-4.3607	0.7294	0.0000
8	12.2605	12.5170	-9.7969	-10.1486	-4.3607	0.7294	0.0000

To quickly find the QP-energy of the highest lying occupied state, try

```
./gap_GW.sh OUTCAR
```

## Beyond the random-phase-approximation

To include local field effects beyond the random-phase-approximation in the description of the frequency dependent dielectric response function (local field effects in DFT) add the following line to your [INCAR](#) file:

```
LRPA = .FALSE.
```

and again restart from the [WAVECAR](#) and [WAVEDER](#) files from step 2.

## Beyond $G_0W_0$ : $GW_0$

The most usual step beyond single-shot GW ( $G_0W_0$ ) is to iterate the quasi-particle energies in the Greens functions. This is the socalled  $GW_0$  approximation. To have VASP do, for instance, 4 iterations of the QP-energies in G, add the following line to the [INCAR](#) file:

```
NELM = 4
```

and again restart from the [WAVECAR](#) and [WAVEDER](#) files from step 2.

To quickly find the QP-energy of the highest lying occupied state after 4 iterations of the QP energies in G, type:

```
./gap_GW.sh OUTCAR
```

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# Bandgap of Si using different DFT+HF methods

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  - 2.4 Calculation
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## Task

Calculation of the band gap in Si using different DFT+HF schemes (PBE, B3LYP, PBE0, HSE06, and HF).

## Input

### POSCAR

```
System: Si
5.430
0.5 0.5 0.0
0.0 0.5 0.5
0.5 0.0 0.5
1
Cartesian
0 0 0
0.25 0.25 0.25
```

### INCAR

```
## Better preconverge with PBE first
## and use the WAVECAR file as inout for the DFT+HF calculation

## Selects the B3LYP hybrid function
#LHFCALC = .TRUE. ; GGA = B3 ; AEXX = 0.2 ; AGGAX = 0.72
#AGGAC = 0.81 ; ALDAC = 0.19
#ALGO = D ; TIME = 0.4

## Selects the PBE0 hybrid function
#LHFCALC = .TRUE. ;
#ALGO = D ; TIME = 0.4

## Selects the HSE06 hybrid function
#LHFCALC = .TRUE. ; HFSCREEN = 0.2 ;
#ALGO = D ; TIME = 0.4

## Selects HF
#LHFCALC = .TRUE. ; AEXX = 1.0 ; ALDAC = 0.0 ; AGGAC = 0
#ALGO = D ; TIME = 0.4

## Leave this in
ISMEAR = 0
SIGMA = 0.01
GGA = PE
```

### KPOINTS

```
k-points
0
Gamma
6 6 6
0 0 0
```

## Calculation

- script to extract eigenvalues and calculate the bandgap

```
homo=`awk '/NELECT/ {print $3/2}' $1`  

lumo=`awk '/NELECT/ {print $3/2+1}' $1`  

nkpt=`awk '/NKPTS/ {print $4}' $1`  

e1=`grep " $homo " $1 | head -$nkpt | sort -n -k 2 | tail -1 | awk '{print $2}'`
```

```
e2=`grep "    $lumo    " $1 | head -$nkpt | sort -n -k 2 | head -1 | awk '{print $2}'  
echo "HOMO: band:" $homo " E=" $e1  
echo "LUMO: band:" $lumo " E=" $e2
```

type

```
./gap.sh OUTCAR
```

■ README.txt

For each HF+DFT method (B3LYP, PBE0, HSE06, and HF) compute the bandgap of Si adopting the following procedure:

- i) Perform a standard PBE calculation
- ii) Perform a HF+DFT run (VASP reads in the WAVECAR from run (i))
- iii) Calculate the value of the bandgap by running the script 'gap':  
$$\text{bandgap} = \min(\text{cband}) - \max(\text{vband})$$

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# Bandstructure of Si in GW (VASP2WANNIER90)

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  - 5.2 Obtain bandstructure (Wannier interpolation)
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## Task

Calculation of the bandstructure of Si in GW using the VASP2WANNIER90 interface.

**Mind:** The procedure to compute bandstructure in GW using V2W is almost identical to the corresponding HSE one described in [Si bandstructure](#).

**Mind:** The standard procedure for GW calculations is described in [Bandgap of Si in GW](#).

## Step 1: a DFT groundstate calculation

Everything starts with a standard DFT groundstate calculation (in this case PBE).

- INCAR

```
ISMEAR = 0
SIGMA = 0.05
GGA = PE
```

- KPOINTS

```
4x4x4
0
G
4 4 4
0 0 0
```

- POSCAR

```
system Si
5.430
0.5 0.5 0.0
0.0 0.5 0.5
0.5 0.0 0.5
2
cart
0.00 0.00 0.00
0.25 0.25 0.25
```

## Step 2: obtain DFT virtual orbitals

To obtain a [WAVECAR](#) file with a reasonable number of virtual orbitals (50-100 per atom) we need to restart from the previous groundstate calculation with [ALGO=Exact](#), and manually set the number of bands by means of the [NBANDS](#)-tag. To obtain the corresponding [WAVEDER](#) file we additionally specify [LOPTICS=.TRUE.](#).

- INCAR

```
ALGO = Exact
NBANDS = 64
LOPTICS = .TRUE.
NEDOS = 2000

ISMEAR = 0
SIGMA = 0.05
GGA = PE
```

## Step 3: GW calculation including LWANNIER90 TAG

Restart from the [WAVECAR](#) and [WAVEDER](#) files of the previous calculation, with

■ [INCAR](#)

```
## Frequency dependent dielectric tensor including
## local field effects within the RPA (default) or
## including changes in the DFT xc-potential (LRPA=.FALSE.).
## N.B.: beware one first has to have done a
## calculation with ALGO=Exact and LOPTICS=.TRUE..
## and a reasonable number of virtual states (see above)
ALGO = GW0 ; LSPECTRAL = .TRUE. ; NOMEGA = 50
#LRPA = .FALSE.
## be sure to take the same number of bands as for
## the LOPTICS=.TRUE. calculation, otherwise the
## WAVEDER file is not read correctly
NBANDS = 64
##VASP2WANNIER90
LWANNIER90=.TRUE.
```

Use the wannier90.win file given below which contains all instructions needed to generate the necessary input files for the WANNIER90 runs (wannier90.amn, wannier90.mmn, wannier90.eig).

■ [wannier90.win](#)

```
num_wann=8
num_bands=8

exclude_bands 9-64

Begin Projections
Si:sp3
End Projections

dis_froz_max=9
dis_num_iter=1000

guiding_centres=true

# Bandstructure plot
#restart = plot
#bands_plot = true
#begin kpoint_path
#L 0.50000 0.50000 0.50000 G 0.00000 0.00000 0.00000
#G 0.00000 0.00000 0.00000 X 0.50000 0.00000 0.50000
#X 0.50000 0.00000 0.50000 K 0.37500 -0.37500 0.00000
#K 0.37500 -0.37500 0.00000 G 0.00000 0.00000 0.00000
#end kpoint_path
#bands_num_points 40
#bands_plot_format gnuplot xmGrace

begin unit_cell_cart
    2.7150000 2.7150000 0.0000000
    0.0000000 2.7150000 2.7150000
    2.7150000 0.0000000 2.7150000
end unit_cell_cart

begin atoms_cart
Si 0.0000000 0.0000000 0.0000000
Si 1.3575000 1.3575000 1.3575000
end atoms_cart

mp_grid = 4 4 4

begin kpoints
    0.0000000 0.0000000 0.0000000
    0.2500000 0.0000000 0.0000000
    0.5000000 0.0000000 0.0000000
    0.2500000 0.2500000 0.0000000
    0.5000000 0.2500000 0.0000000
    -0.2500000 0.2500000 0.0000000
    0.5000000 0.5000000 0.0000000
    -0.2500000 0.5000000 0.2500000
    0.0000000 0.2500000 0.0000000
    0.0000000 0.0000000 0.2500000
    -0.2500000 -0.2500000 -0.2500000
    -0.2500000 0.0000000 0.0000000
    0.0000000 -0.2500000 0.0000000
    0.0000000 0.0000000 -0.2500000
    0.2500000 0.2500000 0.2500000
    0.0000000 0.5000000 0.0000000
    0.0000000 0.0000000 0.5000000
    -0.5000000 -0.5000000 -0.5000000
    0.0000000 0.2500000 0.2500000
    0.2500000 0.0000000 0.2500000
    -0.2500000 -0.2500000 0.0000000
    -0.2500000 0.0000000 -0.2500000
    0.0000000 -0.2500000 -0.2500000
    0.0000000 0.5000000 0.2500000
    0.2500000 0.0000000 0.5000000
    -0.2500000 -0.2500000 0.2500000
    -0.5000000 -0.2500000 -0.5000000
    0.2500000 0.5000000 0.0000000
    0.2500000 -0.2500000 -0.2500000
    -0.5000000 -0.5000000 -0.2500000
    0.0000000 0.2500000 0.5000000
    -0.2500000 0.2500000 -0.2500000
```

```

-0.2500000 -0.5000000 -0.5000000
0.5000000 0.0000000 0.2500000
-0.5000000 -0.2500000 0.0000000
0.0000000 -0.5000000 -0.2500000
-0.2500000 0.0000000 -0.5000000
0.2500000 0.2500000 -0.2500000
0.5000000 0.2500000 0.5000000
-0.2500000 -0.5000000 0.0000000
-0.2500000 0.2500000 0.2500000
0.5000000 0.5000000 0.2500000
0.0000000 -0.2500000 -0.5000000
0.2500000 -0.2500000 0.2500000
0.2500000 0.5000000 0.5000000
-0.5000000 0.0000000 -0.2500000
0.0000000 -0.2500000 0.2500000
0.2500000 0.0000000 -0.2500000
-0.2500000 -0.2500000 -0.5000000
0.2500000 0.5000000 0.2500000
0.2500000 -0.2500000 0.0000000
-0.5000000 -0.2500000 -0.2500000
0.2500000 0.2500000 0.5000000
0.0000000 0.2500000 -0.2500000
-0.2500000 -0.5000000 -0.2500000
0.5000000 0.2500000 0.2500000
-0.2500000 0.0000000 0.5000000
0.2500000 0.5000000 0.5000000
0.5000000 0.0000000 0.5000000
0.2500000 -0.2500000 0.5000000
0.5000000 0.2500000 -0.2500000
-0.5000000 -0.2500000 -0.7500000
0.2500000 -0.5000000 -0.2500000
-0.2500000 0.2500000 -0.5000000
end kpoints

```

## Step 4: WANNIER90

---

### Compute Wannier functions

run wannier90:

wannier90.x wannier90

This run generates the wannier90 standard output (wannier90.wout) and the file wannier90.chk needed for the wannier interpolation (next step)

### Obtain bandstructure (Wannier interpolation)

Uncomment the bandstructure plot flags in wannier90.win and rerun (restart) wannier90:

wannier90.x wannier90

This run generates the following bandstructure files which can be visualized using xmgrace or gnuplot:

wannier90\_band.agr

wannier90\_band.dat

wannier90\_band.gnu

to plot the band structure using gnuplot: `gnuplot -persist wannier90_band.gnu`

### Download

---

[Si\\_bandstructure\\_GW.tgz](#) 

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# Bandstructure of SrVO<sub>3</sub> in GW

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## Task

Calculation of the GW bandstructure of SrVO<sub>3</sub> using VASP and [WANNIER90](#).

Performing a GW calculation with VASP is a 3-step procedure: a DFT groundstate calculation, a calculation to obtain a number of virtual orbitals, and the actual GW calculation itself. In this example we will also see how the results of the GW calculation may be postprocessed with [WANNIER90](#) to obtain the dispersion of the bands along the usual high symmetry directions in reciprocal space.

**N.B.:** This example involves quite a number of individual calculations. The easiest way to run this example is to execute:

```
./doall.sh
```

And compare the output of the different steps (DFT, GW, HSE) by:

```
./plotall.sh
```

In any case, one can consider the doall.sh script to be an overview of the steps described below.

## The DFT groundstate calculation and bandstructure with wannier90

Everthing starts with a conventional DFT (in this case LDA) groundstate calculation:

- [INCAR](#) (see INCAR.DFT)

```
System = SrVO3
NBANDS = 36
ISMEAR = -5
EMIN = -20 ; EMAX = 20 ; NEDOS = 1000 # usefull energy range for density of states
EDIFF = 1E-8                      # high precision for groundstate calculation
KPAR = 2
LORBIT = 11
LWANNIER90_RUN = .TRUE.
```

Copy the aforementioned file to [INCAR](#):

```
cp INCAR.DFT INCAR
```

- [KPOINTS](#)

```
Automatically generated mesh
0
Gamma
4 4 4
0 0 0
```

**Mind:** this is definitely not dense enough for a high-quality description of SrVO<sub>3</sub>, but in the interest of speed we will live with it.

- [POSCAR](#)

```
SrVO3
3.77706 #taken from 9x9x9 with sigma=0.2 ismear=2
+1.0000000000 +0.0000000000 +0.0000000000
+0.0000000000 +1.0000000000 +0.0000000000
+0.0000000000 +0.0000000000 +1.0000000000
Sr V O
1 1 3
Direct
+0.0000000000 +0.0000000000 +0.0000000000
+0.5000000000 +0.5000000000 +0.5000000000
```

```
+0.50000000000 +0.50000000000 +0.00000000000
+0.50000000000 +0.00000000000 +0.50000000000
+0.00000000000 +0.50000000000 +0.50000000000
```

- wannier90.win (see wannier90.win.dft)

**WANNIER90** takes its input from the file [wannier90.win](#). To construct Wannier functions for the Vanadium  $t_{2g}$  manifold in SrVO<sub>3</sub>, and plot the dispersion of the associated bands along R-G-X-M, one may use the following settings:

```
bands_plot = true
begin kpoint_path
R 0.5000000 0.5000000 0.5000000 G 0.0000000 0.0000000 0.0000000
G 0.0000000 0.0000000 0.0000000 X 0.5000000 0.0000000 0.0000000
X 0.5000000 0.0000000 0.0000000 M 0.5000000 0.5000000 0.0000000
M 0.5000000 0.5000000 0.0000000 G 0.0000000 0.0000000 0.0000000
end kpoint_path
num_wann = 3
num_bands= 3
exclude_bands : 1-20, 24-36
begin projections
V:dxz;dxz;dyz
end projections
```

Copy the above to [wannier90.win](#):

```
cp wannier90.win.dft wannier90.win
```

and run vasp.

If all went well, the Vanadium  $t_{2g}$  band dispersion thus obtained, may conveniently be visualized with *gnuplot*:

```
gnuplot -persist ./wannier90_band.gnu
```

**N.B.:** Most modern versions of gnuplot will respond with an error message unless you remove the first line of wannier90\_band.gnu (some deprecated syntax issue).

**Mind:** Here the eigenvalues have been shifted such that the Fermi level is a 0 eV.

## Analysis of the DOS

In the above we have set:

```
LORBIT = 11
```

Therefore, in addition to the total density-of-states (DOS), the [DOSCAR](#) file contains blocks of information with the site-projected  $l_m$ -decomposed DOS as well. The site-projected  $l_m$ -decomposed band character is written to the [PROCAR](#) file.

To plot the total DOS and the Vanadium  $t_{2g}$  and  $e_g$  partial-DOS using *gnuplot*, execute the following command:

```
./plotdos
```

**Mind:** Check the [OUTCAR](#) file for the position of the Fermi level. These DOSs have not been shifted such that the Fermi level is at 0 eV.

## Obtain DFT virtual orbitals

- [INCAR](#) (see INCAR.DIAG)

```
System = SrVO3
#ISMEAR = -5           # does not work for LOPTICS=.TRUE.
ISMEAR = 1 ; SIGMA = 0.2
EMIN = -20 ; EMAX = 20 ; NEDOS = 1000 # usefull energy range for density of states
ALGO = Exact ; NELM = 1      # exact diagonalization one step suffices
EDIFF = 1E-8               # high precision for groundstate calculation
NBANDS = 96                 # need for a lot of bands in GW
LOPTICS = .TRUE.             # we need d phi/ d k for GW calculations
KPAR = 2
```

Copy the aforementioned file to [INCAR](#):

```
cp INCAR.DIAG INCAR
```

and restart VASP.

At this stage it is a good idea to make a safety copy of the [WAVECAR](#) and [WAVEDER](#) files since we will repeatedly need them in the calculations that follow:

```
cp WAVECAR WAVECAR.DFT.96bands
cp WAVEDER WAVEDER.DFT.96bands
```

## The dielectric function

The frequency dependent dielectric function in the independent-particle (IP) picture is written to the **OUTCAR** and **vasprun.xml** files. In the **OUTCAR** you should search for

```
frequency dependent IMAGINARY DIELECTRIC FUNCTION (independent particle, no local field effects)
```

and

```
frequency dependent REAL DIELECTRIC FUNCTION (independent particle, no local field effects)
```

To visualize the real and imaginary parts of the frequency dependent dielectric function (from the **vasprun.xml**) you may execute

```
./plotoptics2
```

## The GW calculation

- **INCAR** (see INCAR.GW0)

```
System = SrVO3
ISMEAR = -5
EMIN = -20 ; EMAX = 20 ; NEDOS = 1000 # usefull energy range for density of states
NBANDS = 96 # need for a lot of bands in GW
ALGO = GW0 #
NELM = 1 # one step so this is really G0W0
PRECFOCK = Fast # select fast mode for FFT's
ENCUTGW = 100 # energy cutoff for response function
NOMEGA = 200 # metal, we need a lot of frequency points
KPAR = 2
```

Copy the aforementioned file to **INCAR**:

```
cp INCAR.GW0 INCAR
```

and restart VASP.

## Analysis of the DOS and bandstructure with wannier90

- **INCAR** (see INCAR.NONE)

```
System = SrVO3
ISMEAR = -5
EMIN = -20 ; EMAX = 20 ; NEDOS = 1000 # usefull energy range for density of states
ALGO = None ; NELM = 1 # exact diagonalization one step suffices
NBANDS = 96 # need for a lot of bands in GW
LORBIT = 11
LWANNIER90_RUN = .TRUE.
```

Again, copy the aforementioned file to **INCAR**:

```
cp INCAR.GW0 INCAR
```

And use the following input for wannier90:

- **wannier90.win** (see wannier90.win.gw)

```
bands_plot = true
begin kpoint_path
R 0.50000000 0.50000000 0.50000000 G 0.00000000 0.00000000 0.00000000
G 0.00000000 0.00000000 0.00000000 X 0.50000000 0.00000000 0.00000000
X 0.50000000 0.00000000 0.00000000 M 0.50000000 0.50000000 0.00000000
M 0.50000000 0.50000000 0.00000000 G 0.00000000 0.00000000 0.00000000
end kpoint_path
num_wann = 3
num_bands= 3
exclude_bands : 1-20, 24-96
begin projections
V:dxy;dxz;dyz
end projections
```

and restart VASP.

If all went well, the Vanadium  $t_{2g}$  band dispersion thus obtained, may conveniently be visualized with **gnuplot**:

```
gnuplot -persist ./wannier90_band.gnu
```

**N.B.:** Most modern versions of gnuplot will respond with an error message unless you remove the first line of wannier90\_band.gnu (some deprecated syntax issue).

To plot the total DOS and the Vanadium  $t_{2g}$  and  $e_g$  partial-DOS using *gnuplot*, execute the following command:

```
./plotdos
```

**Mind:** Check the **OUTCAR** file for the position of the Fermi level. These DOSs have not been shifted such that the Fermi level is at 0 eV.

### The dielectric function

To extract the frequency dependent dielectric constant, both in the independent-particle picture as well as including local field effects (either in DFT or in the RPA) and plot the real and imaginary components using *gnuplot*, execute

```
./plotchi
```

### A comparison to the HSE hybrid functional

To illustrate the kind of results one would obtain for SrVO<sub>3</sub> using the **DFT/Hartree-Fock hybrid functional HSE**, without actually doing a full selfconsistent calculation, we will recalculate the one-electron energies and DOS (**ALGO**=Eigenval) using the HSE functional with DFT orbitals as input:

- **INCAR** (see INCAR.HSE)

```
System = SrVO3
ISMEAR = -5
EMIN = -20 ; EMAX = 20 ; NEDOS = 1000 # usefull energy range for density of states
EDIFF = 1E-8                      # high precision for groundstate calculation
KPAR = 2
LHFCAUC = .TRUE. ; HFSCREEN = 0.2 ; NBANDS = 48
PRECFOCK = Fast ; NELM = 1
ALGO = Eigenval
LWAVE = .FALSE.                   # do not write the wave functions
LORBIT = 11
LWANNIER90_RUN = .TRUE.
```

Copy the aforementioned file to **INCAR**:

```
cp INCAR.HSE INCAR
```

Use the following **WANNIER90** input:

- **wannier90.win** (see wannier90.win.hse)

```
bands_plot = true
begin kpoint_path
R 0.50000000 0.50000000 0.50000000 G 0.00000000 0.00000000 0.00000000
G 0.00000000 0.00000000 0.00000000 X 0.50000000 0.00000000 0.00000000
X 0.50000000 0.00000000 0.00000000 M 0.50000000 0.50000000 0.00000000
M 0.50000000 0.50000000 0.00000000 G 0.00000000 0.00000000 0.00000000
end kpoint_path
num_wann = 3
num_bands= 3
exclude_bands : 1-20, 24-48
begin projections
V:dxy;dxz;dyz
end projections
```

Copy the above to **wannier90.win**:

```
cp wannier90.win.hse wannier90.win
```

- **WAVECAR**

**Mind:** This calculation (and the ones following below) needs to restart from a set of converged DFT wave functions, therefore:

```
cp WAVECAR.DFT.96bands WAVECAR
```

and run **vasp**.

If all went well, the Vanadium  $t_{2g}$  band dispersion thus obtained, may conveniently be visualized with *gnuplot*:

```
gnuplot -persist ./wannier90_band.gnu
```

**N.B.:** Most modern versions of gnuplot will respond with an error message unless you remove the first line of wannier90\_band.gnu (some

deprecated syntax issue).

**Mind:** Here the eigenvalues have been shifted such that the Fermi level is a 0 eV.

To plot the total DOS and the Vanadium  $t_{2g}$  and  $e_g$  partial-DOS using *gnuplot*, execute the following command:

```
./plotdos
```

**Mind:** Check the [OUTCAR](#) file for the position of the Fermi level. These DOSs have not been shifted such that the Fermi level is at 0 eV.

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[SrVO3\\_GW\\_band.tgz](#) 

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# Beta-tin Si

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## Task

Relaxation of the internal coordinates, volume and cell shape in beta-tin Si.

## Input

### POSCAR

```
beta Sn
4.90000000000000
1.0 0.0 0.0
0.0 1.0 0.0
0.5 0.5 0.26
2
Direct
-0.125 -0.375 0.25
0.125 0.375 -0.25
```

### INCAR

```
System = beta Si
ISMEAR = 0; SIGMA = 0.1;
ENMAX = 240
IBRION=2; ISIF=3 ; NSW=15
EDIFF = 0.1E-04
EDIFFG = -0.01
```

### KPOINTS

```
k-points
0
Monkhorst Pack
11 11 11
0 0 0
```

## Calculation

This example is completely analogous to [cd Si volume relaxation](#).

## Download

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**Task**

Volume relaxtion and the calculation of the DOS and bandstructure within cubic diamond (cd) Si.

**Input****POSCAR**

```
cubic diamond
5.5
0.0 0.5 0.5
0.5 0.0 0.5
0.5 0.5 0.0
2
Direct
-0.125 -0.125 -0.125
0.125 0.125 0.125
```

- Cubic diamond Si starting lattice constant of 5.5 .
- Fcc cell.
- 2 atoms in cell.

**INCAR**

```
System = diamond Si
ISTART = 0 ; ICHARG=2
ENCUT = 240
ISMEAR = 0; SIGMA = 0.1
```

**KPOINTS**

```
k-points
0
Monkhorst Pack
11 11 11
0 0 0
```

**Calculation**

The calculation of the optimized volume. DOS and bandstructure is similar as in the examples [fcc\\_Si](#), [fcc\\_Si\\_DOS](#) and [fcc\\_Si\\_bandstructure](#), respectively.

**Volume relaxation**

- The bash-script loop.sh runs Si in the cubic diamond (cd) structure at several different lattice constants (5.1-5.7 Å) and collects free energy versus lattice constant into the file SUMMARY.dia:

```
#!/bin/bash
BIN=/path/to/your/vasp/executable
rm WAVECAR SUMMARY.dia
for i in 5.1 5.2 5.3 5.4 5.5 5.6 5.7 ; do
cat >POSCAR <<!
cubic diamond
$!
0.0 0.5 0.5
0.5 0.0 0.5
0.5 0.5 0.0
2
Direct
-0.125 -0.125 -0.125
0.125 0.125 0.125
!
echo "a= $i" ; mpirun -n 2 $BIN
```

```
E=`awk '/F=/ {print $0}' OSZICAR` ; echo $i $E >>SUMMARY.dia
done
cat SUMMARY.dia
```

- Example output of SUMMARY.dia:

```
5.2 1 F= -.10528151E+02 E0= -.10528137E+02 d E =-.274709E-04
5.3 1 F= -.10713281E+02 E0= -.10713280E+02 d E =-.218410E-05
5.4 1 F= -.10806685E+02 E0= -.10806685E+02 d E =-.114401E-06
5.5 1 F= -.10823039E+02 E0= -.10823039E+02 d E =-.429842E-08
5.6 1 F= -.10775102E+02 E0= -.10775102E+02 d E =-.204668E-09
5.7 1 F= -.10673578E+02 E0= -.10673578E+02 d E =-.112715E-10
5.8 1 F= -.10528393E+02 E0= -.10528393E+02 d E =-.552513E-11
```

- To make a quick plot of SUMMARY.dia try:

```
gnuplot
gnuplot> plot "SUMMARY.dia" using ($1):($4) w lp
```

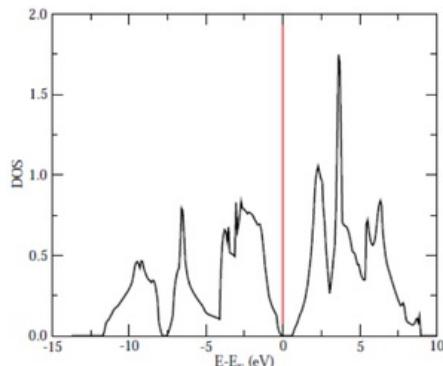
- Extracted lattice parameter should be at 5.465 .

## DOS

- Enter (approximate) volume of 5.5 into the [POSCAR](#) file.
- Change the [INCAR](#) according to DOS calculation (or use INCAR.dos):

```
System = diamond Si
ISTART = 0 ; ICHARG=2
ENCUT = 240
ISMEAR = -5
LORBIT = 11
```

- Use p4vasp or run the script *dos.sh* to calculate the DOS.
- The example DOS should look like this:

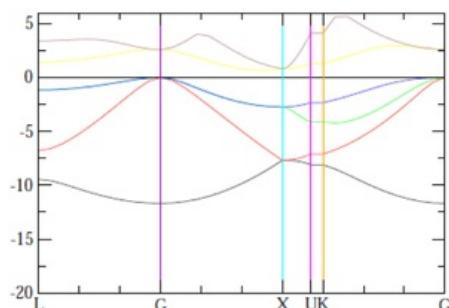


## Bandstructure

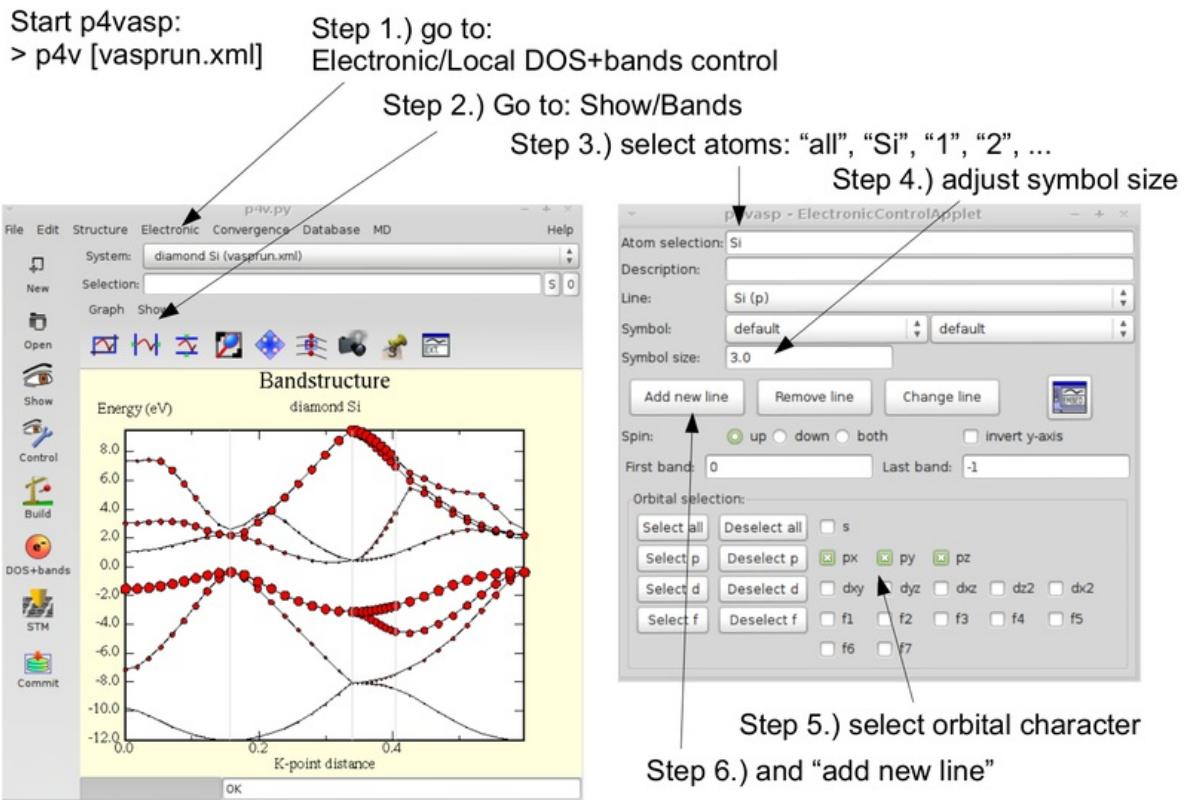
- Enter (approximate) volume of 5.5 into the [POSCAR](#) file.
- Change the [INCAR](#) according to bandstructure calculation (or use INCAR.band):

```
System = diamond Si
ISTART = 0 ; ICHARG=11
ENCUT = 240
ISMEAR = 0; SIGMA = 0.1;
LORBIT = 11
```

- Use p4vasp or run the script *band.sh* to calculate the bandstructure.
- The example bandstructure should look like this:



- For "fat" bands (or orbital character of bands) use p4vasp:



**Mind:** You will have to set the correct path to your VASP executable (i.e., BIN), and invoke VASP with the correct command (e.g., in the above: mpirun -np 2).

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# Cd Si relaxation

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## Task

Relaxation of the internal coordinates of a perturbed cd Si structure.

## Input

### POSCAR

```
cubic diamond
5.5
0.0 0.5 0.5
0.5 0.0 0.5
0.5 0.5 0.0
2
Direct
-0.125 -0.125 -0.125
0.125 0.125 0.130
```

- Break of symmetry in standard diamond structure: change z position from 0.125 to 0.130.

### INCAR

```
System = diamond Si
ISTART = 0 ; ICHARG=2
ENCUT = 240
ISMEAR = 0; SIGMA = 0.1;
NSW = 10; IBRION = 2
ISIF = 2
EDIFFG = -0.0001
```

- 10 relaxation steps ([NSW=10](#)).
- Conjugate-gradient algorithm ([IBRION=2](#)).
- Relaxation only of internal parameters ([ISIF=2](#)).

### KPOINTS

```
k-points
0
Monkhorst Pack
11 11 11
0 0 0
```

## Calculation

- Example output after 10 relaxation steps:

POSITION			TOTAL-FORCE (eV/Angst)		
4.81253	4.81253	4.81250	-0.000724	-0.000724	-0.000031
0.68747	0.68747	0.68750	0.000724	0.000724	0.000031
total drift:			0.000000	0.000000	0.000000

- Files to watch during relaxations:

- [stdout](#) (terminal): each electronic step is written to the terminal:
- [OSZICAR](#): a copy of the terminal output.
- [OUTCAR](#): more detailed information on every electronic and ionic step.

- Other important files:
  - **CONTCAR**: holds the structure of the last ionic step and at the end the structural result (also very important for restarting a relaxation).
  - **STOPCAR**: stops a relaxation.

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# Cd Si volume relaxation

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## Task

Relaxation of the internal coordinates, volume and cell shape in cd Si.

## Input

### POSCAR

```
cubic diamond
5.5
0.0 0.5 0.5
0.5 0.0 0.5
0.5 0.5 0.0
2
Direct
-0.125 -0.125 -0.125
0.125 0.125 0.125
```

### INCAR

```
System = diamond Si
ISMEAR = 0; SIGMA = 0.1;
ENMAX = 240
IBRION = 2; ISIF=3 ; NSW=15
EDIFF = 0.1E-04
EDIFFG = -0.01
```

- [IBRION=2](#) conjugate-gradient algorithm.
- [ISIF=3](#) change of internal parameter, shape and volume simultaneously.

### KPOINTS

```
k-points
0
Monkhorst Pack
1 1 1
0 0 0
```

## Calculation

- To determine the equilibrium volume we can:
  - Fit the energy over a certain volume range to an equation of state (see [cd\\_Si](#)).
  - Alternatively we relax the structure with VASP "on the fly" ([IBRION=2](#) and [ISIF=3](#))
- From equation of states we determine lattice parameter of  $a = 5.4687$  (volume scan plus Murnaghan EOS using [ENMAX=400](#)).
- From relaxations using [IBRION=2](#) and [ISIF=3](#) we get  $a = 5.4684$ .
- Difference can be due to pulay stress (especially when the relaxation starts far away from equilibrium):

```
-----
Total    0.00155   0.00155   0.00155  -0.00000  -0.00000   0.00000
in kB    0.06056   0.06056   0.06056  -0.00000  -0.00000   0.00000
external pressure =      0.06 kB  Pulay stress =      0.00 kB
```

VOLUME and BASIS-vectors are now :

```

energy-cutoff : 400.00
volume of cell : 40.88
direct lattice vectors reciprocal lattice vectors
0.000000000 2.734185321 2.734185321 -0.182869828 0.182869828 0.182869828
2.734185321 0.000000000 2.734185321 0.182869828 -0.182869828 0.182869828
2.734185321 2.734185321 0.000000000 0.182869828 0.182869828 -0.182869828

```

- To remedy this increase the plane wave cutoff by at least 30% (here we used **ENMAX**=400 instead of 240) and use a small **EDIFF**.

## Summary

- Calculation of the equilibrium volume:
  - Fit the energy over a certain volume range to an equation of state.
  - When internal degrees of freedom exist (e.g. c/a), the structure must be optimized. Use a conjugate-gradient algorithm (**IBRION**=2) and at each volume do e.g. 10 ionic steps (**NSW**=10) and allow change of internal parameters and shape (**ISIF**=4).
- Simpler but less reliable: relaxing all degrees of freedom including volume.
  - To relax all degrees of freedom use **ISIF**=3 (internal coordinates, shape and volume).
  - Mind pulay stress problem. Increase plane wave cutoff by 25-30% when the volume is allowed to change.

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CO

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**Task**

Relaxation of the bond length in a CO molecule.

**Input****POSCAR**

```
CO molecule in a box
1.0      ! universal scaling parameters
8.0 0.0 0.0 ! lattice vector a(1)
0.0 8.0 0.0 ! lattice vector a(2)
0.0 0.0 8.0 ! lattice vector a(3)
1 1      ! number of atoms for each species
cart      ! positions in cartesian coordinates
0 0 0      ! first atom
0 0 1.12   ! second atom
```

**INCAR**

```
SYSTEM = CO molecule in a box
ISMEAR = 0 ! Gaussian smearing
NSW = 5   ! 5 ionic steps
IBRION = 2 ! use the conjugate gradient algorithm
```

**KPOINTS**

```
Gamma-point only
0
Monkhorst Pack
1 1 1
0 0 0
```

**POTCAR**

The **POTCAR** file is created by the concatenation of two individual **POTCAR** files corresponding to O and C, e.g.:

```
cat .../O/POTCAR .../C POTCAR > POTCAR
```

**Calculation**

- A similar relaxation as in the previous case ([O\\_dimer](#)) is performed but in this case more steps are required, since the first estimate for the minimum is not very accurate. The trial steps are much too long ([POTIM](#) parameter).

```
1 F= -.14764064E+02 E0= -.14764064E+02 d E =-.147641E+02
curvature: 0.00 expect dE= 0.000E+00 dE for cont linesearch 0.000E+00
trial: gam= 0.00000 g(F)= 0.820E+00 g(S)= 0.000E+00 ort = 0.000E+00 (trialstep = 0.100E+01)
search vector abs. value= 0.820E+00
bond charge predicted
...
...
...
...
2 F= -.12660858E+02 E0= -.12660858E+02 d E =0.210321E+01
trial-energy change: 2.103205 1.order 1.311207 -0.819873 3.442288
step: 0.1924(harm= 0.1924) dis= 0.02705 next Energy= -14.842919 (dE=-0.789E-01)
bond charge predicted
...
...
```

```
...   ...   ...
... 3 F= -.14747869E+02 E0= -.14747869E+02 d E =0.161943E-01
curvature: -0.10 expect dE=-0.902E-01 dE for cont linesearch -0.902E-01
ZBRENT: interpolating
opt : 0.0929 next Energy= -14.802162 (dE=-0.381E-01)
bond charge predicted
...
...
...
... 4 F= -.14796822E+02 E0= -.14796822E+02 d E =-.327586E-01
curvature: -0.04 expect dE=-0.330E-03 dE for cont linesearch -0.330E-03
trial: gam= 0.00000 g(F)= 0.814E-02 g(S)= 0.000E+00 ort =-0.817E-01 (trialstep = 0.819E+00)
search vector abs. value= 0.814E-02
reached required accuracy - stopping structural energy minimisation
```

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# CO on Ni 111 surface

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## Task

Adsorption of a CO molecule at the top site of a Ni (111) surface.

## Input

### POSCAR

```
Ni - (111) + CO on-top
3.53
.70710678 .0000000 .0000000
-0.35355339 0.6123724 .0000000
.0000000 .0000000 5.1961524
5 1 1
selective dynamics
direct
.00000000 .00000000 .00000000 F F F
.33333333 .66666667 .11111111 F F F
.66666667 .33333333 .22222222 F F F
.00000000 .00000000 .33333333 T T T
.33333333 .66666667 .44444444 T T T
.33333333 .66666667 .54029062 T T T
.33333333 .66666667 .60298866 T T T
```

- CO molecule put above surface atom "on-top".
- $z_{\text{CO}} = (.540 - .444) \cdot 5.196 \cdot 3.53 \approx 1.76$
- $d_{\text{CO}} = (.603 - .540) \cdot 5.196 \cdot 3.53 \approx 1.16$

### INCAR

```
ISTART = 0
ICHARG = 2

general:
SYSTEM = CO adsorption on Ni(111)
ENMAX = 400
ISMEAR = 2 ; SIGMA = 0.2
ALGO= Fast
EDIFF = 1E-6

dynamic:
NSW=100
POTIM = 0.2
IBRION = 1
```

### KPOINTS

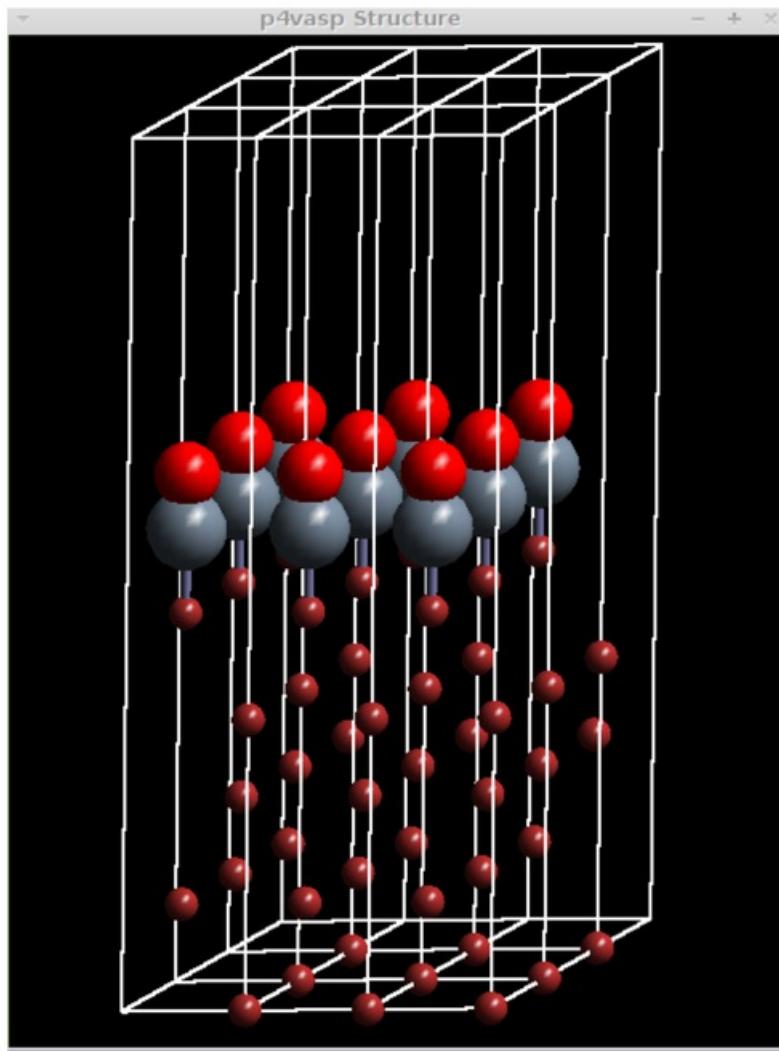
```
K-Points
0
Monkhorst-Pack
9 9 1
0 0 0
```

## Calculation

- Two additional atom types (C and O) in the calculations: append C and O potentials to the POTCAR file.
- The sample output for the forces should look like the following:

POSITION			TOTAL-FORCE (eV/Angst)		
0.00000	0.00000	0.00000	0.000000	0.000000	0.175780
0.00000	1.44112	2.03805	0.000000	0.000000	-0.104008
1.24804	0.72056	4.07609	0.000000	0.000000	-0.036305
0.00000	0.00000	6.10852	0.000000	0.000000	-0.083336
0.00000	1.44112	8.15366	0.000000	0.000000	0.009539
0.00000	1.44112	9.90873	0.000000	0.000000	0.011228
0.00000	1.44112	11.06339	0.000000	0.000000	0.027102
total drift:			-0.000093	-0.000213	0.019852

- Small outward relaxation of surface due to adsorption:  $\Delta d_{12} = (8.154 - 6.109)/2.038 = 0.4\%$
- CO geometry change:  $d_{CO} = 11.063 - 9.909 = 1.155$ ;  $z_C = 9.909 - 8.154 = 1.755$
- Visualize the structure using p4vasp:



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# CO partial DOS

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## Task

Calculation of the DOS of a CO molecule (using p4vasp)

### Input

#### POSCAR

```
CO molecule in a box
1.0 ! universal scaling parameters
8.0 0.0 0.0 ! lattice vector a(1)
0.0 8.0 0.0 ! lattice vector a(2)
0.0 0.0 8.0 ! lattice vector a(3)
1 1 ! number of atoms for each species
sel ! selective degrees of freedom are changed
cart ! positions in cartesian coordinates
0 0 0 F F T ! first atom
0 0 1.43 F F T ! second atom
```

#### INCAR

```
SYSTEM = CO molecule in a box
ISMEAR = 0 ! Gaussian smearing
LORBIT = 11
```

#### KPOINTS

```
Gamma-point only
0
Monkhorst Pack
1 1 1
0 0 0
```

### Calculation

- The [PROCAR](#) file gives valuable information of the character of the one electron states:

<a href="#">LORBIT=10</a>	<a href="#">DOSCAR</a> and I decomposed <a href="#">PROCAR</a> file
<a href="#">LORBIT=11</a>	<a href="#">DOSCAR</a> and Im decomposed <a href="#">PROCAR</a> file

- We'll use [LORBIT=11](#) and see if we can distinguish  $p_x$  and  $p_z$  states.

#### PROCAR

```
band 3 # energy -11.46540832 # occ. 2.00000000
ion s py pz px dxy dyz dz2 dxz dx2 tot
 1 0.000 0.510 0.000 0.036 0.000 0.000 0.000 0.000 0.000 0.546
 2 0.000 0.146 0.000 0.010 0.000 0.000 0.000 0.000 0.000 0.157
tot 0.000 0.656 0.000 0.047 0.000 0.000 0.000 0.000 0.000 0.703

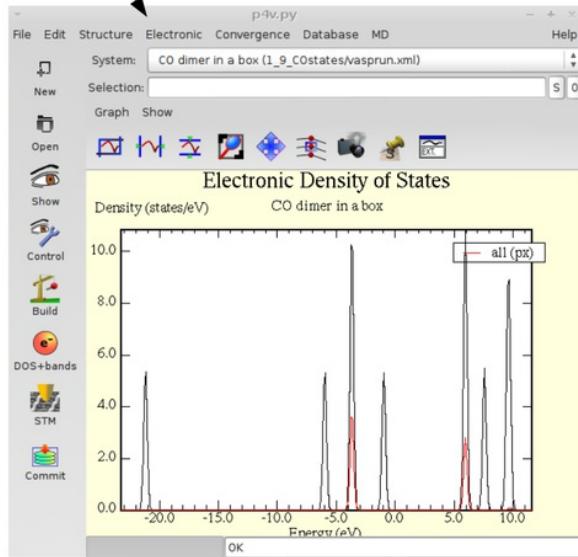
band 4 # energy -11.46540832 # occ. 2.00000000
ion s py pz px dxy dyz dz2 dxz dx2 tot
 1 0.000 0.036 0.000 0.510 0.000 0.000 0.000 0.000 0.000 0.546
 2 0.000 0.010 0.000 0.146 0.000 0.000 0.000 0.000 0.000 0.157
tot 0.000 0.047 0.000 0.656 0.000 0.000 0.000 0.000 0.000 0.703
```

```
band 5 # energy -8.76483386 # occ. 2.00000000
ion s py pz px dxy dyz dz2 dxz dx2 tot
 1 0.001 0.000 0.135 0.000 0.000 0.000 0.000 0.000 0.000 0.136
 2 0.172 0.000 0.261 0.000 0.000 0.000 0.000 0.000 0.000 0.433
tot 0.173 0.000 0.396 0.000 0.000 0.000 0.000 0.000 0.000 0.569
```

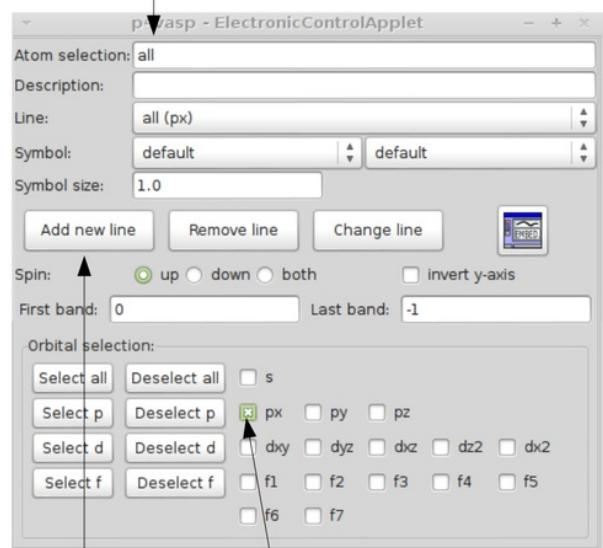
- To plot the DOS start p4vasp:

Start p4vasp:  
> p4v [vasprun.xml]

Step 1.) go to:  
Electronic/Local DOS+bands control



Step 2.) select atoms: "all", "C", "O", "1", "2", ...



Step 3.) select orbital character

Step 4.) and "add new line"

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# CO vibration

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## Task

Calculation of the vibrational frequencies of a CO molecule.

## Input

### POSCAR

```
CO molecule in a box
1.0      ! universal scaling parameters
8.0 0.0 0.0 ! lattice vector a(1)
0.0 8.0 0.0 ! lattice vector a(2)
0.0 0.0 8.0 ! lattice vector a(3)
1 1      ! number of atoms for each species
sel      ! selective degrees of freedom are changed
cart    ! positions in cartesian coordinates
0 0 0   F F T ! first atom
0 0 1.143 F F T ! second atom
```

Alternatively, try to fix one of the atoms completely.

### INCAR

```
SYSTEM = CO molecule in a box
ISMEAR = 0 ! Gaussian smearing
IBRION = 5 ! use the conjugate gradient algorithm
NFREE = 2 ! central differences
POTIM = 0.02 ! 0.02 A stepwidth
NSW = 1   ! ionic steps > 0
```

### KPOINTS

```
Gamma-point only
0
Monkhorst Pack
1 1 1
0 0 0
```

## Calculation

- The selected degrees of freedom are displaced once in the direction  $\hat{x}$  and once in  $-\hat{x}$  by 0.002 (POTIM).
- In the present case this makes 4 displacements plus the equilibrium positions (i.e. a total of five ionic configurations).

### OUTCAR

At the end of the **OUTCAR** file the following output should be obtained:

#### SECOND DERIVATIVES (NOT SYMMETRIZED)

```
-----  
1Z 2Z  
1Z -114.737304 114.737304  
2Z 114.458316 -114.458316
```

#### Eigenvectors and eigenvalues of the dynamical matrix

```
-----  
1 f = 63.887522 THz 401.417139 2PiTHz 2131.058277 cm-1 264.217647 meV
```

X	Y	Z	dx	dy	dz
0.000000	0.000000	0.000000		0	0 -0.655280
0.000000	0.000000	1.143000		0	0 0.755386

2 f/i=	0.038494	THz	0.241864	2PiTHz	1.284016	cm-1	0.159198	meV
X	Y	Z	dx	dy	dz			
0.000000	0.000000	0.000000		0	0	-0.755386		
0.000000	0.000000	1.143000		0	0	-0.655280		

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# Collective jumps of a Pt adatom on fcc-Pt (001): Nudged Elastic Band Calculation

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**Description:** calculate the energy barrier for the self-diffusion (of a Pt-adatom) on Pt (001): The most stable adsorption site of the adatom Pt@Pt(001) is the hollow (h) position. Simple models of the diffusion of the adatom from h to the neighboring h site include two diffusion paths: hollow-top-hollow (hth, eg along [1-10]) or hollow-bridge-hollow (hbh, eg along [100]). A collective jump mechanism involving 2 Pt atoms diffusing along [1-10] is proposed to be the diffusion mechanism with the lowest energy barrier [\[1\]](#)

The calculation of the barrier heights involves the following steps:

1. calculation of the bulk  $a_0$  of Pt for the chosen functional
  2. a clean Pt (001) surface, with a 2D supercell -at minimum- (2x2) reconstruction
  3. the energies of the surface including the Pt-adatom in h, b, and t position
  4. a Nudged Elastic Band (NEB) calculation [\[2\]](#) for the proposed collective jump mechanism
- steps 1-3 are straightforward

inputs for a fast, preliminary estimate are given here and in Pt\_NEB\_fast.tgz (**mind** this "quick and dirty" setup is only suitable to learn about principles of the setup of a NEB calculation; the results of the NEB run with this minimal set of parameters do **not** reproduce the experimentally found behaviour), for a more time-consuming, but more accurate setup (larger number of Pt layers, denser k-mesh, higher PREC and ENCUT) please use the files untarred from Pt\_NEB.tgz:

■ [INCAR](#)

System: fcc Pt (001), 3layers

```

ISTART = 0
EDIFF = 1e-6      # electronic convergence
PREC = Normal
IBRION = 1        # DIIS algorithm
POTIM = 0.5
NSW = 20
EDIFFG = -0.01
NELMIN = 5        # max forces: 0.1eV/AA
                   # at least 5 el. scf steps for each ionic step

```

■ [KPOINTS](#)

```

K-Points
0
Gamma
3 3 1
0 0 0

```

■ [POSCAR](#) (clean surface)

```

fcc Pt, paw-PBE
5.62024
1.0 0.0 0.0
0.0 1.0 0.0
0.0 0.0 3.0
Pt
12
Selective
Direct
0.25 0.25 0.11785 F F F
0.75 0.25 0.11785 F F F
0.25 0.75 0.11785 F F F
0.75 0.75 0.11785 F F F
0.00 0.00 0.23570 F F T
0.00 0.50 0.23570 F F T
0.50 0.00 0.23570 F F T
0.50 0.50 0.23570 F F T
0.25 0.25 0.35355 F F T
0.75 0.25 0.35355 F F T
0.25 0.75 0.35355 F F T
0.75 0.75 0.35355 F F T

```

■ [POSCAR](#) (Pt@Pt(001), hollow)

```

fcc Pt, paw-PBE
5.62024000000000
 1.000000000000000 0.000000000000000 0.000000000000000
 0.000000000000000 1.000000000000000 0.000000000000000
 0.000000000000000 0.000000000000000 3.000000000000000
Pt
13
Selective dynamics
Direct
 0.250000000000000 0.250000000000000 0.117849999999971 F F F
 0.750000000000000 0.250000000000000 0.117849999999971 F F F
 0.250000000000000 0.750000000000000 0.117849999999971 F F F
 0.750000000000000 0.750000000000000 0.117849999999971 F F F
 0.000000000000000 0.000000000000000 0.2341409911878811 T T T
 0.000000000000000 0.500000000000000 0.2344158754007225 T T T
 0.500000000000000 0.000000000000000 0.2377721273226986 T T T
 0.500000000000000 0.500000000000000 0.2341409911878811 T T T
 0.250000000000000 0.250000000000000 0.3517982322412672 T T T
 0.750000000000000 0.250000000000000 0.3517982322412672 T T T
 0.250000000000000 0.750000000000000 0.3517982322412672 T T T
 0.750000000000000 0.750000000000000 0.3517982322412672 T T T
 0.000000000000000 0.500000000000000 0.4492270704381683 T T T

```

■ [POSCAR](#) (Pt@Pt(001), bridge)

```

fcc Pt, paw-PBE
5.62024000000000
 1.000000000000000 0.000000000000000 0.000000000000000
 0.000000000000000 1.000000000000000 0.000000000000000
 0.000000000000000 0.000000000000000 3.000000000000000
Pt
13
Selective dynamics
Direct
 0.250000000000000 0.250000000000000 0.117849999999971 F F F
 0.750000000000000 0.250000000000000 0.117849999999971 F F F
 0.250000000000000 0.750000000000000 0.117849999999971 F F F
 0.750000000000000 0.750000000000000 0.117849999999971 F F F
 0.0002686432543183 0.000000000000000 0.2356407813553420 T T T
 0.0014220524373488 0.500000000000000 0.2356795143373628 T T T
 0.4997313567456815 0.000000000000000 0.2356407813553420 T T T
 0.4985779475626512 0.500000000000000 0.2356795143373628 T T T
 0.250000000000000 0.2341977119064422 0.3525947402192897 F T T
 0.750000000000000 0.2518717446753760 0.3518647397661007 T T T
 0.250000000000000 0.7658022880935580 0.3525947402192897 F T T
 0.750000000000000 0.7481282553246233 0.3518647397661007 T T T
 0.250000000000000 0.500000000000000 0.4716518885541170 F F T

```

■ [POSCAR](#) (Pt@Pt(001), top)

```

fcc Pt, paw-PBE
5.62024000000000
 1.000000000000000 0.000000000000000 0.000000000000000
 0.000000000000000 1.000000000000000 0.000000000000000
 0.000000000000000 0.000000000000000 3.000000000000000
Pt
13
Selective dynamics
Direct
 0.250000000000000 0.250000000000000 0.117849999999971 F F F
 0.750000000000000 0.250000000000000 0.117849999999971 F F F
 0.250000000000000 0.750000000000000 0.117849999999971 F F F
 0.750000000000000 0.750000000000000 0.117849999999971 F F F
 -0.0014262288827347 -0.0014262288827347 0.2348121710889565 T T T
 -0.0014262288827347 0.5014262288827348 0.2348121710889565 T T T
 0.5014262288827348 -0.0014262288827347 0.2348121710889565 T T T
 0.5014262288827348 0.5014262288827348 0.2348121710889565 T T T
 0.250000000000000 0.250000000000000 0.3433443664932221 F F T
 0.750000000000000 0.250000000000000 0.3546231232810972 T T T
 0.250000000000000 0.750000000000000 0.3546231232810972 T T T
 0.750000000000000 0.750000000000000 0.3516055254412989 T T T
 0.250000000000000 0.250000000000000 0.4861522106341429 F F T

```

the NEB calculation should be done a follows:

- run the job from a parent directory containing the files [INCAR](#), [POTCAR](#), [KPOINTS](#) and the run-script of the job
- consider how many intermediate geometries (N) should be chosen between the initial and the final state of the jump in [INCAR](#), this corresponds to the parameter [IMAGES](#)
- generate sub-directories 00 (containing the [POSCAR](#) of the initial geometry i), ... 0(N+1) (containing the [POSCAR](#) of the final geometry f of the jump). The [POSCAR](#) files of the intermediate steps, to be interpolated between [POSCAR](#)<sub>i</sub> and [POSCAR](#)<sub>f</sub> are stored in the directories 01 .. 0N. Calculations are **only** done for these intermediate steps, the optimization of the geometries is done under the constraint that the relaxing atoms remain on a plane perpendicular to the hypotangent of the diffusion path. All all output files [OUTCAR](#), [CONTCAR](#), [OSZICAR](#) .. of the NEB-steps run are written to these subdirectories.

in the present excercise, the required precision,... is reduced to a minimum (the files are found in [Pt\\_NEB\\_fast.tgz](#)) to save computing time, a more reliable setup is saved in [Pt\\_NEB.tgz](#)

## ■ INCAR

System: fcc Pt (001), 3layers

```
ISTART = 0
EDIFF = 1e-6          # electronic convergence
PREC = Normal
IBRION = 1            # DIIS algorithm
NSW = 10
EDIFFG = -0.01        # max forces: 0.1eV/AA
NELMIN = 5            # at least 5 el. scf steps for each ionic step
IMAGES = 2             # 2 intermediate geometries for the NEB
SPRING = -5           # spring constant
```

## ■ KPOINTS

```
K-Points
0
Gamma
3 3 1
0 0 0
```

## ■ POSCAR (of the initial state, in directory 00)

```
fcc Pt, paw-PBE
5.62024000000000
 1.0000000000000000  0.0000000000000000  0.0000000000000000
 0.0000000000000000  1.0000000000000000  0.0000000000000000
 0.0000000000000000  0.0000000000000000  3.0000000000000000
13
Direct
 0.250000  0.250000  0.117850
 0.750000  0.250000  0.117850
 0.250000  0.750000  0.117850
 0.750000  0.750000  0.117850
 0.000000  0.000000  0.230682
 0.000000  0.500000  0.230971
 0.500000  0.000000  0.234757
 0.500000  0.500000  0.230682
 0.256381  0.243619  0.347171
 0.743619  0.243619  0.347171
 0.256381  0.756381  0.347171
 0.743619  0.756381  0.347171
 0.000000  0.500000  0.444316
```

## ■ POSCAR (of the final state, in directory 03)

```
fcc Pt, paw-PBE
5.62024000000000
 1.0000000000000000  0.0000000000000000  0.0000000000000000
 0.0000000000000000  1.0000000000000000  0.0000000000000000
 0.0000000000000000  0.0000000000000000  3.0000000000000000
13
Direct
 0.250000  0.250000  0.117850
 0.750000  0.250000  0.117850
 0.250000  0.750000  0.117850
 0.750000  0.750000  0.117850
 0.000000  0.000000  0.230682
 0.000000  0.500000  0.230971
 0.500000  0.000000  0.234757
 0.500000  0.500000  0.230682
 0.500000  0.000000  0.444316
 0.756381  0.256381  0.347171
 0.243619  0.743619  0.347171
 0.756381  0.743619  0.347171
 0.243619  0.256381  0.347171
```

4. concatenate the [POSCAR](#) files of i and f to the file [POSCAR1\\_POSCAR2](#) MIND:

- these files must not include the lines with the names of the atoms (vasp.5.2 only) and 'Selective Dynamics',
- there must be no blank line between the POSCARs
- the block with the velocities of the atoms must be deleted
- be careful to check that in [POSCAR<sub>i</sub>](#) and [POSCAR<sub>j</sub>](#) all atoms are on the same side of the supercell to avoid that an atom that actually jumps across the origin of the cell is dragged through the cell by the interpolation of the positions.

5. interpolate the starting geometries of the [IMAGES](#), this can be done by using the following script

interpolatePOSCAR [POSCAR1\\_POSCAR2](#), the interpolated files are written into the respective subdirectories 00 ... 0(N+1)

## ■ interpolatePOSCAR

```

file=$1
if [ ! -x $file ]
then
  usage: interpolatePOS POSCAR1_POSCAR2
fi

awk <$file '
BEGIN { rep=4; center=0 }
/center/ { center=1}
/rep/ { rep=$2 }
{ line=line+1
  if ( second != 1 ) {
    if ( line == 6 ) {
      lines = $1 + $2 + $3 + 7
      print "found ",lines," ions"
      head[line] = $0
    } else if ( line < 8 )
      head[line] = $0
    else
      {
        x[line-7] = $1 ; y[line-7] = $2 ; z[line-7] = $3
        if (line==lines) {
          line=0; second=1;
          print "first set read"
        }
      }
    } else{
      if ( line >= 8 )
        {
          x2[line-7] = $1; y2[line-7] = $2 ; z2[line-7] = $3
          if (line==lines) {
            print "second set read"
          }
        }
    }
  }
END {
  lines=lines-7
  for ( line=1; line<=lines ; line ++ ) {
    cx1=cx1+ x[line] ; cy1=cy1+ y[line] ; cz1=cz1+ z[line]
    cx2=cx2+ x2[line]; cy2=cy2+ y2[line]; cz2=cz2+ z2[line]
  }
  if (center) {
    cx=(cx2-cx1)/lines
    cy=(cy2-cy1)/lines
    cz=(cz2-cz1)/lines
    print "center of mass for second cell will be shifted by",cx,cy,cz
  }

  for ( i=0; i<rep ; i++ ) {
    file="0" i "/POSCAR"
    print "writing to " file
    for (line=1; line<=7 ; line++)
      print head[line] >file
    for ( line=1; line<=lines ; line ++ ) {
      b=i/(rep-1)
      a=(rep-1-i)/(rep-1)
      dx=a*x[line] + b*(x2[line]-cx)
      dy=a*y[line] + b*(y2[line]-cy)
      dz=a*z[line] + b*(z2[line]-cz)
      printf " %10.6f %10.6f %10.6f\n",dx,dy,dz >file
    }
  }
}'

```

NOTE: the total number of steps is explicitly given in line 8 of the script (rep=, rep = **IMAGES+2**). If a different number of **IMAGES** is chosen, this parameter has to be changed.

**alternatively** the name of the input file and the number of images can be passed as options to interpolatePOSCAR:  
**interpolatePOSCAR <fn> <IMAGES+2>**

6. run vasp:

**MIND:** the number of CPUs to be used has to be an integer multiple of **IMAGES**

7. if convergence is not reached within **NSW** steps, the calculation can be continued by a continuation run, just like for a standard ionic relaxation.

8. **HINT:** better convergence is usually achieved if the number of **IMAGES** is rather low (up to 4). If the region close to the transition state is to be refined, one can do another NEB-calculation, using the ionic configurations of the **IMAGES** adjacent to the transition state as the new initial and final states for the follow-up run.

9: obtain the barrier along diffusion path 00-03 by interpolation (spline)

## Downloads

[Pt\\_NEB.tgz](#), [Pt\\_NEB\\_fast.tgz](#)

## References

1. ↑ G.L.Kellogg and Peter J.Feibelman, Phys. Rev. Lett. **64** (26), 3143 (1990)
2. ↑ G. Mills, H. Jonsson and G. K. Schenter, Surface Science, **324**, 305 (1995); H. Jonsson, G. Mills and K. W. Jacobsen, 'Nudged Elastic Band Method for Finding Minimum Energy Paths of Transitions', in 'Classical and

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## Constrained MD using a canonical ensemble

**Description:** Compare adsoption of H<sub>2</sub>O on TiO<sub>2</sub>[110] using a simple model structure: the model surface consists of 2 layers TiO<sub>2</sub>, (1x1)

- The bottom layer of the slab will be kept frozen
- 2 setups will be tested:
  - Standard relaxation, minimizing the Hellmann-Feyman forces
  - Constrained MD, fixing the bond lengths and angle of H<sub>2</sub>O, the system is coupled to an ANDERSEN thermostat:
    - Microcanonical NVE ensemble (no collisions with the thermostat)
    - Canonical ensemble at T= 10K, to be close to the standard relaxation (OK)

To keep the computing time reasonable, the number of steps in the MD is limited to 100 (100 fs) which implies that the MD is NOT CONVERGED.

- [INCAR](#) for standard relaxation

```
SYSTEM = H2O_TiO2
ENMAX = 400
ISMEAR = 2
SIGMA = 0.05
EDIFF = 1e-6
EDIFFG = -0.05
IBRION = 2
POTIM = 0.5
NSW = 200
```

- [INCAR](#) for constrained MD using a microcanonical ensemble

```
SYSTEM = H2O_TiO2
ENMAX = 400
ISMEAR = 2
SIGMA = 0.05
ISMEAR = 0
EDIFF = 1e-6
EDIFFG = -0.05
IBRION = 0
POTIM = 1.
MDALGO = 1 # Andersen Thermostat
TEBEG = 10; TEEND = 10
NSW = 100
```

- [ICONST](#) for constrained MD using a microcanonical ensemble

```
R 7 8 0
R 7 9 0
A 8 7 9 0
```

- [INCAR](#) for constrained MD using a canonical ensemble

```
SYSTEM = H2O_TiO2
ENMAX = 400
ISMEAR = 2
SIGMA = 0.05
ISMEAR = 0
EDIFF = 1e-6
EDIFFG = -0.05
IBRION = 0
POTIM = 1.
MDALGO = 1 # Andersen Thermostat
ANDERSEN_PROB = 0.9
TEBEG = 10; TEEND = 10
NSW = 100
```

- [ICONST](#) for constrained MD using a canonical ensemble

```
R 7 8 0
R 7 9 0
A 8 7 9 0
```

- [POSCAR](#)

```
TiO2+H2O
1.0000000000000000
```

```

4.61949 0.00000 0.00000
0.00000 4.61949 0.00000
0.00000 0.00000 14.7788
Ti O H
2 5 2
Selective
Direct
0.00000 0.00000 0.00000 F F F
0.50000 0.50000 0.10000 T T T
0.30374 0.30374 0.00000 F F F
0.69625 0.69625 0.00000 F F F
0.19625 0.80374 0.10000 T T T
0.80374 0.19625 0.10000 T T T
0.50000 0.50000 0.31500 T T T
0.37720 0.62280 0.35881 T T T
0.62280 0.37720 0.35881 T T T

```

#### ■ KPOINTS

```

Automatically generated mesh
0
Gamma
5 5 1

```

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[h2o\\_on\\_tio2.tgz, sub-folder constrMD\\_canonical](#)

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## Constrained MD using a microcanonical ensemble

**Description:** Compare adsoption of H<sub>2</sub>O on TiO<sub>2</sub>[110] using a simple model structure: the model surface consists of 2 layers TiO<sub>2</sub>, (1x1)

- The bottom layer of the slab will be kept frozen
- 2 setups will be tested:
  - Standard relaxation, minimizing the Hellmann-Feyman forces
  - Constrained MD, fixing the bond lengths and angle of H<sub>2</sub>O, the system is coupled to an ANDERSEN thermostat:
    - Microcanonical NVE ensemble (no collisions with the thermostat)
    - Canonical ensemble at T= 10K, to be close to the standard relaxation (OK)

To keep the computing time reasonable, the number of steps in the MD is limited to 100 (100 fs) which implies that the MD is NOT CONVERGED.

- [INCAR](#) for standard relaxation

```
SYSTEM = H2O_TiO2
ENMAX = 400
ISMEAR = 2
SIGMA = 0.05
EDIFF = 1e-6
EDIFFG = -0.05
IBRION = 2
POTIM = 0.5
NSW = 200
```

- [INCAR](#) for constrained MD using a microcanonical ensemble

```
SYSTEM = H2O_TiO2
ENMAX = 400
ISMEAR = 2
SIGMA = 0.05
ISMEAR = 0
EDIFF = 1e-6
EDIFFG = -0.05
IBRION = 0
POTIM = 1.
MDALGO = 1 # Andersen Thermostat
TEBEG = 10; TEEND = 10
NSW = 100
```

- [ICONST](#) for constrained MD using a microcanonical ensemble

```
R 7 8 0
R 7 9 0
A 8 7 9 0
```

- [INCAR](#) for constrained MD using a canonical ensemble

```
SYSTEM = H2O_TiO2
ENMAX = 400
ISMEAR = 2
SIGMA = 0.05
ISMEAR = 0
EDIFF = 1e-6
EDIFFG = -0.05
IBRION = 0
POTIM = 1.
MDALGO = 1 # Andersen Thermostat
ANDERSEN_PROB = 0.9
TEBEG = 10; TEEND = 10
NSW = 100
```

- [ICONST](#) for constrained MD using a canonical ensemble

```
R 7 8 0
R 7 9 0
A 8 7 9 0
```

- [POSCAR](#)

```
TiO2+H2O
1.0000000000000000
```

```

4.61949 0.00000 0.00000
0.00000 4.61949 0.00000
0.00000 0.00000 14.7788
Ti O H
2 5 2
Selective
Direct
0.00000 0.00000 0.00000 F F F
0.50000 0.50000 0.10000 T T T
0.30374 0.30374 0.00000 F F F
0.69625 0.69625 0.00000 F F F
0.19625 0.80374 0.10000 T T T
0.80374 0.19625 0.10000 T T T
0.50000 0.50000 0.31500 T T T
0.37720 0.62280 0.35881 T T T
0.62280 0.37720 0.35881 T T T

```

#### ■ KPOINTS

```

Automatically generated mesh
0
Gamma
5 5 1

```

#### ■ run.sh

```

#
# To run VASP this script calls $vasp_std
# (or possibly $vasp_gam and/or $vasp_ncl).
# These variables can be defined by sourcing vaspcmd
. vaspcmd 2> /dev/null

#
# When vaspcmd is not available and $vasp_std,
# $vasp_gam, and/or $vasp_ncl are not set as environment
# variables, you can specify them here
[ -z "$vasp_std" ] && vasp_std="mpirun -np 8 /path-to-your-vasp/vasp_std"
[ -z "$vasp_gam" ] && vasp_gam="mpirun -np 8 /path-to-your-vasp/vasp_gam"
[ -z "$vasp_ncl" ] && vasp_ncl="mpirun -np 8 /path-to-your-vasp/vasp_ncl"

#
# The real work starts here
#
rm results.dat
drct=$(pwd)

for i in std_relaxation constrMD_microcanonical constr_MD_canonical
do
  cd $drct/$i
  ln -s ./POTCAR .
  ln -s ./POSCAR .
  ln -s ./KPOINTS .
  $vasp_std
  /bin/rm CHG* WAVECAR
done

```

To run the calculations use (and modify if necessary) the run.sh script

## Download

[h2o\\_on\\_tio2.tgz, sub-folder constrMD\\_microcanonical](#)

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## Constraining local magnetic moments

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## Task

## Constraining the local magnetic moments on an Fe dimer.

## Input

POSCAR

INCAR

```

SYSTEM      = Fe dimer
ISTART     = 0
ISYM       = 0
LNONCOLLINEAR = .TRUE.
MAGMOM     = 0 0 3  0 0 3
VOSKOWN    = 1
LORBIT     = 11

! mix slowly when increasing LAMBDA
# AMIX       = 0.1
# BMIX       = 0.00001
# AMIX_MAG   = 0.2
# BMIX_MAG   = 0.00001

# I_CONSTRAINED_M = 1
# RWIGS        = 1.0
# LAMBDA       = 10
# M_CONSTR    = 0 0 1 0 0 1

```

- Symmetry is switched off (**ISYM**=0).
  - Initially moments for ferromagnetic calculation are initialized.

## KPOINTS

```

k-points
0
Monkhorst Pack
 1 1 1
 0. 0. 0.

```

- A single k point in the calculation is sufficient.

## Calculation

- By using the initial ferromagnetic initialization of **MAGMOM** = 0 0 3 0 0 3 we get the following magnetic moments in the **OSZICAR** file:

DAV: 20 -0.929676054634E+01 -0.26101E-03 -0.16780E-03 60 0.102E-01 0.537E-02  
 DAV: 21 -0.929679955346E+01 -0.39007E-04 -0.30319E-04 60 0.590E-02  
 $F_1 = -92967996E+01$   $F_0 = -93047629F+01$   $d_F = 0.238900E-01$   $mag = -0.0006$   $-0.0003$   $6.0537$

- By using a different initial magnetization of **MAGMOM** = 0 0 3 0 2 2 the system converges to a ferromagnetic solution:

magnetization (y)						magnetization (z)					
# of ion	s	p	d	tot	# of ion	s	p	d	tot		
1	0.018	-0.001	1.071	1.087	1	0.045	-0.003	2.587	2.628		
2	0.019	-0.001	1.069	1.087	2	0.045	-0.003	2.588	2.629		
tot	0.037	-0.003	2.140	2.174	tot	0.089	-0.007	5.175	5.257		

- A penalty functional is added to the system, driving the integrated local moments into the desired directions, when the following steps are modified in the input (beware the penalty functional contributes to the total energy):
  - Switching on constraints on magnetic moments (**I\_CONSTRAINED\_M**=1).
  - Setting integration radius to determine local moments (**RWIGS**=1.0).
  - Weight in penalty functional (**LAMBDA**=10).
  - Target directions for constraints on magnetic moments (**M\_CONSTR**= 0 0 1 0 1 1).
- The necessary information is found in the **OSZICAR** file:

```
E_p = 0.35424E-02 lambda = 0.100E+02
ion   MW_int      M_int
1 0.000 0.013 1.557 0.000 0.014 2.674
2 0.000 1.092 1.110 0.000 1.880 1.901
DAV: 35 -0.905322335169E+01 0.58398E-04 -0.60872E-04 60 0.734E-02
1 F= -.90532234E+01 E0= -.90355617E+01 d E =-.529849E-01 mag= -0.0005 2.1161 5.1088
```

- **E\_p** is the energy arising from the penalty function. It decreases with increasing **LAMBDA**.
- By increasing **LAMBDA** stepwise one can bring **E\_p** down (slowly so the solution remains stable from one run to another):

```
E_p = 0.22591E-03 lambda = 0.500E+02
ion   MW_int      M_int
1 0.000 0.002 1.545 0.001 -0.005 2.654
2 0.000 1.086 1.087 0.001 1.871 1.862
DAV: 33 -0.907152551238E+01 0.48186E-04 -0.33125E-04 60 0.163E-01
1 F= -.90715255E+01 E0= -.90541505E+01 d E =-.521251E-01 mag= 0.0042 2.0902 5.0659
```

- This way one approaches the LSDA total energy for a given magnetic configuration.

- What can one do when convergence is bad:

- Start from charge density of non-spin-polarized calculation using **ISTART**=0 (or remove the **WAVECAR** file) and **ICHARG**=1.
- Use linear mixing by setting **BMIX**=0.0001 and **BMIX\_MAG**=0.0001.
- Mix slowly, i.e., reduce **AMIX** and **AMIX\_MAG**.
- REDUCE **MAXMIX**, the number of steps stored in the Broyden mixer (default **MAXMIX**=45).
- Restart from partially converged results (stop a calculation after say 20 steps and restart from the **WAVECAR** file).
- Use constraints to stabilize the magnetic configuration.
- Pray.

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## Constraining the local magnetic moments

Description: Constraining the local magnetic moments on NiO.

To orientate locally each spin, a penalty energy  $E_p$  is added, inversely proportional to the LAMBDA parameter. Thus, the process has to begin with a low LAMBDA, which is increased step by step.

For additional informations, go to the [I\\_CONSTRAINED\\_M](#) page.

**Exercise :** Verify the  $E_p=f(1/\text{LAMBDA})$  relation by constraining the spin directions. Check the efficiency of the method by constraining only the direction, then the direction and the size of spins.

### ■ INCAR

```
NiO GGA+U Constr.
SYSTEM      = "NiO"

Electronic minimization
ENCUT      = 450
EDIFF      = 1E-5
LORBIT     = 11
LREAL       = .False.
ISYM        = -1
NELMIN     = 6
LSORBIT    = .True.
GGA_COMPAT  = .FALSE.

DOS
ISMEAR     = -5

Magnetism
ISPIN      = 2
I_CONSTRAINED_M = 1 # direction
# I_CONSTRAINED_M = 2 # size and direction
M_CONSTR   = 2 0 0 0 -2 0 6*0
LAMBDA     = 1
RWIGS      = 1.30 0.70

Orbital moment
LORBMMOM   = T

Mixer
AMIX       = 0.2
BMIX       = 0.00001
AMIX_MAG   = 0.8
BMIX_MAG   = 0.00001

GGA+U
LDAU       = .TRUE.
LDAUTYPE   = 2
LDAUL      = 2 -1
LDAUU     = 5.00 0.00
LDAUJ     = 0.00 0.00
LDAUPRINT = 2
LMAXMIX   = 4
```

### ■ KPOINTS

```
k-points
0
gamma
4 4 4
0 0 0
```

### ■ POSCAR

```
NiO
4.17
1.0 0.5 0.5
0.5 1.0 0.5
0.5 0.5 1.0
2 2
Cartesian
0.0 0.0 0.0
1.0 1.0 1.0
0.5 0.5 0.5
1.5 1.5 1.5
```

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# Determining the Magnetic Anisotropy

Description: Magnetocrystalline Anisotropy Energy determined non-self-consistently

The Magnetocrystalline Anisotropy Energy is determined by rotating all spins according to different directions. First of all, an accurate (**PREC** = Accurate, **LREAL** = .False.) collinear calculation (using the `vasp-std` script) in the ground state has to be done. Next, the Spin-Orbit Coupling (**LSORBIT** = .True. ; using the `vasp-ncl` script) is took into account non-self-consistently (**ICHARG** = 11) for several spin orientations. In most of cases, the changes in energies are very low (sometimes, it could be about the micro-eV). The number of bands has to be twice compared to a collinear run).

To modify the orientation of the spins in the crystal, we consider the second approach describes [here](#). For the **MAGMOM**-tag, the total local magnetic moment is written according to the z direction (necessarily, the x and y-directions are equal to 0). The spin orientation [uvw] is defined by the **SAXIS**-tag in the Cartesian frame. The Magnetocrystalline Anisotropy Energy is calculated by orientating the spins in different directions and the following equation :  $E_{MAE} = E_{[uvw]} - E_{\min}$ , with  $E_{\min}$  the energy of the most stable spin orientation.

More details are available in the [SAXIS](#) and [LSORBIT](#) pages.

Exercise : Determine the Magnetocrystalline Anisotropy Energy of NiO in a non self-consistent approach by orientating the spins along the following path : (2,2,2) --> (2,2,1) --> (2,2,0) --> ... --> (2,2,-6). Compare to the [self-consistent approach](#).

## ■ INCAR

```
NiO MAE
SYSTEM = "NiO"

Electronic minimization
PREC = Accurate
ENCUT = 450
EDIFF = 1E-7
LORBIT = 11
LREAL = .False.
ISYM = -1
NELMIN = 6
# ICHARG = 11
# LCHARG = .FALSE.
# LWAVE = .FALSE.
# NBANDS = 52
# GGA_COMPAT = .FALSE.

DOS
ISMEAR = -5
```

```
Magnetism
ISPIN = 2
MAGMOM = 2.0 -2.0 2*0.0
# MAGMOM = 0 0 2 0 0 -2 6*0 # Including Spin-orbit
# LSORBIT = .True.
# SAXIS = 1 0 0 # Quantization axis used to rotate all spins in a direction defined in the (O,x,y,z) Cartesian frame
```

Orbital mom.  
LORBMMOM = T

```
Mixer
AMIX = 0.2
BMIX = 0.00001
AMIX_MAG = 0.8
BMIX_MAG = 0.00001
```

```
GGA+U
LDAU = .TRUE.
LDAUTYPE = 2
LDAUL = 2 -1
LDAUU = 5.00 0.00
LDAUJ = 0.00 0.00
LDAUPRINT = 2
LMAXMIX = 4
```

## ■ KPOINTS

```
k-points
0
gamma
4 4 4
0 0 0
```

## ■ POSCAR

NiO  
4.17  
1.0 0.5 0.5  
0.5 1.0 0.5  
0.5 0.5 1.0  
2 2  
Cartesian  
0.0 0.0 0.0  
1.0 1.0 1.0  
0.5 0.5 0.5  
1.5 1.5 1.5

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# Dielectric properties of Si

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## Task

Calculation of the static and frequency dependent dielectric properties of Si. Please have a look at the example on [calculation of the static and frequency dependent dielectric properties of SiC](#) first. The same procedures apply to this example.

## Input

### POSCAR

```
system Si
5.430
0.5 0.5 0.0
0.0 0.5 0.5
0.5 0.0 0.5
2
cart
0.00 0.00 0.00
0.25 0.25 0.25
```

### INCAR

- INCAR file for the static calculation:

```
## Static dielectric properties by means of DFPT
#NBANDS = 4
#EDIFF = 1E-6
#LEPSILON = .TRUE.
## try to add this to the DFPT calculation
#LPEAD = .TRUE.
## to get the ionic contributions to the
## static dielectric properties from
## perturbation theory
#IBRION = 8

## Static dielectric properties by means of PEAD
#EDIFF = 1E-8 # finite field requires very tight convergence
#LCALCEPS = .TRUE.
#NELM = 100

## Leave this in
ISMEAR = 0
SIGMA = 0.01
GGA = PE
```

- INCAR for the frequency dependent calculation:

```
## Frequency dependent dielectric tensor without
## local field effects
#ALGO = Exact
#NBANDS = 64
#LOPTICS = .TRUE. ; CSHIFT = 0.1
#NEDOS = 2000
## and you might try with the following
#LPEAD = .TRUE.

## Frequency dependent dielectric tensor with and
## without local field effects in RPA and due to
## changes in the DFT xc-potential
## N.B.: beware one first has to have done a
## calculation with LOPTICS = .TRUE. (see above)
#ALGO = CHI ; LSPECTRAL = .FALSE.
#LRPA = .FALSE.
## be sure to take the same number of bands as for
## the LOPTICS = .TRUE. calculation, otherwise the
## WAVEDER file is not read correctly
```

```
# NBANDS = 64
```

```
## Leave this in  
ISMEAR = 0  
SIGMA = 0.01  
GGA = PE
```

## Calculation

## Download

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# Dielectric properties of Si using BSE

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- 3.3 Step 3: RPA quasiparticles with single-shot GW (G0W0)
- 3.4 Step 4 (optional): Plot IPA dielectric function using GW0 quasiparticle energies
- 3.5 Step 5: The BSE calculation

#### 4 Download

## Task

Description: Calculate the dielectric function of Si including excitonic effects by solving the Bethe-Salpeter equation (BSE) on top of G0W0.

## Input

### POSCAR

```
Si
5.4300
0.5 0.5 0.0
0.0 0.5 0.5
0.5 0.0 0.5
2
cart
0.00 0.00 0.00
0.25 0.25 0.25
```

### INCAR

- This is the [INCAR](#) file for the basic DFT calculation:

```
System = Si
PREC = Normal ; ENCUT = 250.0
ISMEAR = 0 ; SIGMA = 0.01
KPAR = 2
EDIFF = 1.E-8
```

### KPOINTS

```
Automatic
0
Gamma
6 6 6
0 0 0
```

## Calculation

- The workflow of GW0+BSE calculations is given in doall.sh and consists of the following consecutive steps:
  1. "Standard" DFT groundstate calculation.
  2. Obtain virtual orbitals: needs [WAVECAR](#) file from step 1.
  3. The GW0 calculation: need [WAVECAR](#) and [WAVEDER](#) from step 2.
  4. Optional step: use [LOPTICS=.TRUE.](#) to plot dielectric function in the independent particle approximation (IPA) using GW0 quasiparticle energies instead of DFT energies.
  5. The BSE calculation: needs [WAVECAR](#) from step 3 and [WAVEDER](#) from step 2.

### Step 1: DFT groundstate calculation

- We perform standard DFT calculation using the INCAR.DFT file.

### Step 2: Obtain DFT "virtual" orbitals (empty states)

- This step uses the INCAR.DIAG file:

```
System = Si
PREC = Normal ; ENCUT = 250.0
ALGO = EXACT ; NELM = 1
ISMEAR = 0 ; SIGMA = 0.01
KPAR = 2
NBANDS = 128
LOPTICS = .TRUE. ; LPEAD = .TRUE.
OMEGAMAX = 40
```

- We use exact diagonalization for this step (`ALGO=EXACT`) and keep 128 bands after diagonalization (`NBANDS=128`).
- With `LPEAD=.TRUE.` we use an alternative way of computing the derivates of the orbitals with respect to the Bloch wave vectors.
- It is important that this calculations needs the orbitals (`WAVECAR` file) written in step 1.

### Step 3: RPA quasiparticles with single-shot GW (G0W0)

- This step uses the INCAR.GW0 file:

```
System = Si
PREC = Normal ; ENCUT = 250.0
ALGO = GWO
ISMEAR = 0 ; SIGMA = 0.01
ENCUTGW = 150 ; NELM = 1 ; NOMEGA = 50 ; OMEGATL = 280
KPAR = 2
#NBANDSO=4 ; NBANDSV=8 ; LADDER=.TRUE. ; LUSEW=.TRUE.
NBANDS = 128
NBANDSGW = 12
LWAVE = .TRUE.
PRECFOCK = Normal
```

- We select the G0W0 method by specifying `ALGO=GWO` and `NELM=1`.
- The energy cut off for the response function is select by `ENCUTGW`.
- The number of point used in the frequency integration is given by `NOMEGA`.
- Use the same number of bands (`NBANDS`) as in step 2, otherwise the `WAVEDER` file is not read correctly.
- The quasiparticle energies are calculated for the first few bands given by `NBANDSGW`.
- It is important that this calculation needs the orbitals (`WAVECAR` file) and the derivatives of the orbitals with respect to the Bloch vectors (`WAVEDER` file).
- The quasiparticle energies can be found in the `OUTCAR` file (saved as OUTCAR.GW0 in this example):

```
QP shifts <psi_nk| G(iteration)W_0 |psi_nk>: iteration 1
for sc-GW calculations column KS-energies equals QP-energies in previous step
and V_xc(KS)= KS-energies - (<T + V_ion + V_H > + <T+V_H+V_ion>^1 + <V_x>^1)

k-point 1 : 0.0000 0.0000 0.0000
band No. KS-energies QP-energies sigma(KS) V_xc(KS) V^pw_x(r,r') Z occupation
```

### Step 4 (optional): Plot IPA dielectric function using GW0 quasiparticle energies

- This step uses the INCAR.NONE file:

```
System = Si
PREC = Normal ; ENCUT = 250.0
ALGO = Nothing ; NELM = 1
ISMEAR = 0 ; SIGMA = 0.01
KPAR = 2
NBANDS = 128
LWAVE = .FALSE.
LOPTICS = .TRUE. ; LPEAD = .TRUE.
OMEGAMAX = 40
```

- By specifying `ALGO=Nothing` we do nothing except reading the `WAVECAR` file.
- Using `LOPTICS=.TRUE.` and `LPEAD=.TRUE.` we compute the dielectric function in the IPA.

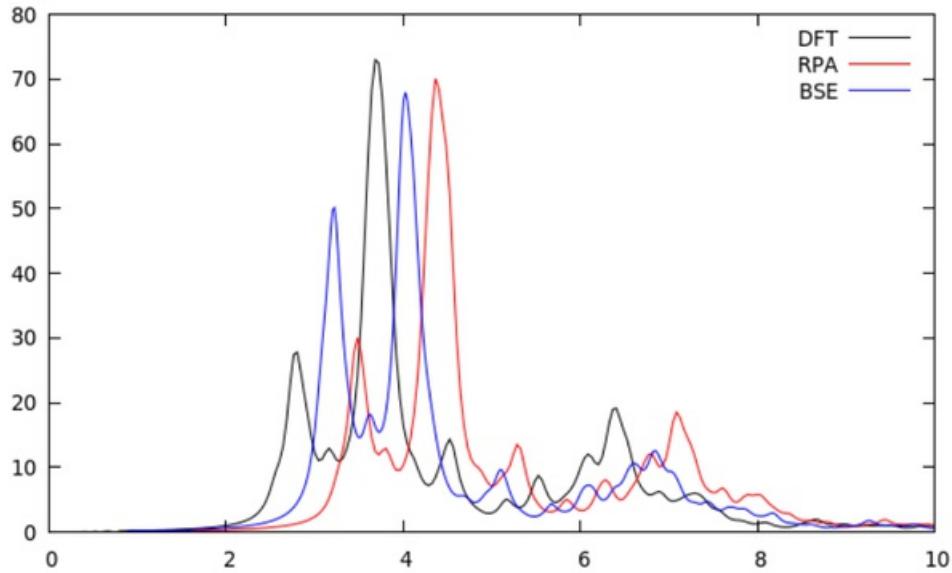
### Step 5: The BSE calculation

- This step uses the INCAR.BSE file:

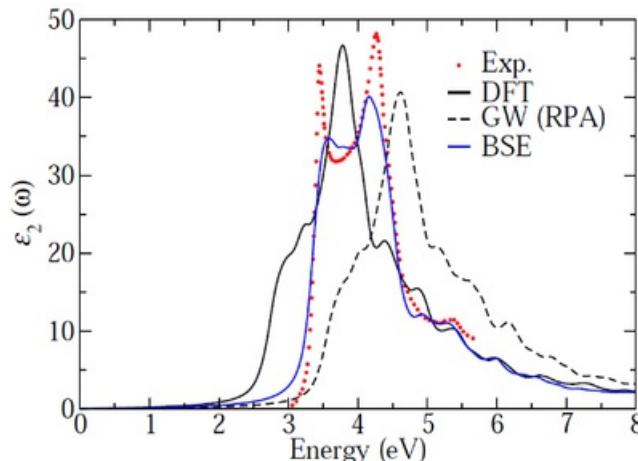
```
PREC = Normal ; ENCUT = 250.0
ALGO = BSE
ANTIRES = 0
ISMEAR = 0 ; SIGMA = 0.01
ENCUTGW = 150
EDIFF = 1.E-8
NBANDS = 128
NBANDSO = 4
NBANDSV = 8
OMEGAMAX = 20
PRECFOCK = Normal
```

- By specifying `ANTIRES=0` we use the Tamm-Dancoff approximation.

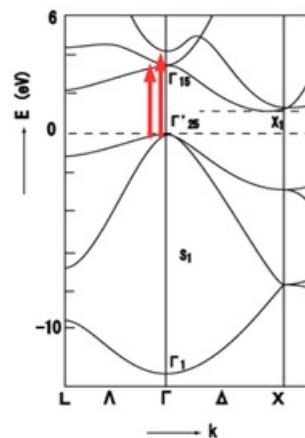
- `ENCUTGW=150` specifies the energy cut-off of the response function.
- `NBANDSO` and `NBANDSV` define the number of valence and conduction bands in the calculations.
- This calculation needs the orbitals (`WAVECAR` file) from step 3 and the derivative of the orbitals with respect to the Bloch vectors (`WAVEDER` file) written in step 2.
- By using the script `./plotall.sh` we get the absorption spectra within the independent particle picture and with BSE:



- The calculated dielectric function of Si is at this point (GW+BSE) already in much better agreement with experiment. However we can do even better as shown in the following figure:



- The problem comes from the coarse k-point grid that we have used. A denser grid samples more (direct) transitions between the bands.



- Simply using a denser grid is mostly not an option because of the computational expense.

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[Si\\_BSE.tgz](#)

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# Dielectric properties of SiC

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## Task

Calculation of the static and frequency dependent dielectric properties of SiC.

### Static dielectric properties

#### Density functional perturbation theory

Let us start with the calculation of the static dielectric properties. The most convenient way to determine the Born effective charges, dielectric-, piezoelectric tensors is by means of density functional perturbation theory ([LEPSILON=.TRUE.](#)).

- [INCAR](#) (see INCAR.LEPSILON)

```
ISMEAR = 0
SIGMA = 0.01
EDIFF = 1.E-8

## to get the Born effective charges
## and the macroscopic dielectric tensor
LEPSILON = .TRUE.

#LRPA = .TRUE.
#LPEAD = .TRUE.

## to get the ionic contribution
## to the macroscopic dielectric tensor
#IBRION = 8

## As an alternative to LEPSILON = .TRUE.
## you might try the following:
#LCALCEPS = .TRUE.

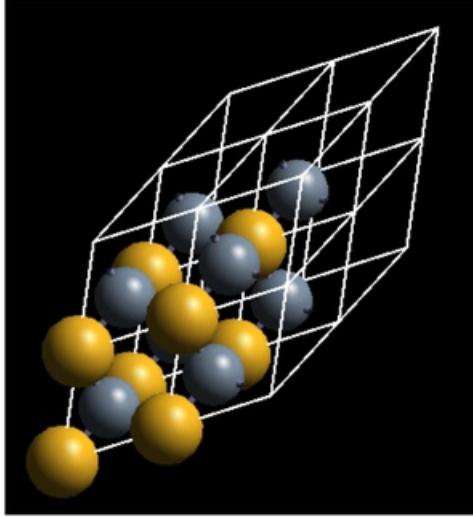
## and:
#IBRION = 6
#NFREE = 2
```

- [KPOINTS](#) (see KPOINTS.8)

```
8x8x8
0
G
8 8 8
0 0 0
```

- [POSCAR](#)

```
system SiC
4.35
0.5 0.5 0.0
0.0 0.5 0.5
0.5 0.0 0.5
1 1
cart
0.00 0.00 0.00
0.25 0.25 0.25
```



- The [LRPA](#)-tag

By default the dielectric tensor is calculated in the independent-particle (IP) approximation, you should see the following lines in the [OUTCAR](#) file:

```
HEAD OF MICROSCOPIC STATIC DIELECTRIC TENSOR (independent particle, excluding Hartree and local field effects)
```

and

```
MACROSCOPIC STATIC DIELECTRIC TENSOR (including local field effects in DFT)
```

which comes later in the [OUTCAR](#) file.

If one adds

```
LRPA=.TRUE.
```

to the [INCAR](#) above, the second instance will include local field effect only with respect to the response in the Hartree part of the potential, i.e., in the *random-phase-approximation* (RPA). Search for

```
MACROSCOPIC STATIC DIELECTRIC TENSOR (including local field effects in RPA (Hartree))
```

in the [OUTCAR](#).

- The Born effective charge tensors ( $Z_{ij}^*$ )

Roughly speaking, the Born effective tensors provide a measure of how much charge effectively moves with an atom when you displace it. For a definition see the article on [Berry phases and finite electric fields](#). For [LEPSILON=.TRUE.](#), the Born effective charge tensors are written near the end of the [OUTCAR](#) file.

Look for

```
BORN EFFECTIVE CHARGES (in e, cummulative output)
```

**Mind:** you will find this entry only if [LRPA=.FALSE.](#) (default), since the Born-effective charges in the RPA tend to be nonsensical.

- The [LPEAD](#)-tag

As an alternative to solving a linear Sternheimer equation (Eq. 32 of [\[1\]](#)), one may compute  $|\nabla_{\mathbf{k}} \tilde{u}_{\mathbf{nk}}\rangle$  from finite differences by specifying

```
LPEAD=.TRUE.
```

in the [INCAR](#) file. The derivative of the cell-periodic part of the wave function w.r.t. the Bloch vector is then computed by means of a fourth-order finite difference stencil, in the spirit of Eqs. 96 and 97 of [\[2\]](#). The results of the calculation of static dielectric properties by means of [LEPSILON=.TRUE.](#) tend to converge more rapidly w.r.t.  $\mathbf{k}$ -point sampling with [LPEAD=.TRUE.](#).

Rerun the example with

```
ISMEAR = 0
SIGMA = 0.01
EDIFF = 1.E-8
```

```

## to get the Born effective charges
## and the macroscopic dielectric tensor
LEPSILON = .TRUE.
LPEAD = .TRUE.

```

This will allow for a clean comparison with the next topic.

## Response to finite electric fields

The second way one may compute the static dielectric properties is from [self-consistent response of the system to a finite electric field](#).<sup>[3]</sup>

- [INCAR](#)

```

ISMEAR = 0
SIGMA = 0.01
EDIFF = 1.E-8

LCALCEPS = .TRUE.

```

## Ionic contributions to the static dielectric properties

To obtain the ionic contributions to the static dielectric properties one needs to compute the force-constant matrices (Hessian of the total energy w.r.t. the ionic positions) and internal strain tensors (second derivative of the total energy w.r.t. strain fields and ionic postions). These properties may be obtained from finite differences ([IBRION](#)=5 or 6) or from perturbation theory ([IBRION](#)=7 or 8). Try the following

- [INCAR](#)

```

ISMEAR = 0
SIGMA = 0.01
EDIFF = 1.E-8

## to get the Born effective charges
## and the macroscopic dielectric tensor
LEPSILON = .TRUE.
LPEAD = .TRUE.

## to get the ionic contribution
## to the macroscopic dielectric tensor
IBRION = 8

```

and search for

[MACROSCOPIC STATIC DIELECTRIC TENSOR IONIC CONTRIBUTION](#)

[ELASTIC MODULI IONIC CONTR \(kBar\)](#)

[PIEZOELECTRIC TENSOR IONIC CONTR for field in x, y, z \(C/m^2\)](#)

in the [OUTCAR](#) file.

## Frequency dependent dielectric response

Frequency dependent dielectric functions may be computed at various levels of approximation:

1. In the independent-particle approximation.
2. Including local field effects in the random-phase-approximation.
3. Including local field effects in DFT.

Whatever we may choose to do afterwards in terms of dielectric response calculations, we have to start with a standard DFT (or hybrid functional) calculation

- [INCAR](#) (see INCAR.DFT)

```

ISMEAR = 0
SIGMA = 0.01
EDIFF = 1.E-8

```

- [KPOINTS](#) (see KPOINTS.6)

```

6x6x6
0
G
6 6 6
0 0 0

```

**Mind:** keep the **WAVECAR** file, you're going to need it in the following.

## The independent-particle picture

To compute the frequency dependent dielectric function in the independent-particle (IP) picture we restart from the **WAVECAR** of the previous run, with the following **INCAR**

- **INCAR** (see **INCARLOPTICS**)

```
ALGO = Exact
NBANDS = 64
LOPTICS = .TRUE. ; CSHIFT = 0.100
NEDOS = 2000

## and you might try with the following
#LPEAD = .TRUE.

ISMEAR = 0
SIGMA = 0.01
EDIFF = 1.E-8
```

The frequency dependent dielectric functions is written to the **OUTCAR** file. Search for

```
frequency dependent IMAGINARY DIELECTRIC FUNCTION (independent particle, no local field effects)
```

and

```
frequency dependent REAL DIELECTRIC FUNCTION (independent particle, no local field effects)
```

To visualize the real and imaginary parts of the frequency dependent dielectric function you may use p4vasp

```
p4v vasprun.xml
```

or run the following bash-script (**plotoptics2**)

```
awk 'BEGIN{i=1} /imag/,\
    /\Vimag/ \
    {a[i]="$2 ; b[i]="$3 ; i=i+1} \
END{for (j=12;j<i-3;j++) print a[j],b[j]}' vasprun.xml > imag.dat

awk 'BEGIN{i=1} /real/,\
    /\Vreal/ \
    {a[i]="$2 ; b[i]="$3 ; i=i+1} \
END{for (j=12;j<i-3;j++) print a[j],b[j]}' vasprun.xml > real.dat

cat >plotfile<<!
# set term postscript enhanced eps colour lw 2 "Helvetica" 20
# set output "optics.eps"
plot [0:25] "imag.dat" using ($1):($2) w lp, "real.dat" using ($1):($2) w lp
!

gnuplot -persist plotfile
```

- **LPEAD-tag**

As an alternative to the perturbative expression (Eq. 31 of [\[1\]](#)), one may compute  $|\nabla_{\mathbf{k}} \tilde{u}_{\mathbf{n}\mathbf{k}}\rangle$  from finite differences by specifying

```
LPEAD=.TRUE.
```

in the **INCAR** file. The derivative of the cell-periodic part of the wave function w.r.t. the Bloch vector is then computed by means of a fourth-order finite difference stencil, in the spirit of Eqs. 96 and 97 of [\[2\]](#).

**Mind:** keep the **WAVECAR** and **WAVEDER** files, you're going to need them in the following. You might also want to keep a copy of the **vasprun.xml**.

```
cp vasprun.xml vasprun_loptics.xml
```

## Including local field effects

To determine the frequency dependent dielectric function including local field effects one needs the **WAVECAR** and **WAVEDER** files from the previous calculation (**ALGO**=Exact and **LOPTICS**=.TRUE., and sufficient virtual orbitals), and

- **INCAR** (see **INCAR.CHI**)

```
# Frequency dependent dielectric tensor with and
# without local field effects in RPA
# N.B.: beware one first has to have done a
# calculation with ALGO=Exact, LOPTICS=.TRUE.
```

```

# and a reasonable number of virtual states (see above)
ALGO = CHI

# be sure to take the same number of bands as for
# the LOPTICS=.TRUE. calculation, otherwise the
# WAVEDER file is not read correctly
NBANDS = 64

ISMEAR = 0
SIGMA = 0.01
EDIFF = 1.E-8

LWAVE = .FALSE.
LCHARG= .FALSE.

```

Information concerning the dielectric function in the independent-particle picture is written after the line

**HEAD OF MICROSCOPIC DIELECTRIC TENSOR (INDEPENDENT PARTICLE)**

in the **OUTCAR** file.

Per default, for **ALGO=CHI**, local field effects are included at the level of the RPA (**LRPA=.TRUE.**), i.e., limited to Hartree contributions only.

See the information after

**INVERSE MACROSCOPIC DIELECTRIC TENSOR (including local field effects in RPA (Hartree))**

in the **OUTCAR** file.

To include local field effects beyond the RPA, i.e., contributions from DFT exchange and correlation, one has to specify

**LRPA=.FALSE.**

in the **INCAR** file.

In this case look at the output after

**INVERSE MACROSCOPIC DIELECTRIC TENSOR (test charge-test charge, local field effects in DFT)**

in the **OUTCAR** file.

The following bash-script (plotchi) uses *awk* to extract the frequency dependent dielectric constant, both in the independent-particle picture as well as including local field effects (either in DFT or in the RPA) and plots the real and imaginary components using *gnuplot*:

```

awk 'BEGIN{i=1} /HEAD OF MICRO/,\
/XI_LOCAL/ \
{if ($4=="dielectric") {a[i]="$1 ; b[i]="$2 ; c[i]="$3 ; i=i+1}} \
END{for (j=1;j<i;j++) print a[j],b[j],c[j]}' OUTCAR > chi0.dat

awk 'BEGIN{i=1} /INVERSE MACRO/,\
/XI_TO_W/ \
{if ($4=="dielectric") {a[i]="$1 ; b[i]="$2 ; c[i]="$3 ; i=i+1}} \
END{for (j=1;j<i;j++) print a[j],b[j],c[j]}' OUTCAR > chi.dat
cat >plotfile<<!
# set term postscript enhanced eps colour lw 2 "Helvetica" 20
# set output "optics.eps"
plot "chi0.dat" using ($1):($2) w lp lt -1 lw 2 pt 4 title "chi0 real", \
"chi0.dat" using ($1):(-$3) w lp lt 0 lw 2 pt 4 title "chi0 imag", \
"chi.dat" using ($1):($2) w lp lt 1 lw 2 pt 2 title "chi real", \
"chi.dat" using ($1):(-$3) w lp lt 0 lw 2 pt 2 lc 1 title "chi imag"
!
gnuplot -persist plotfile

```

If you have kept a copy of the **vasprun.xml** of the **LOPTICS=.TRUE.** run (e.g., **vasprun\_loptics.xml**), you might execute **plotall** to compare the dielectric functions computed with **LOPTICS=.TRUE.** and **ALGO=CHI**.

```

vasprun_LOPTICS=vasprun_loptics.xml
OUTCAR_CHI=OUTCAR

awk 'BEGIN{i=1} /imag/,\
/\imag/ \
{a[i]="$2 ; b[i]="$3 ; i=i+1} \
END{for (j=12;j<i-3;j++) print a[j],b[j]}' $vasprun_LOPTICS > imag.dat

awk 'BEGIN{i=1} /real/,\
/\real/ \
{a[i]="$2 ; b[i]="$3 ; i=i+1} \
END{for (j=12;j<i-3;j++) print a[j],b[j]}' $vasprun_LOPTICS > real.dat

```

```

awk 'BEGIN{i=1} /HEAD OF MICRO/,\
    /XI_LOCAL/ \
    {if ($4=="dielectric") {a[i]=$("#1"; b[i]=$("#2"; c[i]=$("#3; i=i+1})} \
END{for (j=1;j<i;j++) print a[j],b[j],c[j])' $OUTCAR_CHI > chi0.dat

awk 'BEGIN{i=1} /INVERSE MACRO/,\
    /XI_TO_W/ \
    {if ($4=="dielectric") {a[i]=$("#1"; b[i]=$("#2; c[i]=$("#3; i=i+1})} \
END{for (j=1;j<i;j++) print a[j],b[j],c[j])' $OUTCAR_CHI > chi.dat

cat >plotfile<<!
# set term postscript enhanced eps colour lw 2 "Helvetica" 20
# set output "optics.eps"

plot "chi0.dat" using ($1):($2) w lp lt -1 lw 2 pt 4 title "chi0 real", \
"chi0.dat" using ($1):(-$3) w lp lt 0 lw 2 pt 4 title "chi0 imag", \
"chi.dat" using ($1):($2) w lp lt 1 lw 2 pt 2 title "chi real", \
"chi.dat" using ($1):(-$3) w lp lt 0 lw 2 pt 2 lc 1 title "chi imag", \
"real.dat" using ($1):($2) w l lt -1 title "optics real", \
"imag.dat" using ($1):(-$2) w l lt 0 lc -1 title "optics imag"
!

gnuplot -persist plotfile

```

Why are the dielectric functions in independent-particle picture from the `LOPTICS=.TRUE.` and the `ALGO=CHI` calculations different?

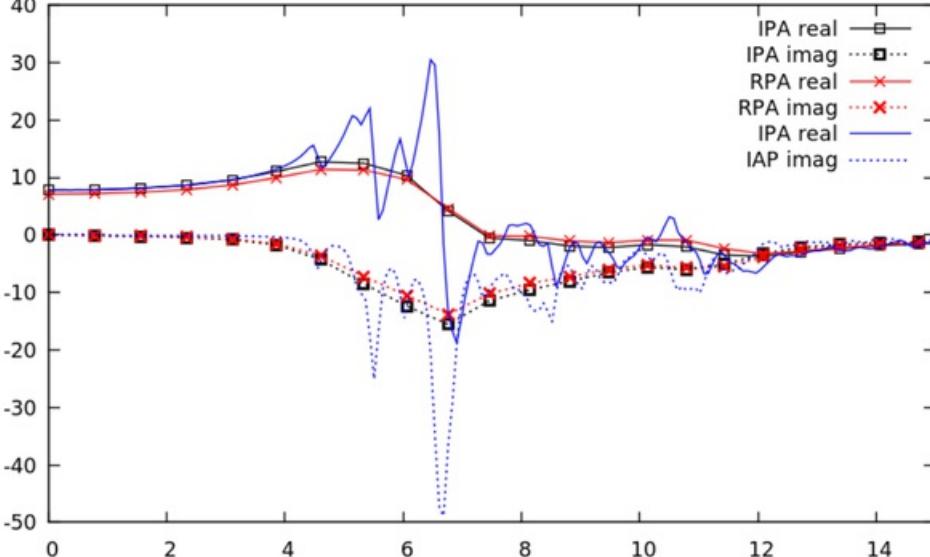
Hints:

- What `CSHIFT` is used in the `ALGO=CHI` calculation?

Try redoing the `LOPTICS=.TRUE.` calculation with the same `CSHIFT` as VASP chose for the `ALGO=CHI` calculation (see INCAR.LOPTICS2):

`CSHIFT=0.466`

- Redo the `ALGO=CHI` calculation with `LSPECTRAL=.FALSE.` in the `ALGO=CHI` calculation (see INCAR.CHII2). and compare the dielectric functions again.
- The sample output (using a  $6 \times 6 \times 6$  mesh for the k points) should look like the following:



## Download

[SiC\\_dielectric.tgz](#)

## References

- ↑ a b M. Gajdoš, K. Hummer, G. Kresse, J. Furthmüller, and F. Bechstedt, Phys. Rev. B 73, 045112 (2006).
- ↑ a b R. W. Nunes and X. Gonze, Phys. Rev. B 63, 155107 (2001).
- ↑ I. Souza, J. Iñiguez, and D. Vanderbilt, Phys. Rev. Lett. 89, 117602 (2002).

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**Task**

Calculation of the equilibrium lattice constant of Si in the RPA (ACFDT).

**Input****POSCAR**

```
system Si
5.8
0.5 0.5 0.0
0.0 0.5 0.5
0.5 0.0 0.5
2
cart
0.00 0.00 0.00
0.25 0.25 0.25
```

**Calculation**

The workflow of RPA total energy calculations consists of five consecutive steps:

- Step 1: a "standard" DFT groundstate calculation with a "dense" mesh of k-points.
- Step 2: compute the Hartree-Fock energy using the orbitals of Step 1. Needs [WAVECAR](#) file from step 1.
- Step 3: a "standard" DFT groundstate calculation with "coarse" mesh of k-points.
- Step 4: obtain DFT "virtual" orbitals (empty states). Needs [WAVECAR](#) file from step 3.
- Step 5: the RPA correlation energy (ACFDT) calculation. Needs [WAVECAR](#) and [WAVEDER](#) files from step 4.

In case of metallic systems there is an additional step between Steps 4 and 5, that is beyond the scope of this example.

All of the calculation steps are prepared in the script doall.sh.

**Step 1**

- DFT groundstate calculation with a "dense" mesh of k-points
- The following [INCAR](#) file is used (INCAR.DFT):

```
ISMEAR = 0 ; SIGMA = 0.05
EDIFF = 1E-8
```

- The following [KPOINTS](#) file is used (KPOINTS.12):

```
12x12x12
0
G
12 12 12
0 0 0
```

**Step 2**

- Compute the Hartree-Fock energy using the DFT orbitals ([WAVECAR](#)) of Step 1.
- The [INCAR](#) file INCAR.EXX is used in this step:

```
ALGO = EIGENVAL ; NELM = 1
LWAVE = .FALSE.
LHFCA = .TRUE.
AEXX = 1.0 ; ALDAC = 0.0 ; AGGAC = 0.0
NKRED = 2
ISMEAR = 0 ; SIGMA = 0.05
KPAR = 8
NBANDS = 4
```

- **NKRED=2** is used for the downsample the k-space representation of the Fock-potential to save time.
- Using **NBANDS=4** only occupied states are considered to save time.

**Step 3**

- DFT groundstate calculation with a "coarse" mesh of k-points.
- The following [INCAR](#) file is used (INCAR.DFT):

```
ISMEAR = 0 ; SIGMA = 0.05
EDIFF = 1E-8
```

- The following coarse [KPOINTS](#) file is used (KPOINTS.12):

```
6x6x6
0
G
6 6 6
0 0 0
```

## Step 4

- Obtain DFT "virtual" orbitals (empty states).
- The following **INCAR** file is used in this step (INCAR.DIAG):

```
ALGO = Exact  
NBANDS = 64  
NELM = 1  
LOPTICS = .TRUE.  
ISMEAR = 0 ; SIGMA = 0.05
```

- In this step one needs to set **LOPTICS=.TRUE.** to have VASP calculate the derivative of the orbitals w.r.t. the Bloch wavevector (stored in the **WAVEDER** file). These are needed to correctly describe the long-wavelength limit of the dielectric screening.
- We use exact diagonalization (**ALGO=Exact**) and keep 64 bands after diagonalization (**NBANDS=64**).
- This calculations needs the orbitals (**WAVECAR** file) written in Step 3.

## Step 5

- The RPA correlation energy (ACFDT) calculation.
- The following **INCAR** file is used in this step (INCAR.ACFDT):

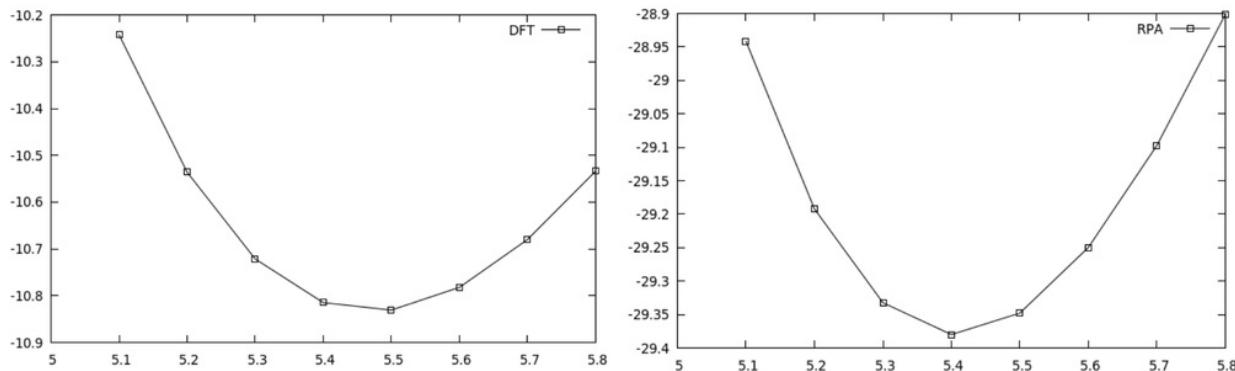
```
ALGO = ACFDT  
NBANDS = 64  
ISMEAR = 0 ; SIGMA = 0.05
```

- In OUTCAR.ACFDT.X.X one finds the RPA correlation energy, e.g.:

cutoff energy	smooth cutoff	RPA	correlation	Hartree contr. to MP2
163.563	130.851	-10.7869840331	-19.0268026572	
155.775	124.620	-10.7813600055	-19.0200457142	
148.357	118.685	-10.7744584182	-19.0118291822	
141.292	113.034	-10.7659931963	-19.0017871991	
134.564	107.651	-10.7555712745	-18.9894197881	
128.156	102.525	-10.7428704760	-18.9742991317	
122.054	97.643	-10.7273118140	-18.9556871679	
116.241	92.993	-10.7085991597	-18.9331679971	

linear regression converged value -10.9079580568 -19.1711146204

- Take the "converged value", in this case:  $EC(RPA) = -10.9079580568\text{eV}$  (an approximate "infinite basis set" limit).
- This calculations needs the orbitals (**WAVECAR** file) and the derivative of the orbitals w.r.t. the Bloch wavevectors (**WAVEDER** file) written in Step 4.
- The RPA total energy is calculated as the,  $E(RPA)=EC(RPA)+EXX$  sum of the RPA correlation energy of step 5  $EC(RPA)$  and the Hartree fock energy  $EXX$ . To get the Hartree fock energy grep "free energy" in the OUTCAR.EXX.\* file (there are two spaces between free and energy).
- The sample output for the total energy vs volume curves for DFT and RPA should look like the following:



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## Estimation of J magnetic coupling

Description: Estimation of the J magnetic exchange coupling using the GGA+U method.

Switching off the symmetry ([ISYM = 0](#)) is often necessary to generate different magnetic configurations.

**Exercise :** Study the change of the 180° superexchange coupling  $J_2$  between the next nearest neighbors ( $d_{Ni-Ni} = 4.17 \text{ \AA}$ ) by varying the  $U_{eff}$  value. The following equation  $J_2 = (E_{FM} - E_{AFM}) / 12$  expresses the super exchange Ni-O-Ni coupling as a function of the energy difference of the ferromagnetic (FM) and antiferromagnetic (AFM) configurations. In this case, the superexchange coupling  $J_1$  between the nearest neighbors is neglected. The theoretical results can be compared to the experimental one :  $J_2 = 19.01 \text{ meV}$  (Hutchings M. T., Samuels E. J., *Phys. Rev. B* 6, 9, **1972**, 3447)

### ■ INCAR

```
NiO GGA+U AFM
SYSTEM = "NiO"
```

```
Electronic minimization
ENCUT = 450
EDIFF = 1E-4
LORBIT = 11
LREAL = .False.
ISTART = 0
ISYM = 0
NELMIN = 6
```

```
DOS
ISMEAR = -5
```

```
Magnetism
ISPIN = 2
MAGMOM = 2.0 -2.0 2*0 # AFM conf.
# MAGMOM = 2*2.0 2*0 # FM conf.
```

```
Mixer
AMIX = 0.2
BMIX = 0.00001
AMIX_MAG = 0.8
BMIX_MAG = 0.00001
```

```
GGA+U
LDAU = .TRUE.
LDAUTYPE = 2
LDAUL = 2 -1
LDAUU = 5.00 0.00
LDAUJ = 0.00 0.00
LDAUPRINT = 2
LMAXMIX = 4
```

### ■ KPOINTS

```
k-points
0
gamma
4 4 4
0 0 0
```

### ■ POSCAR

```
NiO
4.17
1.0 0.5 0.5
0.5 1.0 0.5
0.5 0.5 1.0
2 2
Cartesian
0.0 0.0 0.0
1.0 1.0 1.0
0.5 0.5 0.5
1.5 1.5 1.5
```

Necessarily, the J magnetic coupling decreases with the increasing of the  $U_{eff}$  value. To assess the obtained value, similar calculations could be done using a [hybrid functional](#).

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# Fcc Ni

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## Task

Lattice parameter optimization, calculation of the DOS and bandstructure in (spin-polarized) fcc Ni.

## Input

### POSCAR

```
fcc:
3.53
0.5 0.5 0.0
0.0 0.5 0.5
0.5 0.0 0.5
1
cartesian
0 0 0
```

### INCAR

```
SYSTEM = fcc Ni
ISTART = 0 ; ICHARG=2
ENCUT = 270
ISMEAR = 1 ; SIGMA = 0.2
LORBIT = 11
ISPIN = 2
MAGMOM = 1
```

- Initial charge-density from overlapping atoms in starting job.
- Default energy cutoff of 270 eV used ([ENCUT](#)=270).
- MP smearing used since we have a metal.
- Spin-polarized calculation [ISPIN](#)=2, initial moments of 1 ([MAGMOM](#)=1).
- Static calculation.

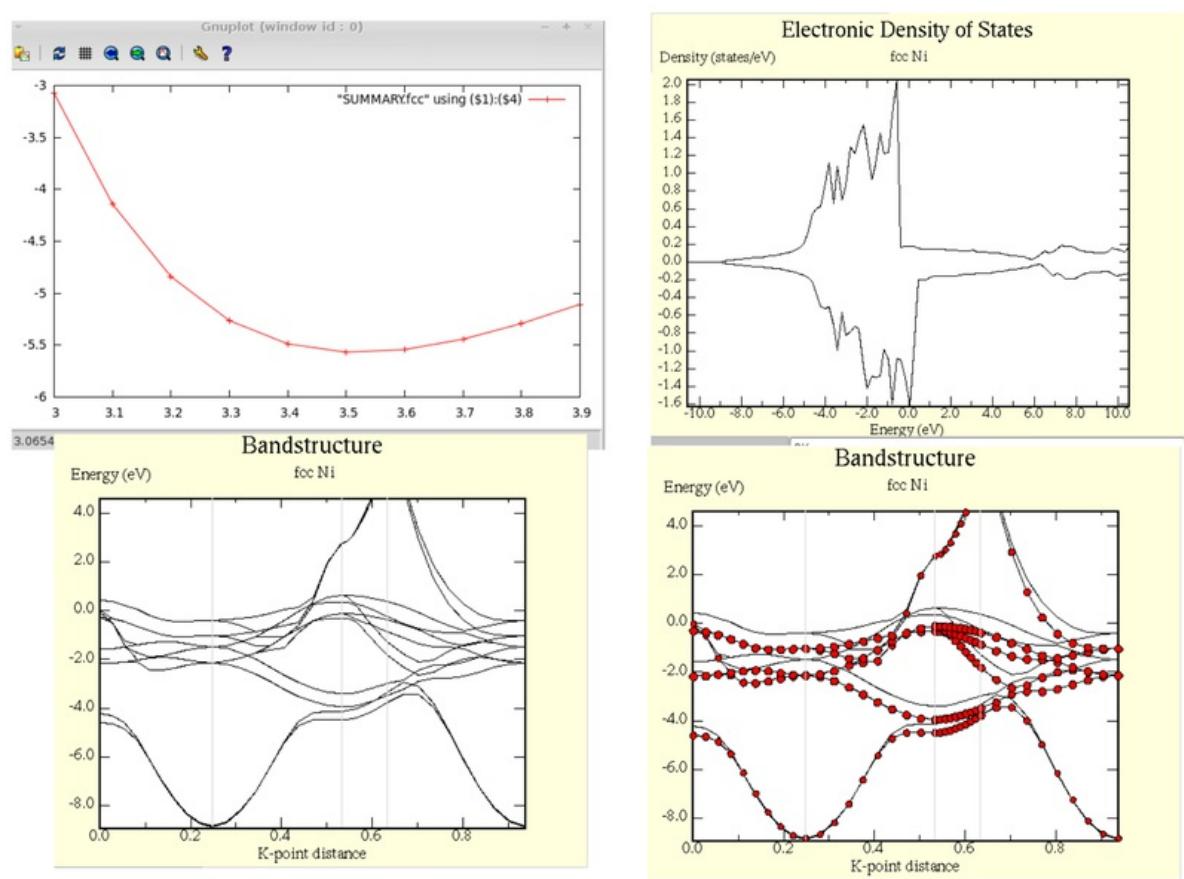
### KPOINTS

```
k-points
0
Monkhorst Pack
11 11 11
0 0 0
```

- Equally spaced k mesh with 56 points in the IBZ.
- Odd,  $\Gamma$ -centered mesh.

## Calculation

- The calculations are carried out in analogy to [cd Si](#). Please follow the instructions in that example.
- Here is a sample output of the results:



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# Fcc Ni (revisited)

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## Task

Calculation of the partial DOS of spin-polarized fcc Ni, a ferromagnet.

## Input

### POSCAR

```
fcc:
-10.93
0.5 0.5 0.0
0.0 0.5 0.5
0.5 0.0 0.5
1
Cartesian
0 0 0
```

### INCAR

```
SYSTEM = Ni fcc bulk
ISTART = 0
ISPIN = 2
MAGMOM = 1.0
ISMEAR = -5
VOSKOWN = 1
LORBIT = 11
```

- Spin-polarized calculation with initial magnetic moment of 1  $\mu\text{B}$ .
- Interpolation scheme of Vosko, Wilk and Nusair is used (see VOSKOWN=1).
- Im-decomposed DOSCAR is created.
- Tetrahedron method with Blöchl's corrections used for k-mesh integration.

### KPOINTS

```
k-points
0
Gamma
11 11 11
0 0 0
```

## Calculation

### Collinear case

- The output for the magnetic moments in the OSZICAR should look like the following:

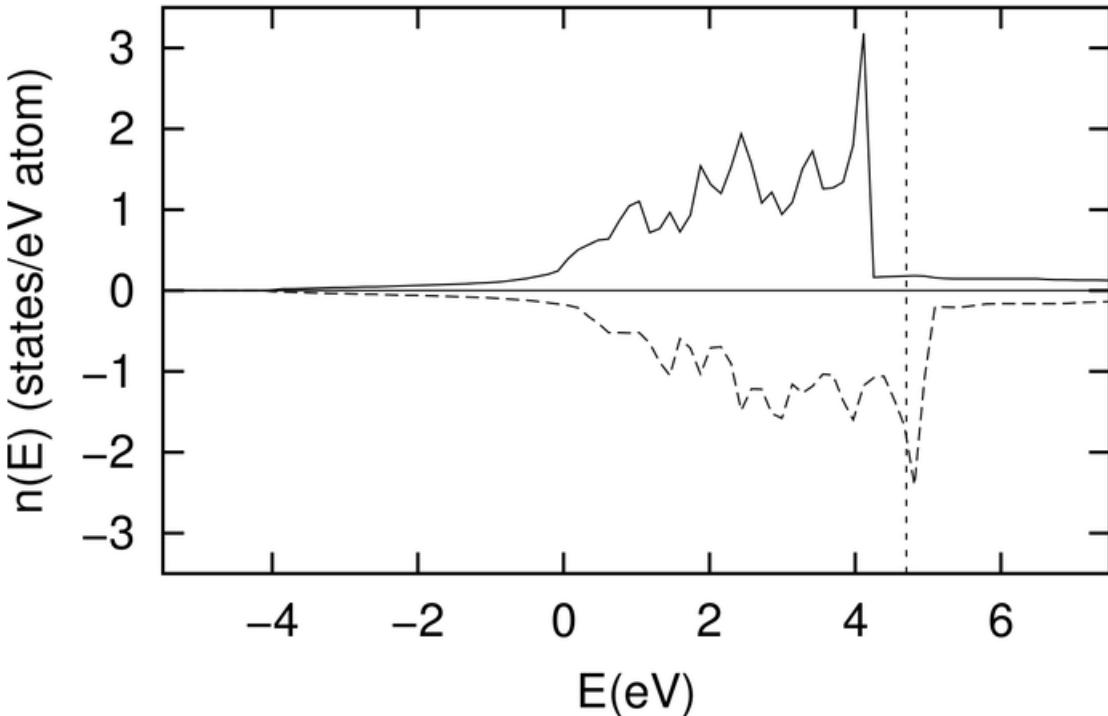
```
N      E
DAV: 1   0.139935173959E+02  0.13994E+02  -0.35801E+03  2338  0.828E+02
DAV: 2   -0.623612680591E+01  -0.20230E+02  -0.19281E+02  2282  0.123E+02
DAV: 3   -0.643764005251E+01  -0.20151E+00  -0.19906E+00  2536  0.140E+01
DAV: 4   -0.643786482872E+01  -0.22478E-03  -0.22442E-03  2344  0.459E-01
DAV: 5   -0.643786514671E+01  -0.31798E-06  -0.31687E-06  1832  0.173E-02  0.793E+00
...
DAV: 9   -0.545953126374E+01  0.48409E-02  -0.96206E-03  2946  0.839E-01  0.847E-02
DAV: 10  -0.545946513577E+01  0.66128E-04  -0.77007E-05  1364  0.126E-01
1 F= -.54594651E+01 E= -.54594651E+01 d E = 0.000000E+00 mag=  0.5781
```

- The I decomposed parts of the magnetic moment are written in the **OUTCAR** file:

```
magnetization (x)
```

# of ion	s	p	p	tot
1	-0.007	-0.026	0.625	0.591

- The example output for the spin up and down DOS shows an exchange splitting of approximately 0.5 eV:



- Proper initialization of magnetic moments is very important:

- Too small initial magnetic moments will/may lead to nonmagnetic solution (by starting with an initial moment of 0.0 we arrive only to a magnetic of 0.002).
- Badly initialized calculations take longer to converge.
- Coexistence of low- and high spin solutions.

### Noncollinear case

- For a noncollinear calculation replace **ISPIN=2** and **MAGMOM=1.0** in the **INCAR** file by the following:

```
LNONCOLLINEAR = .TRUE.
MAGMOM      = 0.0 0.0 1.0
```

- The last three lines of the **OSZICAR** file using this parameter should look like the following:

```
DAV: 9  -0.546480633680E+01  0.41628E-02  -0.49402E-04  7532  0.330E-01  0.695E-02
DAV: 10 -0.546475032360E+01  0.56013E-04  -0.52286E-05  4328  0.446E-02
1 F= -.54647503E+01 E0= -.54647503E+01 d E =0.000000E+00 mag= 0.0000  0.0000  0.5792
```

- By using **MAGMOM = 1.0 0.0 0.0** we get the following output:

```
DAV: 9  -0.546481348871E+01  0.41496E-02  -0.50294E-04  7548  0.330E-01  0.692E-02
DAV: 10 -0.546474438319E+01  0.69106E-04  -0.51451E-05  4288  0.432E-02
1 F= -.54647444E+01 E0= -.54647444E+01 d E =0.000000E+00 mag= 0.5792  0.0000  0.0000
```

- Analogously if we set **MAGMOM = 0.0 1.0 0.0** we get the following output:

```
DAV: 9  -0.546481179459E+01  0.41515E-02  -0.50430E-04  7552  0.330E-01  0.692E-02
DAV: 10 -0.546474640011E+01  0.65394E-04  -0.51658E-05  4292  0.434E-02
1 F= -.54647464E+01 E0= -.54647464E+01 d E =0.000000E+00 mag= 0.0000  0.5792  0.0000
```

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## Fcc Ni DOS

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## Task

Calculation of the DOS in fcc Ni.

## Incar

### POSCAR

```
fcc:
3.53
0.5 0.5 0.0
0.0 0.5 0.5
0.5 0.0 0.5
1
cartesian
0 0 0
```

## INCAR

```
SYSTEM = fcc Ni
ISTART = 0 ; ICHARG = 2
ENCUT = 270
ISMEAR = -5
LORBIT = 11

ISPIN = 2
MAGMOM = 1
```

## KPOINTS

```
k-points
0
Monkhorst Pack
11 11 11
0 0 0
```

## Calculation

- The bash-script `plotdos` invokes `awk` and `gnuplot` to get the DOS from the `vasprun.xml` file and plot it.

```
awk 'BEGIN{i=1} /dos>/,\n    /\dos>/\n    {a[i]=$2 ; b[i]=$3 ; i=i+1}\nEND{for (j=12;j<i-5;j++) print a[j],b[j]}' vasprun.xml > dos.dat\n\nef=`awk '/efermi/ {print $3}' vasprun.xml`\n\n cat >plotfile<<!\n# set term postscript enhanced eps colour lw 2 "Helvetica" 20\n# set output "optics.eps"\nplot "dos.dat" using ($1-$ef):($2) w lp\n!\n\n gnuplot -persist plotfile\nrm dos.dat plotfile
```

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# Fcc Ni DOS with hybrid functional

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## Task

Calculate fcc Ni DOS using HSE and PBE0 (comparison with PBE).

## Input

### POSCAR

```
fcc Ni
3.53
0.5 0.5 0.0
0.0 0.5 0.5
0.5 0.0 0.5
1
cartesian
0 0 0
```

### INCAR

```
## Plot the spin-polarized DOS of fcc Ni
## at HSE and PBE0 level, and compare with
## standard PBE.
## Better preconverge with PBE first!

SYSTEM = fcc Ni
ISMEAR = -5
LORBIT = 11

ISPIN = 2
MAGMOM = 1

## Selects the HSE06 hybrid function
#LHFCALC = .TRUE. ; HFSCREEN = 0.2 ;
#ALGO = D ; TIME = 0.4 ; LSUBROT = .TRUE.

## Selects the PBE0 hybrid function
#LHFCALC = .TRUE. ;
#ALGO = D ; TIME = 0.4 ; LSUBROT = .TRUE.
```

### KPOINTS

```
k-points
0
Gamma
5 5 5
0 0 0
```

## Calculation

## Download

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# Fcc Si

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## Task

Lattice constant optimization for fcc Si.

## Input

### POSCAR

```
fcc Si:  
3.9  
0.5 0.5 0.0  
0.0 0.5 0.5  
0.5 0.0 0.5  
1  
cartesian  
0 0 0
```

- Fcc Si lattice constant of 3.9 .
- 1 atom per unit cell.

### INCAR

```
System = fcc Si  
ISTART = 0 ; ICHARG = 2  
ENCUT = 240  
ISMEAR = 0; SIGMA = 0.1
```

- Initial charge density form overlapping atoms.
- Energy cutoff of 240 eV from [POTCAR](#) file.

### KPOINTS

```
k-points  
0  
Monkhorst Pack  
11 11 11  
0 0 0
```

- Equally spaced k mesh.
- Odd number of k points in each direction results in a  $\Gamma$  centered mesh.
- 56 k points in IBZ.

## Calculation

- Calculate energy for different lattice parameters.
- Fit to some equation of states to obtain the equilibrium volume.
- The bash-script loop.sh runs fcc Si at several different lattice constants (3.5-4.3 Å) and collects free energy versus lattice constant into the file SUMMARY.fcc

```
#!/bin/bash  
BIN=/path/to/your/vasp/executable  
rm WAVECAR SUMMARY.fcc  
for i in 3.5 3.6 3.7 3.8 3.9 4.0 4.1 4.2 4.3 ; do  
cat >POSCAR <<!  
fcc:  
$i  
0.5 0.5 0.0  
0.0 0.5 0.5  
0.5 0.0 0.5  
1  
cartesian  
0 0 0  
!  
echo "a= $i" ; mpirun -np 2 $BIN  
E=`awk '/F=/ {print $0}' OSZICAR` ; echo $i $E >>SUMMARY.fcc  
done  
cat SUMMARY.fcc
```

The output for the SUMMARY.fcc file within this example should look like this:

```
3.5 1 F= -.44256712E+01 E0= -.44233993E+01 d E =-.454388E-02
3.6 1 F= -.46614699E+01 E0= -.46600410E+01 d E =-.285796E-02
3.7 1 F= -.47979864E+01 E0= -.47959298E+01 d E =-.411323E-02
3.8 1 F= -.48645042E+01 E0= -.48630063E+01 d E =-.299564E-02
3.9 1 F= -.48773847E+01 E0= -.48758538E+01 d E =-.306176E-02
4.0 1 F= -.48487436E+01 E0= -.48481092E+01 d E =-.126878E-02
4.1 1 F= -.47852634E+01 E0= -.47844854E+01 d E =-.155599E-02
4.2 1 F= -.46936947E+01 E0= -.46922530E+01 d E =-.288339E-02
4.3 1 F= -.45831167E+01 E0= -.45811837E+01 d E =-.386598E-02
```

- To make a quick plot of SUMMARY.fcc try:

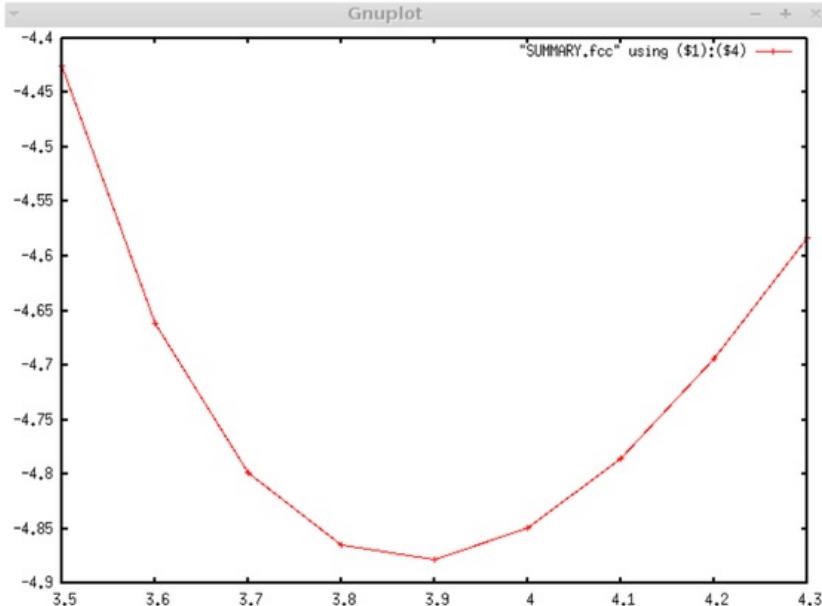
```
gnuplot
gnuplot> plot "SUMMARY.fcc" using ($1):($4) w lp
```

- The equilibrium lattice constant is found at roughly 3.9 . Adjust your [POSCAR](#) file to reflect this and rerun VASP.
- Keep your [CHGCAR](#) file from this run. We will need it in the following examples.
- A quick look at the results:

>gnuplot

```
gnuplot> plot "SUMMARY.fcc" using ($1):($4) w lp
gnuplot> exit
```

"kill the window with"



**Mind:** You will have to set the correct path to your VASP executable (i.e., BIN), and invoke VASP with the correct command (e.g., in the above: mpirun -np 2).

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# Fcc Si bandstructure

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## Task

Computation of the bandstructure in fcc Si along L- $\Gamma$ -X-U and K- $\Gamma$ .

## Input

### POSCAR

```
fcc Si:
3.9
0.5 0.5 0.0
0.0 0.5 0.5
0.5 0.0 0.5
1
cartesian
0 0 0
```

### INCAR

```
System = fcc Si
ICHARG = 11 #charge read file
ENCUT = 240
ISMEAR = 0; SIGMA = 0.1;
LORBIT = 11
```

### KPOINTS

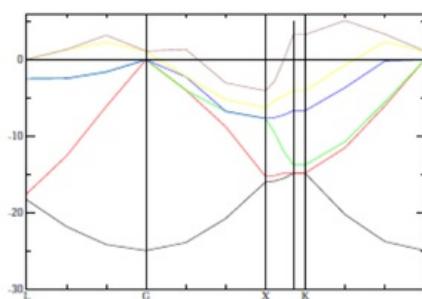
```
k-points for bandstructure L-G-X-U K-G
10
line
reciprocal
0.50000 0.50000 0.50000 1
0.00000 0.00000 0.00000 1

0.00000 0.00000 0.00000 1
0.00000 0.50000 0.50000 1

0.00000 0.50000 0.50000 1
0.25000 0.62500 0.62500 1

0.37500 0.7500 0.37500 1
0.00000 0.00000 0.00000 1
```

- k points along the line  $L - \Gamma - X - U\bar{K} - \Gamma$ .
- 10 points per line.
- Keyword *line* to generate bandstructure.
- In reciprocal coordinates.
- All points with weight 1.
- Example bandstructure should look like this:



### CHGCAR

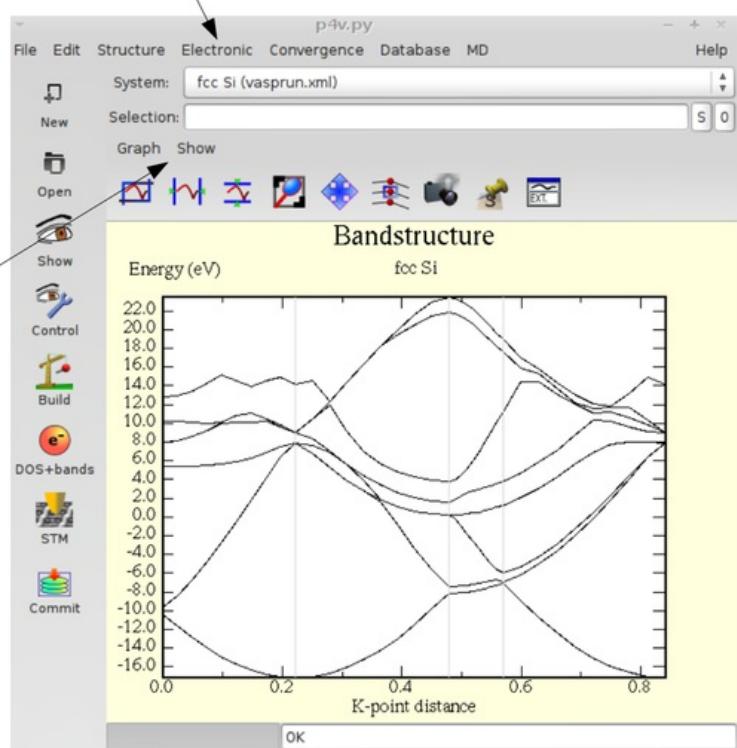
This calculation needs a converged charge density as input (`ICHARG=11`). You may use the `CHGCAR` file of the [fcc Si DOS](#) example.

## CALCULATION

- To copy the self-consistent charge density of example fccSidos to your current working directory, type: `$ cp ./fccSidos/CHGCAR`. You must do this otherwise VASP can not read the `CHGCAR` and will terminate.
- To plot the bandstructure use p4vasp:

Start p4vasp:  
> p4v [vasprun.xml]

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**Mind:** For this calculations you need the `CHGCAR` file of the [fcc Si DOS](#) example.

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# Fcc Si DOS

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## Task

Calculation of the DOS in fcc Si.

## Input

### POSCAR

```
fcc Si:  
3.9  
0.5 0.5 0.0  
0.0 0.5 0.5  
0.5 0.0 0.5  
1  
cartesian  
0 0 0
```

### INCAR

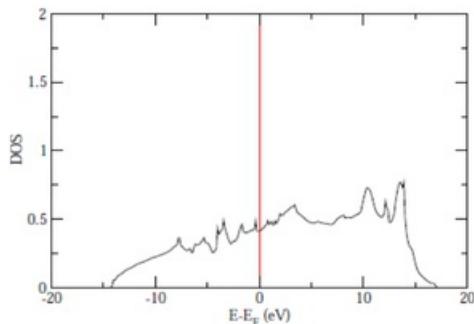
```
System = fcc Si  
# ICHARG = 11 #charge read file  
ENCUT = 240  
ISMEAR = -5 #tetrahedron  
LORBIT = 11
```

### KPOINTS

```
k-points  
0  
Monkhorst Pack  
21 21 21  
0 0 0
```

## Calculation

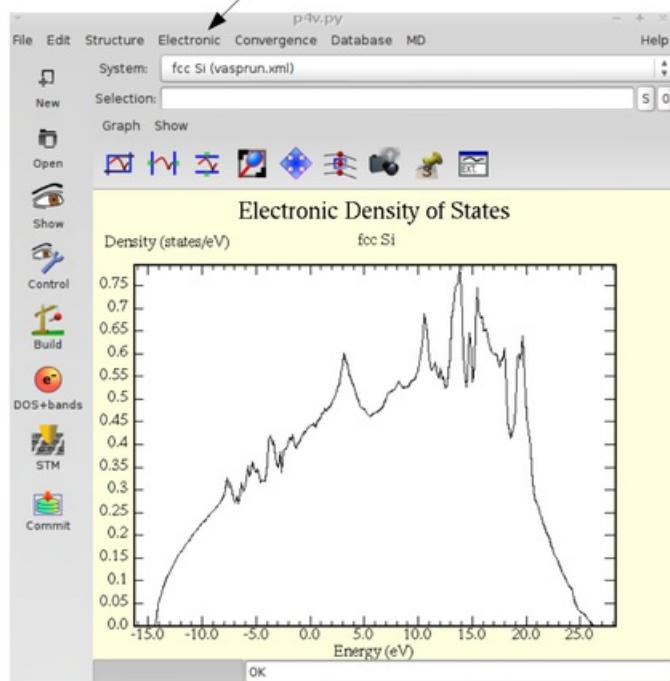
- Perform a static ([NSW=0](#), [IBRION=-1](#)) self consistent calculation for the DOS (the DOS is found in the [DOSCAR](#) file).
- For large systems:
  - Converge with a small number of k points.
  - Increase the number of k points for the DOS and set [ICHARG=11](#) (charge density from the last self-consistent run). [ICHARG=11](#) treats each k point independently and keeps the charge density and the potential fixed.
- Read [CHGCAR](#) from previous run. To copy the self-consistent charge density of example [fcc\\_Si](#) to your current working directory (assumed to be `fccSidos`), type: `$ cp ..//fccSi/CHGCAR .` You must do this otherwise VASP can not read the [CHGCAR](#) and will terminate.
- The smearing of the k points is set to the tetrahedron method with Blöchl corrections ([ISMEAR=-5](#) to fix the problem)



- To plot the DOS use p4vasp:

Start p4vasp:  
> p4v [vasprun.xml]

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- Alternatively the bash-script `plotdos.sh` invokes `awk` and `gnuplot` to get the DOS from the `vasprun.xml` file and plot it.

```

awk 'BEGIN{i=1} /dos>/, \
      /\dos-/ \
      {a[i]="$2 ; b[i]="$3 ; i=i+1} \
END{for (j=12;j<i-5;j++) print a[j],b[j]}' vasprun.xml > dos.dat

ef=`awk '/efermi/ {print $3}' vasprun.xml` 

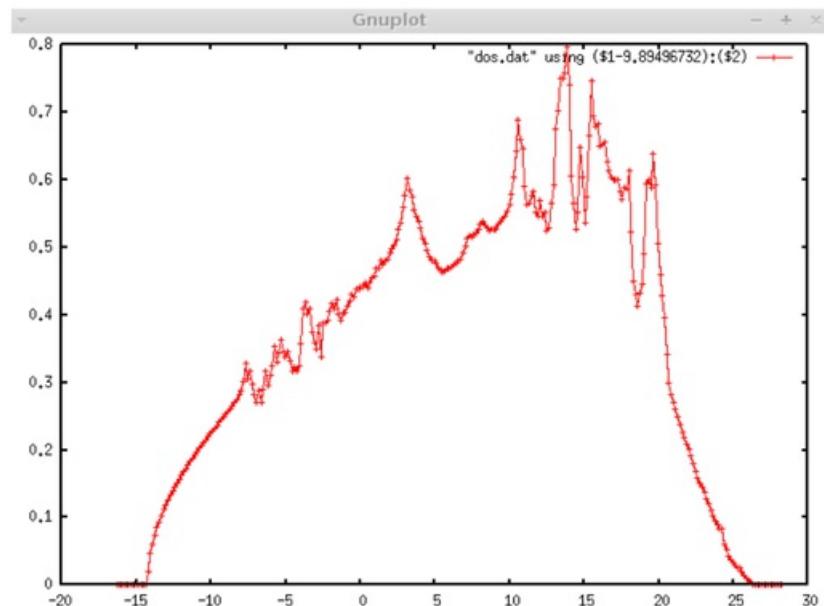
cat >plotfile <<!
# set term postscript enhanced eps colour lw 2 "Helvetica" 20
# set output "optics.eps"
plot "dos.dat" using ($1-$ef):($2) w lp
!

gnuplot -persist plotfile

rm dos.dat plotfile

```

```
>./plotdos.sh
```



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## Task

Determine the interlayer distance of graphite in the stacking direction using the method of Tchatchenko and Scheffler to account for van der Waals interactions.

## Input

### POSCAR

```
graphite
1.0
1.22800000 -2.12695839 0.00000000
1.22800000 2.12695839 0.00000000
0.00000000 0.00000000 7.0
4
direct
0.00000000 0.00000000 0.25000000
0.00000000 0.00000000 0.75000000
0.33333333 0.66666667 0.25000000
0.66666667 0.33333333 0.75000000
```

### INCAR

```
IVDW = 20
LVDW_EWALD = .TRUE.
NSW = 1
IBRION = 2
ISIF = 4
PREC = Accurate
EDIFFG = 1e-5
LWAVE = .FALSE.
LCHARG = .FALSE.
ISMEAR = -5
SIGMA = 0.01
EDIFF = 1e-6
ALGO = Fast
NPAR = 2
```

### KPOINTS

```
Monkhorst Pack
0
gamma
16 16 8
0 0 0
```

## Calcualtion

Semilocal DFT at the GGA level underestimates long-range dispersion interactions. This problem causes a bad overestimation of graphite lattice in the stacking direction (8.84 Å (PBE) vs. 6.71 Å (exp)).

In this example, dispersion correction method of Tchatchenko and Scheffler (see [Tkatchenko-Scheffler method](#)) is used to cope with this problem.

Optimal length of the lattice vector c normal to the stacking direction is determined in a series of single point calculations with varied value of c (all other degrees of freedom are fixed at their experimental values).

The computed c vs. energy dependence is written in the file results.dat and can be visualized e.g. using xmgrace. The optimal value can be obtained using the attached utility (python with numpy or Numeric is needed):

```
./utilities/fit.py results.dat
```

```
200 iterations performed  
Ch-square: 4.30305519481e-09  
-----
```

```
E0(eV): -37.433456779  
d0(A): 6.65603352689
```

The computed value of 6.66 Å agrees well with experiment (6.71 Å).

## Download

[graphiteDistance\\_ts.tgz](#) 

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# Graphite MBD binding energy

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## Task

Determine the interlayer binding energy of graphite in its experimental structure using the MBD@rsSCS method of Tchatchenko *et al.* to account for van der Waals interactions.

## Input

### POSCAR

- Graphite:

```
graphite
1.0
1.22800000 -2.12695839 0.00000000
1.22800000 2.12695839 0.00000000
0.00000000 0.00000000 6.71
4
direct
 0.00000000 0.00000000 0.25000000
 0.00000000 0.00000000 0.75000000
 0.33333333 0.66666667 0.25000000
 0.66666667 0.33333333 0.75000000
```

- Graphene:

```
graphite
1.0
1.22800000 -2.12695839 0.00000000
1.22800000 2.12695839 0.00000000
0.00000000 0.00000000 20.
2
direct
 0.00000000 0.00000000 0.25000000
 0.33333333 0.66666667 0.25000000
```

### INCAR

```
IVDW = 202
LVDWEXPANSION =.TRUE.
NSW = 1
IBRION = 2
ISIF = 4
PREC = Accurate
EDIFFG = 1e-5
LWAVE = .FALSE.
LCHARG = .FALSE.
ISMEAR = -5
SIGMA = 0.01
EDIFF = 1e-6
ALGO = Fast
NPAR = 2
```

### KPOINTS

- Graphite:

```
Monkhorst Pack
0
gamma
```

```
16 16 8  
0 0 0
```

■ Graphene:

```
Monkhorst Pack  
0  
gamma  
16 16 1  
0 0 0
```

## Calculation

Semilocal DFT at the GGA level underestimates long-range dispersion interactions. In the case of graphite, PBE predicts the interlayer binding energy of ~1 meV/atom which is too small compared to the RPA reference of 0.048 eV/atom [1]. In contrast, the pairwise correction scheme of Tkatchenko and Scheffler, overestimates this quantity strongly (0.083 eV/atom, see example [Graphite TS binding energy](#)). In this example we show that this problem can be eliminated by if many-body effects in dispersion energy are taken into account using the MBD@rsSCS method of Tchatchenko et al. (see [Many-body dispersion energy](#)).

Once again, the calculation is performed in two steps (single-point calculations) in which the energy for bulk graphite and for graphene are obtained. The binding energy is computed automatically and it is written in the file results.dat.

The computed value of 0.050 eV/A is now fairly close to the RPA reference of 0.048 eV/atom [1].

## Download

[graphiteBinding\\_mdb.tgz](#) ↗

## References

- ↑ <sup>a b</sup> S. Lebègue, J. Harl, Tim Gould, J. G. Ángyán, G. Kresse, and J. F. Dobson, Phys. Rev. Lett. 105, 196401 (2010). ↗

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# Graphite TS binding energy

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## Task

Determine the interlayer binding energy of graphite in its experimental structure using the method of Tchatchenko and Scheffler to account for van der Waals interactions.

## Input

### POSCAR

- Graphite:

```
graphite
1.0
1.22800000 -2.12695839 0.00000000
1.22800000 2.12695839 0.00000000
0.00000000 0.00000000 6.71
4
direct
 0.00000000 0.00000000 0.25000000
 0.00000000 0.00000000 0.75000000
 0.33333333 0.66666667 0.25000000
 0.66666667 0.33333333 0.75000000
```

- Graphene:

```
graphite
1.0
1.22800000 -2.12695839 0.00000000
1.22800000 2.12695839 0.00000000
0.00000000 0.00000000 20.
2
direct
 0.00000000 0.00000000 0.25000000
 0.33333333 0.66666667 0.25000000
```

### INCAR

```
IVDW = 20
LVDW_EWALD = .TRUE.
NSW = 1
IBRION = 2
ISIF = 4
PREC = Accurate
EDIFFG = 1e-5
LWAVE = .FALSE.
LCHARG = .FALSE.
ISMEAR = -5
SIGMA = 0.01
EDIFF = 1e-6
ALGO = Fast
NPAR = 2
```

### KPOINTS

- Graphite:

Monkhorst Pack

```
0  
gamma  
16 16 8  
0 0 0
```

■ Graphene:

```
Monkhorst Pack  
0  
gamma  
16 16 1  
0 0 0
```

There is no interaction of layers in z-direction for graphene so we need only 1 k point in this direction.

## Calculation

Semilocal DFT at the GGA level underestimates long-range dispersion interactions. In the case of graphite, PBE predicts the interlayer binding energy of ~1 meV/atom which is too small compared to the RPA reference of 0.048 eV/atom [1].

In this example, the interlayer binding energy of graphite in its experimental structure is determined using the [Tkatchenko-Scheffler method](#), which performs well in description of the structure of graphite (see e.g. example [graphite interlayer distance](#)).

The calculation is performed in two steps (single-point calculations) in which the energy for bulk graphite and for graphene are obtained. The binding energy is computed automatically and it is written in the file results.dat.

Even though the TS method predicts a reasonable geometry it overestimates the energetics strongly: the computed binding energy of -0.083 eV/atom is too large compared to the RPA reference of 0.048 eV/atom. This overestimation is - at least in part - due to neglecting the many-body interactions (see example [Graphite MBD binding energy](#)).

## Download

[graphiteBinding\\_ts.tgz](#) ↗

## References

- ↑ S. Lebègue, J. Harl, Tim Gould, J. G. Ángyán, G. Kresse, and J. F. Dobson, Phys. Rev. Lett. 105, 196401 (2010). ↗

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# H<sub>2</sub>O

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## Task

Relaxation of an H<sub>2</sub>O molecule.

## Input

### POSCAR

```
H2O_2
0.52918 ! scaling parameter
15 0 0
0 15 0
0 0 15
1 2
select
cart
0.00 0.00 0.00 F F F
1.10 -1.43 0.00 T T F
1.10 1.43 0.00 T T F
```

All coordinates are scaled by the factor 0.52918.

### INCAR

```
PREC = Normal ! standard precision
ENMAX = 400 ! cutoff should be set manually
ISMEAR = 0 ; SIGMA = 0.1
IBRION = 1 ! use DIIS algorithm to converge
NFREE = 2 ! 2 independent degrees of freedom
NSW = 10 ! 10 ionic steps
EDIFFG = -0.02 ! forces smaller 0.02 A/eV
```

### KPOINTS

```
Gamma-point only
0
Monkhorst Pack
1 1 1
0 0 0
```

## Calculation

- Use PREC=Normal (Default for VASP.5.X)
- It is strongly urged that the energy cutoffs are set manually in the INCAR file, as it provides more control over the calculations.
- For the ionic optimization the DIIS algorithm is used. This algorithm builds an approximation of the Hessian matrix and converges usually faster than the conjugate gradient algorithm. It is however recommended to set the independent degrees of freedom manually. \*EDIFFG determines when to terminate the relaxation. Positive values: energy change between steps must be less than the value set by EDIFFG. Negative values:  $|F_i| < |EDIFFG| \forall i = 1, N_{ions}$ .

## Download

[H<sub>2</sub>O.tgz](#)

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## H<sub>2</sub>O molecular dynamics

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### Task

Molecular dynamics calculation for a H<sub>2</sub>O molecule.

### Input

#### POSCAR

```
H2O_2
0.52918 ! scaling parameter
12 0 0
0 12 0
0 0 12
1 2
select
cart
0.00 0.00 0.00 T T F
1.10 -1.43 0.00 T T F
1.10 1.43 0.00 T T F
```

To save time the box size is reduced to 12 a.u.

#### INCAR

```
PREC = Normal ! standard precision
ENMAX = 400 ! cutoff should be set manually
ISMEAR = 0 ; SIGMA = 0.1
ISYM = 0 ! strongly recommended for MD
IBRION = 0 ! molecular dynamics
NSW = 100 ! 100 steps
POTIM = 1.0 ! timestep 1 fs
SMASS = -3 ! Nose Hoover thermostat
TEBEG = 2000 ; TEEND = 2000 ! temperature
```

#### KPOINTS

```
Gamma-point only
0
Monkhorst Pack
1 1 1
0 0 0
```

### Calculation

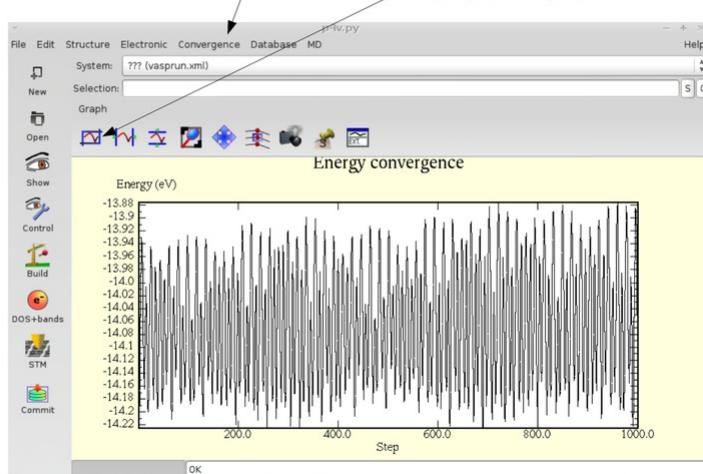
- An example OSZICAR file (with 1000 steps and a step size of 0.5 fs) looks like this:

```
1 T= 2134. E= -.13655511E+02 F= -.14207209E+02 E0=.. EK= 0.55170E+00 SP= 0.00E+00 SK= 0.00E+00
2 T= 1971. E= -.13643254E+02 F= -.14152912E+02 E0=.. EK= 0.50966E+00 SP= 0.00E+00 SK= 0.00E+00
3 T= 1336. E= -.13629241E+02 Fd, which just encloses the cutoff sphere corresponding to the plane wave cutoff, is used. This accelerates the calculations by roughly a factor two to three, but causes slight changes
4 T= 1011. E= -.13624149E+02 F= -.13885486E+02 E0=.. EK= 0.26134E+00 SP= 0.00E+00 SK= 0.00E+00
5 T= 1307. E= -.13629772E+02 F= -.13967549E+02 E0=.. EK= 0.33778E+00 SP= 0.00E+00 SK= 0.00E+00
```

Start p4vasp:  
> p4v [vasprun.xml]

Step 1.) go to: Convergence/Energy

Step 2.) update graph



- The pair correlation function can be visualized using e.g. the following script:
- `plot_PCDAT`

```
awk <PCDAT>PCDAT.dat'
NR==8 {pcskal=$1}
NR==9 {pcfein=$1}
NR==13
line=line+1
if (line==257) {
    print ""
    line=0
}
else
    print (line-0.5)*pcfein/pcskal,$1
}
cat >plotfile<<
# set term postscript enhanced colour lw 2 "Helvetica" 20
# set output "pair_correlation.eps"
set title "pair-correlation of H2O at 2000 K"
set xlabel "r [Angstrom]"
set ylabel "g(r)"
plot [0:15] "PCDAT.dat" w lines
```

```
! gnuplot -persist plotfile
```

## Download

H2Omd.tgz 

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d, which just encloses the cutoff sphere corresponding to the plane wave cutoff, is used. This accelerates the calculations by roughly a factor two to three, but causes slight changes in the tot Back to the [main page](#).

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# H<sub>2</sub>O vibration

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## Task

Calculation of the vibrational frequencies of a H<sub>2</sub>O molecule.

## Input

### POSCAR

```
H2O_2
1.0000000
8.0000000 0.0000000 0.0000000
0.0000000 8.0000000 0.0000000
0.0000000 0.0000000 8.0000000
 1 2
cart
0.0000000 0.0000000 0.0000000
0.5960812 -0.7677068 0.0000000
0.5960812 0.7677068 0.0000000
```

### INCAR

```
SYSTEM = H2O vibration
PREC = A
# IBRION = 1 ; NSW = 10 ; NFREE = 2 ; EDIFFG = -1E-4
ENMAX = 400
ISMEAR = 0 # Gaussian smearing
IBRION = 6 # finite differences with symmetry
NFREE = 2 # central differences (default)
POTIM = 0.015 # default as well
EDIFF = 1E-8
NSW = 1 # ionic steps > 0
```

### KPOINTS

```
Gamma-point only
0
Monkhorst Pack
1 1 1
0 0 0
```

## Calculation

How many zero frequency modes should be observed and why? Try to use the linear response code (**IBRION**=8 and **EDIFF**=1E-8) to obtain reference results. For finite differences, are the results sensitive to the step width **POTIM**. In this specific case, the drift in the forces is too large to obtain the zero frequency modes "exactly", and it is simplest to increase the cutoff **ENCUT** to 800 eV. The important and physically meaningful frequencies are, however, insensitive to the choice of the cutoff.

## Download

[H2Ovib.tgz](#)

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# Improving the dielectric function

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## Task

Calculate the dielectric function of Si using an averaging over multiple grids or a model-BSE to improve k-sampling in BSE calculations.

## Input

```
Si
5.4300
0.5 0.5 0.0
0.0 0.5 0.5
0.5 0.0 0.5
2
cart
0.00 0.00 0.00
0.25 0.25 0.25
```

## INCAR

- This is the [INCAR](#) file for the basic DFT calculation:

```
System = Si
PREC = Normal ; ENCUT = 250.0
ISMEAR = 0 ; SIGMA = 0.01
KPAR = 2
EDIFF = 1.E-8
```

## KPOINTS

```
Automatic
0
Gamma
4 4 4
0 0 0
```

## Calculation

The calculated spectra can be improved in two ways:

- Averaging over multiple grids:

Compute  $N$  independent dielectric functions using BSE (or any other method), using *shifted* grids of  $\mathbf{k}$ -points, and take the average over the results.

- Model-BSE:

Use a parametrized model<sup>[1]</sup> for the dielectric screening, and DFT eigenenergies moved with a *scissor* operator, instead of RPA screening and GW quasiparticle energies.

## Averaging over multiple grids

- Construct shifted  $\mathbf{k}$ -point grid with the same density.
- $n \times n \times n$   $\mathbf{k}$ -point grid  $\rightarrow \mathbf{X}_n$  irreducible  $\mathbf{k}$ -points  $\mathbf{K}_n$  with weights  $\mathbf{W}_n$ . We do  $\omega_n$  calculations on a  $m \times m \times m$  grid, shifted of Gamma by  $\mathbf{K}_n$ .
- Extract the dielectric function of each calculation and average over them with respect to the weights  $\mathbf{W}_n$ :

We have now effectively constructed the result for a  $(n \times m) \times (n \times m) \times (n \times m)$  grid. But interactions of range longer than  $m$  times the supercell size have been ignored.

- In our example we use  $n = 4$  and  $m = 4$ : Effectively we use  $16 \times 16 \times 16$  k-points.

Do 8 calculations with different KPOINTS files:

KPOINTS:

4x4x4

0

G

4 4 4

Kx Ky Kz

4x4x4 Gamma centered grid:  
Found 8 irreducible k-points:

Following reciprocal coordinates:		
Coordinates		Weight
0.000000 0.000000 0.000000		1.000000
0.250000 -0.000000 0.000000		8.000000
0.500000 -0.000000 0.000000		4.000000
0.250000 0.250000 0.000000		6.000000
0.500000 0.250000 0.000000		24.000000
-0.250000 0.250000 0.000000		12.000000
0.500000 0.500000 0.000000		3.000000
-0.250000 0.500000 0.250000		6.000000

$\mathbf{K}_n$

$W_n$

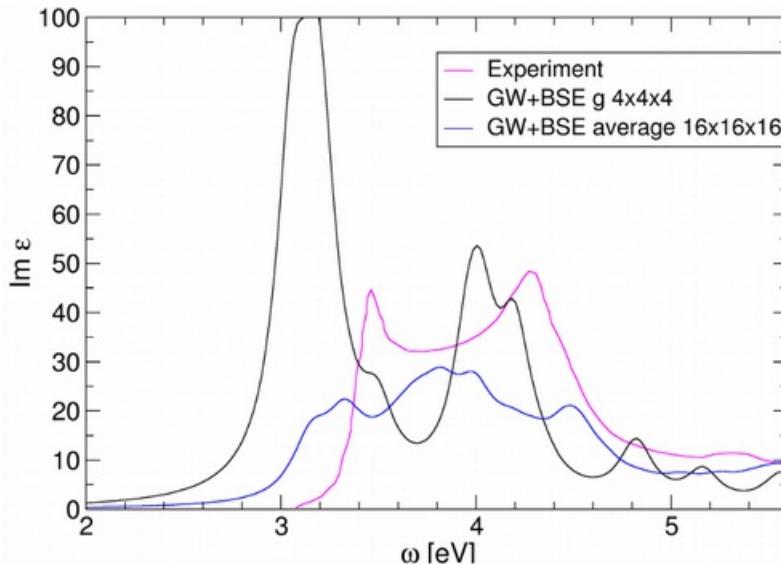
- In the script `doall-average.sh` the scheme is written for  $n = 4$  and  $n = \$NKPT$ . At the end the dielectric functions are extracted and averaged accordingly. You can choose up to which level of theory (DFT, RPA, BSE) the dielectric function is computed by commenting out the corresponding lines in the script (default is all the way up to BSE).
- Because of the shifted grids we have to use density functional perturbation theory to calculate the derivatives of the wave functions with respect to  $\mathbf{k}$  and not the finite difference scheme. We also have to switch off all k-points symmetry in all `INCAR` files. These two important parameters look like the following in the `INCAR` file:

```
PREC = Normal ; ENCUT = 250.0
```

```
ALGO = EXACT ; NELM = 1
ISMEAR = 0 ; SIGMA = 0.01
KPAR = 2
```

```
NBANDS = 32 # The number of bands in the consecutive BSE calculation should be the same!
LOPTICS = .TRUE.; LPEAD = .FALSE.
ISYM = -1
OMEGAMAX = 40
```

- Finally the averaging over multiple grids should give spectra that are in much closer agreement than the calculations using  $4 \times 4 \times 4$  k-points:



## Model-BSE

The dielectric function  $\epsilon_{\mathbf{G}, \mathbf{G}'}^{-1}(\mathbf{k})$  is replaced by the local model function:

$$\epsilon^{-1}(\mathbf{k} + \mathbf{G}) = 1 - (1 - \epsilon_{\infty}^{-1}) \exp\left(\frac{-(2\pi|\mathbf{k} + \mathbf{G}|)^2}{4\lambda^2}\right) .$$

This makes the screened Coulomb kernel diagonal ( $\mathbf{G} = \mathbf{G}'$ ) in the screened Coulomb potential:

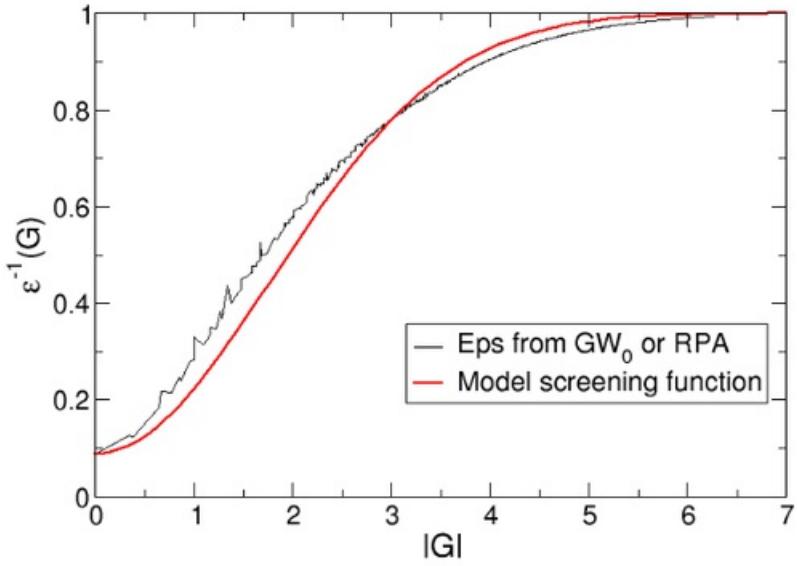
$$W_{c'v'k}^{ck} = \frac{4\pi e^2}{\Omega} \sum_{\mathbf{G}} B_{c'k}^{\mathbf{k}}(\mathbf{G}) \frac{\epsilon^{-1}(\mathbf{k} + \mathbf{G})}{|\mathbf{k} + \mathbf{G}|^2} B_{v'k}^{\mathbf{k}}(\mathbf{G}) ,$$

where  $B_{n'k}^{\mathbf{k}}(\mathbf{G})$  denote Bloch integrals of the cell-periodic part of the Bloch waves.

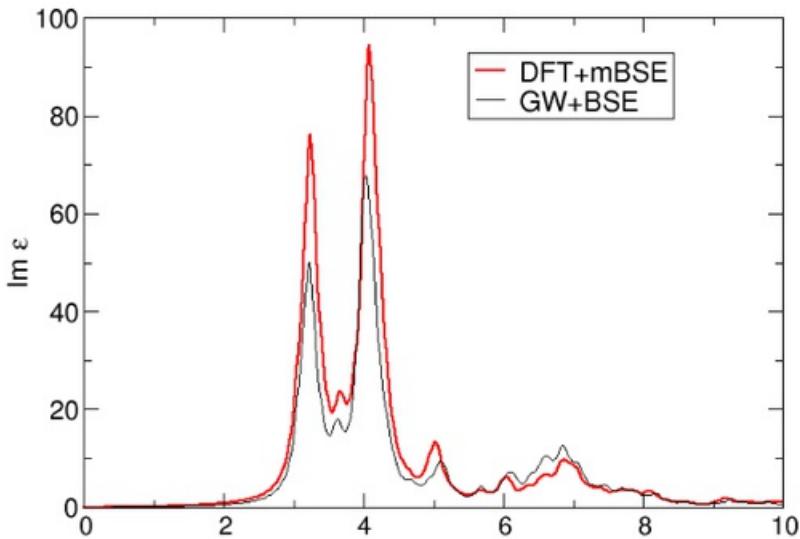
- In addition to a model dielectric function we need approximate quasiparticle energies and wave functions.

Approximation:

- Use DFT single particle eigenvalues + SCISSOR (SCISSOR=GW band gap - DFT band gap).
- Use DFT single particle orbitals.
- Extract  $\mathbf{G} = \mathbf{G}'$  dielectric function from the `vasprun.xml` file from the previous GW calculation using the script `extract_optics.sh` or view the file `dieG_g6x6x6-GW0.dat`. Use `AEXX=0.088` for  $\epsilon_{\infty}^{-1}$  and `HSCREEN=1.26` for  $\lambda$ . Then fit the model to get:



- Check the GW+BSE and DFT+mBSE calculations for consistency:



- The sequence of calculations as given in the script `doall-model.sh` consists of two steps:

- Step 1: standard DFT calculation. The [INCAR](#) file (INCAR.DFT) for this step looks as follows:

```

PREC = Normal ; ENCUT = 250.0
ISMEAR = 0 ; SIGMA = 0.01
EDIFF = 1.E-8
NBANDS = 16
PRECFOCK = Normal

#WAVEDER file must be made:
LOPTICS = .TRUE.
LPEAD = .TRUE.
OMEGAMAX = 40

```

- Step2: model BSE calculation. The [INCAR](#) file (INCAR.mBSE) for this step looks as follows:

```

PREC = Normal ; ENCUT = 250.0
ALGO = TDHF
ANTIRES = 0 ; SIGMA = 0.01
ENCUTGW = 150

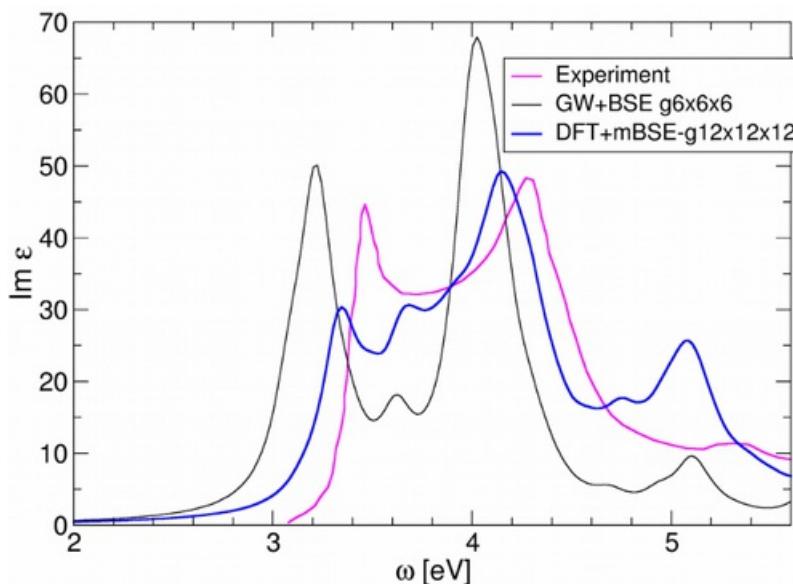
EDIFF = 1.E-8
NBANDS = 16
NBANDSO = 4
NBANDSV = 8
OMEGAMAX = 20

PRECFOCK = Normal

LMODELHF = .TRUE.
HFSCREEN = 1.26
AEXX = 0.088
SCISSOR = 0.69

```

- Finally the result of the DFT+mBSE should be of similar accuracy as the GW+BSE calculations when compared to experiment:



## Download

[Si\\_improve\\_eps.tgz](#)

## References

- ↑ M.Bokdam et al., *Scientific Reports* 6, 28618 (2016).

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## Including the Spin-Orbit Coupling

Description: Spin-Orbit Coupling (SOC) included self-consistently

The Magnetocrystalline Anisotropy Energy is determined by rotating all spins according to different directions. To modify the orientation of the spins in the crystal, we consider the second approach described in the [SAXIS](#) page. For the **MAGMOM**-tag, the total local magnetic moment is written according to the z direction (necessarily, the x and y-directions are equal to 0). The spin orientation [uvw] is defined by the **SAXIS**-tag in the Cartesian frame. The Magnetocrystalline Anisotropy Energy is calculated by orientating the spins in different directions and the following equation :  $E_{MAE} = E_{[uvw]} - E_{\min}$ , with  $E_{\min}$  the energy of the most stable spin orientation.

More details are available in the [SAXIS](#) and [LSORBIT](#) pages.

Exercise : Determine the total magnetic moment by adding the orbital moment of the Ni atoms. Calculate the Magnetocrystalline Anisotropy Energy of NiO by orientating the spins along the following path : (2,2,2) --> (2,2,1) --> (2,2,0) --> ... --> (2,2,-6). Identify the most stable spin orientation according to this path.

### ■ INCAR

```
NiO GGA+U SOC
SYSTEM = "NiO"
```

```
Electronic minimization
ENCUT = 450
EDIFF = 1E-7
LORBIT = 11
LREAL = .False.
ISTART = 0
ISYM = -1
NELMIN = 6
LSORBIT = .True.
LWAVE = .False.
LCHARG = .False.
```

```
DOS
ISMEAR = -5
```

```
Magnetism
ISPIN = 2
MAGMOM = 0 0 2 0 0 -2 6*0
SAXIS = 2 2 2
```

```
Orbital Moment
LORBMMOM = T
```

```
Mixer
AMIX = 0.2
BMIX = 0.00001
AMIX_MAG = 0.8
BMIX_MAG = 0.00001
```

```
GGA+U
LDAU = .TRUE.
LDAUTYPE = 2
LDAUL = 2 -1
LDAUU = 5.00 0.00
LDAUJ = 0.00 0.00
LDAUPRINT = 2
LMAXMIX = 4
```

### ■ KPOINTS

```
k-points
0
gamma
4 4 4
0 0 0
```

### ■ POSCAR

```
NiO
4.17
1.0 0.5 0.5
0.5 1.0 0.5
0.5 0.5 1.0
2 2
Cartesian
0.0 0.0 0.0
1.0 1.0 1.0
0.5 0.5 0.5
1.5 1.5 1.5
```

## Download

nio\_SOC.tgz 

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# Input

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VASP basically gives 4 input files for standard production runs:

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- 1 INCAR
- 2 POSCAR
- 3 KPOINTS
- 4 POTCAR

## INCAR

- The [INCAR](#) file gives the input parameters which "steer" the calculation.
- The default values set by VASP itself are a clever choice to do standard calculations.
- These standard settings can be modified to specify:
  - What do you want to do? (scf calculation, DOS, dielectric properties ...)
  - You can give parameters to fulfill your requirements concerning required precision, requested convergence, calculation time ...

## POSCAR

- A sample [POSCAR](#) file can look as the following:

```
fcc: Ni
3.53
0.5 0.5 0.0
0.0 0.5 0.5
0.5 0.0 0.5
Ni
1
Selective Dyn
Cartesian
0 0 0 ( T T T )
```

- The description of each line is given as follows:
  - 1: Header (comment).
  - 2: Overall scaling constant.
  - 3-6: Bravais matrix.
  - 4: Name(s) of the atom(s).
  - 5: Number of the atoms (of each atom type).
  - 6: (optional: selective dynamics).
  - 7: Specifies which coordinate system is used (cartesian or direct).
  - 8-x: Positions of the atoms.

## KPOINTS

- A sample [KPOINTS](#) file can look like the following:

```
Automatic mesh
0
G (M)
4 4 4
0. 0. 0.
```

- The description of each line is given as follows:
  - 1: Header (comment).
  - 2: Specifies the k mesh generation type.  $\frac{N_k}{k} = 0$  : automatic generation scheme.
  - 3:  $\Gamma$ -centered (Monkhorst-Pack) grid.
  - 4: Number of subdivisions in each direction.
  - 5: Optional shift of the mesh.

## POTCAR

- The [POTCAR](#) file contains the relevant information concerning the pseudo potentials that are necessary to run the calculation:
  - Data that was required for generating the pseudo potentials.
  - Number of valence electrons.
  - Atomic mass.

- Energy cut-off.
- If the cell contains different atoms, the atomic [POSCAR](#) files have to be concatenated, in the same order as the atoms are given in the [POSCAR](#) file.
- Different XC-types must not be mixed.

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# Liquid Si

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## Task

## Input

### POSCAR

```

Si
15.12409564534287297131
 0.5000000000000000 0.5000000000000000 0.0000000000000000
 0.0000000000000000 0.5000000000000000 0.5000000000000000
 0.5000000000000000 0.0000000000000000 0.5000000000000000

48
Direct
 0.8550657259653851 0.3204575801875221 0.6180363868822553
 0.6045454476433229 0.0546379652195404 0.1629680405553871
 0.4803889256776521 0.2999635319377835 0.0131251454718051
 0.8413504226620471 0.7598095803296524 0.1917781560970181
 0.9754163118144437 0.6134171268457649 0.7421364242876367
 0.2668229391055025 0.0066502741664650 0.0031140604380929
 0.8935777664000575 0.3324172908647429 0.9535738516718881
 0.0527608886321274 0.5249316429131962 0.5293744880144071
 0.4396089233132741 0.7564833235979471 0.5665855438788387
 0.5907859878830199 0.5198033580597228 0.3581725847640679
 0.2120832721474721 0.4042899613004446 0.7921535013319151
 0.0225803885096466 0.8414911198321031 0.1209255489569852
 0.0992500701525566 0.3917384466892963 0.3612433325214984
 0.9673794138223195 0.5206425706394114 0.1719623236201897
 0.2774602656926126 0.8480860088162007 0.2673309412777037
 0.0196991774214161 0.8282178425383616 0.6986213756952502
 0.3570927152895376 0.2951488295546784 0.2651851032568589
 0.1663829731894614 0.9766237917413699 0.6051764245375237
 0.4931841331696695 0.8689890620771937 0.2612357008392290
 0.8006473407426477 0.1033419073227807 0.4706563716777467
 0.0161340851939779 0.9953827418297991 0.8853439845676159
 0.7827740166661069 0.1821830067208054 0.9399555168314748
 0.0720651739141343 0.2539424963694544 0.6857919074324333
 0.4443385370769313 0.0486404637002326 0.4180706114402839
 0.7055263679666055 0.6802623819082319 0.7983614866719116
 0.2237125282521105 0.4055474352416297 0.0077044950891134
 0.2963682069847125 0.5771265542042112 0.2019757061665083
 0.2782449529809642 0.0451513130915826 0.7644934848784113
 0.9312079203181675 0.9090938018377080 0.3429249881187518
 0.6341882597200124 0.2969253226419481 0.3227590981305088
 0.3587691103780569 0.1061057273904179 0.0931868777500710
 0.8710437838676732 0.6541301230631744 0.4261617089364881
 0.6784300588817769 0.3263889355408940 0.5560491395978739
 0.5597052314845080 0.0174390112509929 0.6129003207931863
 0.0595962318875451 0.1019295953521402 0.3340999072062676
 0.7689671766774326 0.1768870209149794 0.1604177484299765
 0.9603661624482890 0.3311649224573259 0.1439224909303592
 0.3792868784787023 0.2806150985211180 0.4921541531665999
 0.8079860889823454 0.9194188799048340 0.9131036494263627
 0.3002081239026374 0.7834053620019006 0.8650323716139056
 0.4704528574512951 0.7221628305989689 0.9746107190983403
 0.2886552568292480 0.5927625600330780 0.4239421203107919
 0.4116743942942291 0.2198943758058664 0.7072597030225044
 0.210494234814825 0.6457654201409418 0.8275863924787099
 0.6784628197745537 0.7205455185203838 0.1093053357228383
 0.6344130299021448 0.1650970001101275 0.8037018707797643
 0.3965793440603315 0.5364088146415013 0.6064549771969059
 0.6686412136025504 0.7848666926903073 0.5681234351534038

```

### Script for INCAR

```

for i in 2000 1900 1800 1700 1600 1500 1400 1300 1200 1100 1000 900 800
do
cat >INCAR <<!

```

```

SYSTEM = Si
# electronic degrees
LREAL = A          # real space projection
PREC = Normal      # chose Low only after tests
EDIFF = 1E-5        # do not use default (too large drift)
ISMEAR = -1 ; SIGMA = 0.130 # Fermi smearing: 1500 K 0.086 10-3
ALGO = Very Fast   # recommended for MD (fall back ALGO = Fast)
MAXMIX = 40         # reuse mixer from one MD step to next
ISYM = 0            # no symmetry
NELMIN = 4          # minimum 4 steps per time step, avoid breaking after 2 steps

# MD (do little writing to save disc space)
IBRION = 0 ; NSW = 400 ; NWRITE = 0 ; LCHARG = .FALSE. ; LWAVE = .FALSE.
TEBEG = $i ; TEEND = $i
# canonic (Nose) MD with XDATCAR updated every 10 steps
SMASS = 3 ; NBLOCK = 10 ; POTIM = 3
!
mpirun -np 2 /path/to/your/vasp/executable
cp XDATCAR XDATCAR.$i
cp OUTCAR OUTCAR.$i
cp PCDAT PCDAT.$i
cp CONTCAR CONTCAR.$i
cp POSCAR POSCAR.$i
cp OSZICAR OSZICAR.$i
cp CONTCAR POSCAR
done

```

script performs molecular dynamics runs on liquid Si at decreasing temperatures, starting at 2000 K and ending at 800 K. This should contain the transition from liquid Si to crystalline Si (amorphous).

## KPOINTS

```

test
0 0 0
monk
1 1 1
0 0 0

```

## Calculation

- To analyse the diffusion behaviour at a certain temperature T, the data read from [[XDATCAR.[T]]] can be processed using the script diffusion:

```

awk <XDATCAR >diffusion.xy '
#
# simple module function
#
function mod(x,y) { return x-int(x/y)*y }
function minim(x) { return mod(x+2.5,1.0)-0.5 }
#
# calculate mean square displacement
#
function diff() {
    d=0
    for (ion=1; ion<=ions; ion++) {
        dx=minim(xn[ion]-x[ion])
        dy=minim(yn[ion]-y[ion])
        dz=minim(zn[ion]-z[ion])

        xn[ion]=x[ion]+dx
        yn[ion]=y[ion]+dy
        zn[ion]=z[ion]+dz

        d=d+(xn[ion]-x0[ion])*(xn[ion]-x0[ion])*a1*a1
        d=d+(yn[ion]-y0[ion])*(yn[ion]-y0[ion])*a2*a2
        d=d+(zn[ion]-z0[ion])*(zn[ion]-z0[ion])*a3*a3
    }
    d=d/(set*t)/6
    d=d/6
    print set*t,d
}
#
# set the number of ions
#
NR==1 { ions = $1 }
NR==2 { a1=$2*10^10 ; a2=$3*10^10 ; a3=$4*10^10 ; t=$5*10^12 }
#
# at this point a complete set of ionic positions has been found
#
mod(NR-6,ions+1)==0 {
    if (set>=2) diff()
    if (set==1) {
        for (ion=1; ion<=ions; ion++) {
            x0[ion]=xn[ion]
            y0[ion]=yn[ion]
            z0[ion]=zn[ion]
        }
    }
    for (ion=1; ion<=ions; ion++) {

```

```

        x[ion]=xn[ion]
        y[ion]=yn[ion]
        z[ion]=zn[ion]
    }
    head=headn
    headn=$0
    set=set+1
}
# store coordinates
mod(NR-6,ions+1)>0 {
    ion=mod(NR-6,ions+1)
    xn[ion]=$1
    yn[ion]=$2
    zn[ion]=$3
}

```

- The pair-correlation function written on [[PCDAT.[T]]] should be processed using the script PCDATtoPCDATxy:

```

awk <PCDAT>PCDAT.xy '
NR==8 { pcscal=$1}
NR==9 { pcfein=$1}
NR>=13 {
line=line+1
if (line==257) {
    print ""
    line=0
}
else
    print (line-0.5)*pcfein/pcscal,$1
}

```

**Mind:** You will have to set the correct path to your VASP executable and invoke VASP with the correct command (e.g., in the above: mpirun -np 2).

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[Si\\_liquid.tgz](#)

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# MgO optimum mixing

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## Task

Find optimum HSE mixing parameter for MgO.

## Input

### POSCAR

```
MgO
-18.7935000000000000000000000000
0.5 0.5 0.0
0.0 0.5 0.5
0.5 0.0 0.5
1 1
cart
0.00 0.00 0.00
0.50 0.0 0.0
```

### INCAR =

```
#####
## Optimum HSE mixing parameter (AEXX) for MgO
## Expt gap = 7.8 eV
## fit gap wrt. 0<AEXX<1
## Compute the bandgap using different value of AEXX
## in the range (0,1) and find the value which leads
## to the best agreement with the experimental gap.
## hint: the gap grows linearly with AEXX
## Better preconverge with PBE first!
#####

## Selects the HSE06 hybrid function
#LHFCALC = .TRUE. ; HFSCREEN = 0.2 ; AEXX=0.25
#ALGO = D ; TIME = 0.4

## Leave this in
ISMEAR = 0
SIGMA = 0.01
GGA = PE
```

### KPOINTS

```
k-points
0
Gamma
4 4 4
0 0 0
```

## Calculation

- script to extract G-eigenvalues and calculate the bandgap

```
grep "    4    " OUTCAR | head -8 | \
awk 'BEGIN{for (j=1;j<i;j++) print j,a[j]}' > vband.dat
grep "    5    " OUTCAR | head -8 | \
awk 'BEGIN{for (j=1;j<i;j++) print j,a[j]}' > cband.dat
```

The bandgap is obtained by subtracting the eigenvalues written in cband.dat (conduction band minimum at Gamma) and vband.dat (valence band maximum at Gamma)

## Download

[5\\_2\\_MgO\\_mixing.tgz](#) ↗

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# Ni 100 surface bandstructure

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## Task

Calculation of the bandstructure of a Ni (100) surface.

## Input

### POSCAR

```

fcc (100) surface
3.53000000000000
 0.500000000000000 0.500000000000000 0.000000000000000
 -0.500000000000000 0.500000000000000 0.000000000000000
 0.000000000000000 0.000000000000000 5.000000000000000
Ni
 5
Selective dynamics
Direct
 0.000000000000000 0.000000000000000 0.000000000000000 F F F
 0.500000000000000 0.500000000000000 0.100000000000014 F F F
 0.000000000000000 0.000000000000000 0.200000000000028 F F F
 0.500000000000000 0.500000000000000 0.3004245271852446 T T T
 0.000000000000000 -0.000000000000000 0.3959414474619545 T T T

 0.0000000E+00 0.0000000E+00 0.0000000E+00
 0.0000000E+00 0.0000000E+00 0.0000000E+00
 0.0000000E+00 0.0000000E+00 0.0000000E+00
 0.0000000E+00 0.0000000E+00 0.0000000E+00
 0.0000000E+00 0.0000000E+00 0.0000000E+00

```

## INCAR

```

ICHARG = 11
general:
 SYSTEM = clean (100) nickel surface
 ENMAX = 270
 ISMEAR = 2 ; SIGMA = 0.2
 ALGO = Normal

spin:
 ISPIN = 2
 MAGMOM = 5*1

LORBIT = 11

```

- ICHARG=11: Read in charge density (1) and do not update it (+10) - non-selfconsistent run.
- N.B.: You need to copy the CHGCAR file of example [Ni 100 surface DOS](#) into the directory where you want to run this calculation.

## KPOINTS

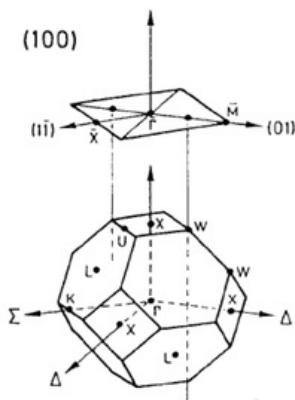
```

kpoints for band-structure G-X-M-G
 13
reziprok
 .00000 .00000 .00000 1
 .12500 .00000 .00000 1
 .25000 .00000 .00000 1
 .37500 .00000 .00000 1
 .50000 .00000 .00000 1

 .50000 .12500 .00000 1
 .50000 .25000 .00000 1
 .50000 .37500 .00000 1
 .50000 .50000 .00000 1

 .37500 .37500 .00000 1
 .25000 .25000 .00000 1
 .12500 .12500 .00000 1
 .00000 .00000 .00000 1

```



- 13 k points along line  $\Gamma - X - M - \Gamma$ .
- The coordinates are given in reciprocal coordinates.
- Each point has weight 1.

## Calculation

- In the **OUTCAR** file the status message on the actual job (non-selfconsistent calculation) is given:

```
...
Static calculation
charge density remains constant during run
spin polarized calculation
...
```

- The bandstructure can be plotted using p4vasp:

Select “Electronic/local DOS+bands control”

Select orbital character

Choose symbol size

Select spin channel

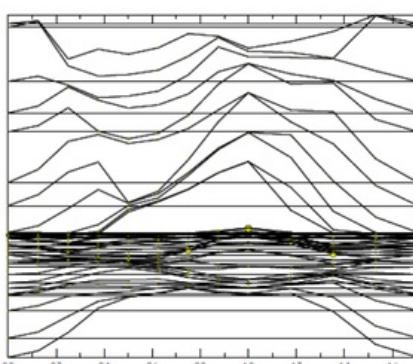
Place pointer over atom, and press space to select/deselect.

The selection should appear in the Electronic Control applet above

Press “Show” to show structure

Atom selection: S  
Description:  
Line: 5 spin down  
Symbol: default  
Symbol size: 2.0  
Add new line Remove line Change line  
Spin: up down both invert y-axis  
First band: 0 Last band: -1  
Orbital selection:  
Select all Deselect all s  
Select p Deselect p px py pz  
Select d Deselect d dx dy dz dx2 dy2 dz2  
Select f Deselect f f1 f2 f3 f4 f5 f6

- The example output for the projected bandstructure consists mainly out of bulk like bands. The Yellow dots mark the surface localizations:



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# Ni 100 surface DOS

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## Task

Calculation of the local density of states (LDOS) of a Ni (100) surface.

## Input

### POSCAR

```

fcc (100) surface
3.53000000000000
 0.500000000000000 0.500000000000000 0.000000000000000
 -0.500000000000000 0.500000000000000 0.000000000000000
 0.000000000000000 0.000000000000000 5.000000000000000
Ni
 5
Selective dynamics
Direct
 0.000000000000000 0.000000000000000 0.000000000000000 F F F
 0.500000000000000 0.500000000000000 0.100000000000014 F F F
 0.000000000000000 0.000000000000000 0.200000000000028 F F F
 0.500000000000000 0.500000000000000 0.3004245271852446 T T T
 0.000000000000000 -0.000000000000000 0.3959414474619545 T T T

 0.0000000E+00 0.0000000E+00 0.0000000E+00
 0.0000000E+00 0.0000000E+00 0.0000000E+00
 0.0000000E+00 0.0000000E+00 0.0000000E+00
 0.0000000E+00 0.0000000E+00 0.0000000E+00
 0.0000000E+00 0.0000000E+00 0.0000000E+00

```

### INCAR

```

general:
 SYSTEM = clean (100) Ni surface
 ENMAX = 270
 ISMEAR = -5
 ALGO = Normal

```

```

spin:
 ISPIN = 2
 MAGMOM = 5*1

```

```
LORBIT = 11 # LM and site decomposed DOS inside PAW spheres
```

- Using the tetrahedron method (with Blöchl corrections).
- LM and site decomposed DOS.
- N.B.: We want to use the optimized structure of [Ni 100 surface relaxation](#). Normally this would mean copying the [CONTCAR](#) file of [Ni 100 surface relaxation](#) to the [POSCAR](#) file in the directory where you want to run **Ni 100 surface DOS**.

In this case, however, that has already been taken care of and the [POSCAR](#) file from the downloadable tar file is the correct one.

### KPOINTS

```

k-points
0
Monkhorst-Pack
9 9 1
0 0 0

```

## Calculation

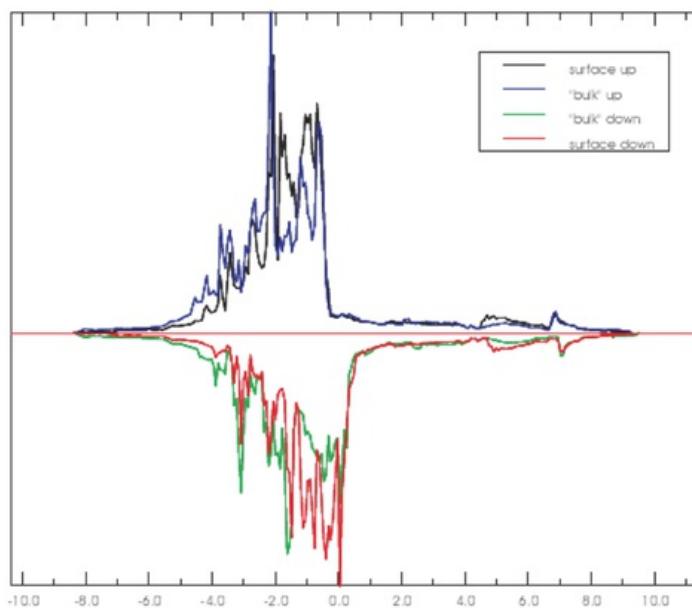
- At the end of the [OUCAR](#) file the information on the local charge and magnetization is given.

total charge					
# of ion	s	p	d	tot	

1	0.461	0.316	8.331	9.108
2	0.483	0.466	8.323	9.273
3	0.484	0.462	8.324	9.270
4	0.490	0.481	8.329	9.300
5	0.472	0.337	8.341	9.150
tot	2.390	2.062	41.648	46.100

total charge					
# of ion	s	p	d	tot	
1	-0.003	-0.019	0.715	0.692	
2	-0.008	-0.023	0.619	0.588	
3	-0.007	-0.024	0.620	0.589	
4	-0.008	-0.024	0.622	0.591	
5	-0.004	-0.020	0.705	0.681	
tot	-0.030	-0.110	3.281	3.141	

- Using **LORBIT=1** and changing **RWIGS** the total number of electrons within the spheres could be adapted (nickel pseudo-potential has a valence of 10).
- Enhancement of the magnetic moment at the surface.
- Magnetic moment int the center "bulk like".
- The surface and bulk projected-DOS plotted for each spin component separately should show a band narrowing and larger exchange splitting at the surface:



- The DOS of can be plotted using p4vasp:

Select “Electronic/local DOS+bands control”

Select orbital character

Select spin channel

Invert y-axis (optional)

Place pointer over atom, and press space to select/deselect.

The selection should appear in the Electronic Control applet above

Press “Show” to show structure

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# Ni 100 surface relaxation

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## Task

Relaxation of the first two layers of a Ni (100) surface.

## Input

### POSCAR

```
fcc (100) surface
3.53
.50000 .50000 .00000
-.50000 .50000 .00000
.00000 .00000 5.00000
5
Selective Dynamics
Kartesisch
.00000 .00000 .00000 F F F
.00000 .50000 .50000 F F F
.00000 .00000 1.00000 F F F
.00000 .50000 1.50000 T T T
.00000 .00000 2.00000 T T T
```

- Ni lattice constant of 3.53 .
- 1 atom per layer: p(1x1) cell.
- 5 nickel layers.
- First two layers (of one side) relaxed.
- **3 × 3.53 = 10.59** vacuum.

### INCAR

```
ISTART = 0; ICHARG = 2
general:
SYSTEM = clean Ni(100) surface
ENCUT = 270
ISMEAR = 2 ; SIGMA = 0.2
ALGO = Fast
EDIFF = 1E-6
spin:
ISPIN=2
MAGMOM = 5*1
dynamic:
NSW = 100
POTIM = 0.8
IBRION = 1
```

- Initial charge-density in startjob from overlapping atoms.
- Default energy cut-off of 270 eV.
- MP-smearing (metal).
- Spin-polarized calculation with initial moment of 1.
- Ionic relaxation used.

### KPOINTS

```
k-points
0
Monkhorst-Pack
9 9 1
0 0 0
```

- Equally spaced mesh.
- Odd mesh, centered on  $\Gamma$  .

- 15 k points in irreducible Brillouin zone (IBZ).
- Only one k point in z-direction for surface.

## Calculation

- The sample output for the forces in the **OUTCAR** file should look like this (first and last step):

First step:

POSITION			TOTAL-FORCE (eV/Angst)		
0.00000	0.00000	0.00000	0.0000000	0.0000000	0.391352
0.00000	1.76500	1.76500	0.0000000	0.0000000	-0.397024
0.00000	0.00000	3.53000	0.0000000	0.0000000	0.005117
0.00000	1.76500	5.29500	0.0000000	0.0000000	0.391161
0.00000	0.00000	7.06000	0.0000000	0.0000000	-0.390607
total drift:			0.0000000	0.0000000	0.016391

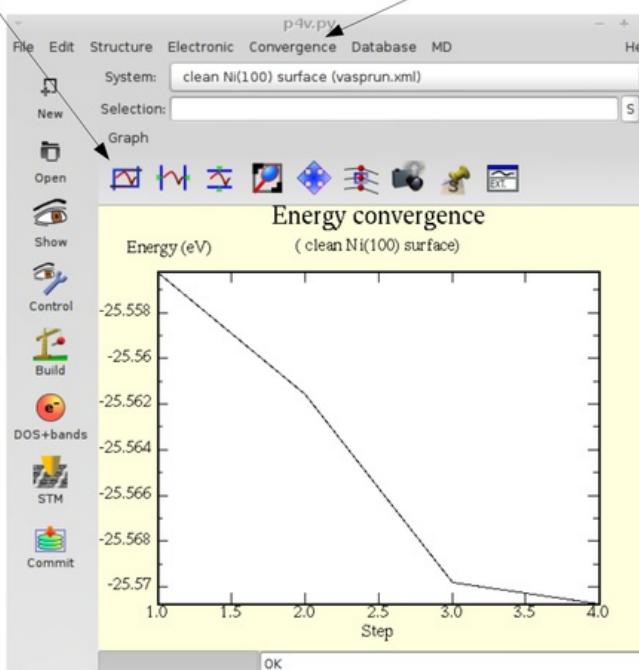
Last step:

POSITION			TOTAL-FORCE (eV/Angst)		
0.00000	0.00000	0.00000	0.0000000	0.0000000	0.399012
0.00000	1.76500	1.76500	0.0000000	0.0000000	-0.377003
0.00000	0.00000	3.53000	0.0000000	0.0000000	0.105799
0.00000	1.76500	5.32685	0.0000000	0.0000000	-0.062054
0.00000	0.00000	7.02377	0.0000000	0.0000000	-0.065753
total drift:			0.0000000	0.0000000	-0.042925

- Energy changes during relaxation from -25.556 to -25.571 eV which gives a relaxation energy of  $E^{\text{rel}} = -15$  meV. Use p4vasp to check the convergence:

“Update” graph

Go to “Convergence/Energy”



- The surface energy of 0.86 eV for the unrelaxed surface is calculated in the following:

$$\sigma^{\text{unrel}} = \frac{1}{2}(E_{\text{surf}} - N_{\text{atoms}} \cdot E_{\text{bulk}}) = \frac{1}{2}(-25.556 - 5 \cdot (-5.457)) = 0.86 \text{ eV.}$$

- The surface energy of 0.84 eV for the relaxed surface is then calculated as:

$$\sigma = \sigma^{\text{unrel}} + E^{\text{rel}} = 0.84 \text{ eV.}$$

- The final geometry (from the **CONTCAR** or **OUTCAR** file) should look as follows:

```

fcc (100) surface
3.530000000000000
0.500000000000000 0.500000000000000 0.000000000000000
-0.500000000000000 0.500000000000000 0.000000000000000
0.000000000000000 0.000000000000000 5.000000000000000
Ni
5
Selective Dynamics
Direct
0.000000000000000 0.000000000000000 0.000000000000000 F F F
0.000000000000000 0.500000000000000 0.10000000000000014 F F F
0.000000000000000 0.000000000000000 0.20000000000000028 F F F
0.500000000000000 0.500000000000000 0.3018043743226639 T T T
0.000000000000000 0.000000000000000 0.3979474020596729 T T T

```

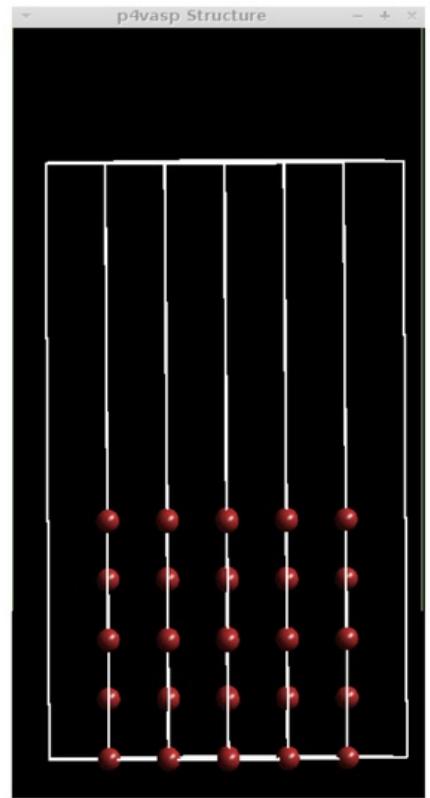
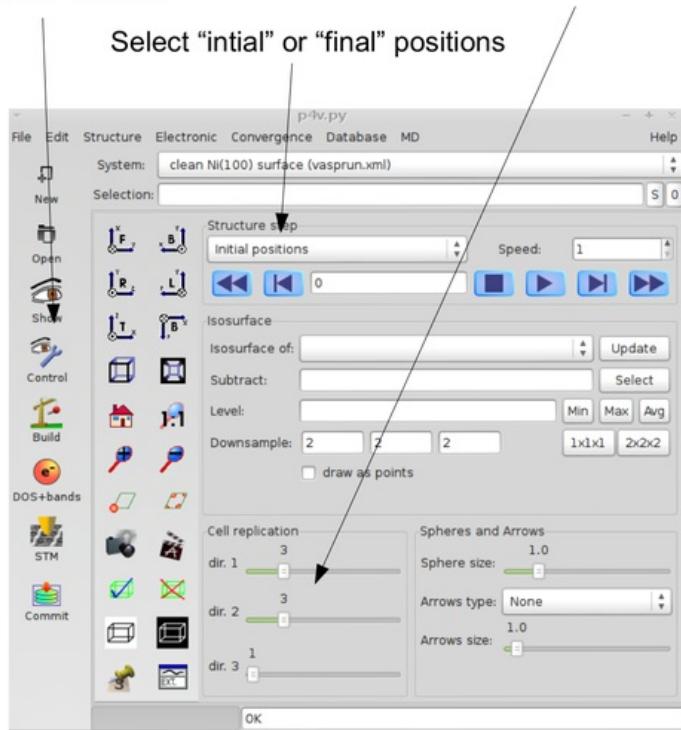
- Inward relaxation of surface layers:

- $\Delta d_{12} = ((0.3979-0.3018)-0.1)/0.1*100=-3.9\%$ .
- $\Delta d_{12} = ((0.3018-0.2000)-0.1)/0.1*100=+1.8\%$ .

■ Use p4vasp to visualize the relaxation:

Go to “Control”

Possibly replicate cells



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# Ni 111 surface high precision

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## Task

Calculation of the adsorption energies and the work function of a Ni (111) surface with high precision.

## Input

### POSCAR

```
fcc (111) surface
3.53000000000000
0.7071067800000000 0.0000000000000000 0.0000000000000000
-0.3535533900000000 0.6123724000000000 0.0000000000000000
0.0000000000000000 0.0000000000000000 5.1961523999999999
Ni
5
Selective dynamics
Direct
0.0000000000000000 0.0000000000000000 0.0000000000000000 F F F
0.3333333300000021 0.6666666699999979 0.111111100000031 F F F
0.6666666699999979 0.3333333300000021 0.2222222199999990 F F F
-0.0000000000000000 -0.0000000000000000 0.3320935940210170 T T T
0.3333333300000021 0.6666666699999979 0.4413539967541983 T T T
0.00000000E+00 0.00000000E+00 0.00000000E+00
```

### INCAR

```
ENMAX = 400
general:
  SYSTEM = clean nickel (111) surface
  ISTART = 0
  ICHARG = 2
  ISMEAR = 2 ; SIGMA = 0.2
  ALGO = Fast
  EDIFF = 1E-6
special:
  LVHAR = .TRUE.
#  LVTOT = .TRUE.
```

- Run a single point calculation for the Ni(111) clean surface at a higher cutoff (400eV), which is needed to compute the adsorption energy.
- Potentials for O and C require an energy cut-off of 400eV:
  - Previous calculation for clean cannot be used as reference.
  - Recalculate with same energy cut-off.

### KPOINTS

```
K-Points
0
Monkhorst-Pack
```

9 9 1  
0 0 0

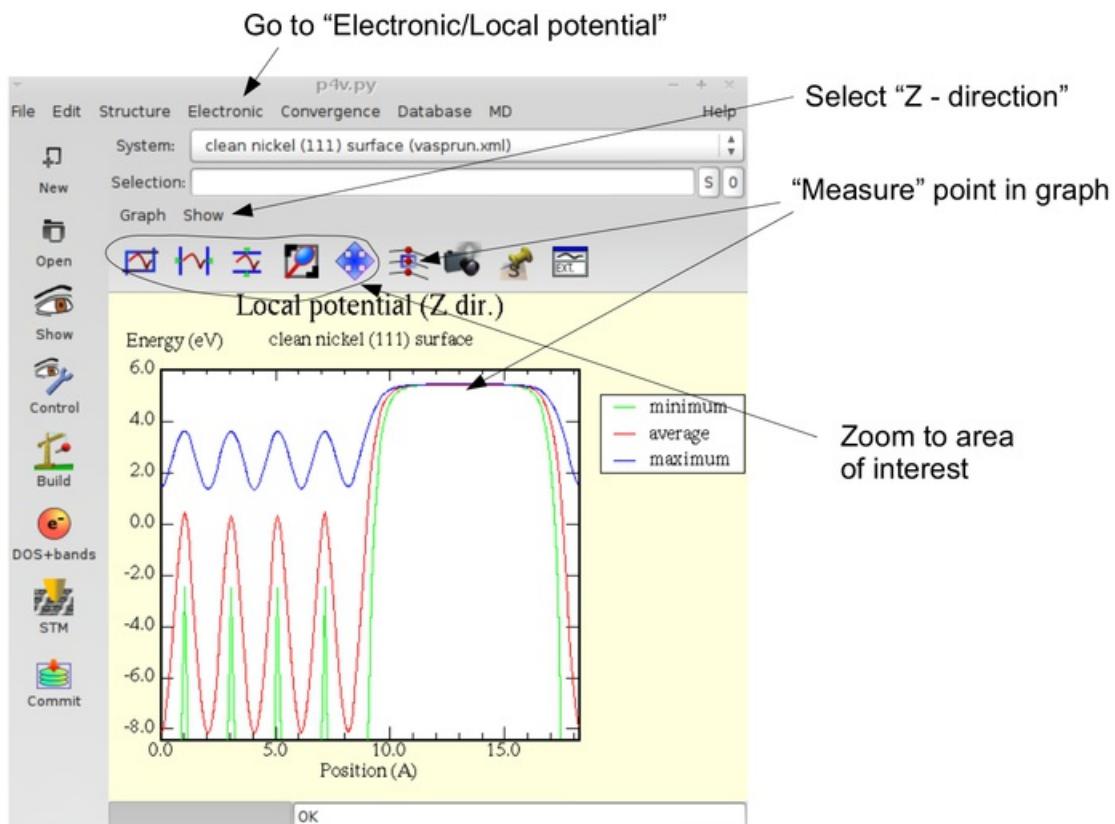
## Calculation

### Adsorption energies

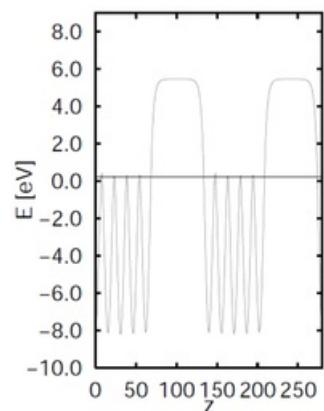
- Change of cut-off lowers total energy:
  - -25.732 eV (270 eV); -25.737 eV (400 eV).
  - Becomes more important for larger cells.
- The adsorption energy is calculated in the following way:
  - $E_{\text{ads}} = E_{\text{total}} - E_{\text{clean}} - E_{\text{CO}}$ .
  - $E_{\text{ads}} = -40.829 + 25.737 + 14.835 = -0.257 \text{ eV}.$

### Work function

- We use this run also to calculate the work-function of Ni(111).
- Use p4vasp to show the planar average of the potential:



- The plot of the planar average of the potential for this example should look like the following:



- Vacuum potential  $E^{\text{vac}} = 5.45 \text{ eV}.$
- Fermi level  $\epsilon_F = 0.224 \text{ eV}$ . (from OUTCAR file).
- Work function  $\Phi = E^{\text{vac}} - \epsilon_F = 5.23 \text{ eV}.$

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# Ni 111 surface relaxation

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## Task

Relaxation of the first two layers of a Ni (111) surface.

## Input

### POSCAR

```
fcc (111) surface
3.53
.70710678 .0000000 .0000000
-0.35355339 0.6123724 .0000000
.000000 .000000 5.1961524
5
selective dynamics
direct
.00000000 .00000000 .00000000 F F F
.33333333 .66666667 .11111111 F F F
.66666667 .33333333 .22222222 F F F
.00000000 .00000000 .33333333 T T T
.33333333 .66666667 .44444444 T T T
```

- Similar setup as for [Ni 100 surface relaxation](#).
- Again 2 of 5 layers relaxed.
- $(1 - .444) \cdot 5.196 \cdot 3.53 \approx 10.2$  of vacuum.

### INCAR

```
general:
ISTART = 0
ICHARG = 2
SYSTEM = clean (111) surface
ENMAX = 270
ISMEAR = 2 ; SIGMA = 0.2
ALGO = Fast
EDIFF = 1E-6

dynamic:
NSW = 100
POTIM = 0.8
IBRION = 1
```

- Same [INCAR](#) file as for [Ni 100 surface relaxation](#), but spin polarization neglected.

## KPOINTS

```
k-points
0
Monkhorst-Pack
9 9 1
0 0 0
```

## Calculation

- N.B.: The setup for the calculation of the "bulk" energy can be found in the *Ni111clean\_rel/bulk* subdirectory of the tar file.
- The sample output for the forces should look like the following:

POSITION			TOTAL-FORCE (eV/Angst)		
0.00000	0.00000	0.00000	0.000000	0.000000	0.178848
0.00000	1.44112	2.03805	0.000000	0.000000	-0.060127
1.24804	0.72056	4.07609	0.000000	0.000000	0.004418
0.00000	0.00000	6.11522	0.000000	0.000000	0.036384
0.00000	1.44112	8.14905	0.000000	0.000000	-0.159523
total drift:			-0.000084	0.000107	-0.017457

■ Forces are already small at the beginning (small relaxations for compact surfaces).

■ For surface energy non-spin-polarized bulk nickel as reference:

■  $\sigma^{\text{unrel}} = \frac{1}{2}(-25.731 - 5 \cdot (-5.407)) = 0.65 \text{ eV}$ .

■ (111) surface more stable than (100) surface.

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## Task

Calculation of NiO, an antiferromagnet.

## Input

## POSCAR

```
AFM NiO
4.17
1.0 0.5 0.5
0.5 1.0 0.5
0.5 0.5 1.0
2 2
Cartesian
0.0 0.0 0.0
1.0 1.0 1.0
0.5 0.5 0.5
1.5 1.5 1.5
```

- AFM coupling: 4 atoms in the basis (instead of 2).

## INCAR

```
SYSTEM = NiO
ISTART = 0
ISPIN = 2
MAGMOM = 2.0 -2.0 2*0
ENMAX = 250.0
EDIFF = 1E-3
ISMEAR = -5
AMIX = 0.2
BMIX = 0.0001
AMIX_MAG = 0.8
BMIX_MAG = 0.00001
LORBIT = 11
```

- Initial magnetic moments of  $2\mu_B$  (Ni) and  $0\mu_B$  (O).
- **AMIX=0.2** and **AMIX\_MAG=0.8** (default), **BMIX** and **BMIX\_MAG** practically zero, i.e. linear mixing.

## KPOINTS

```
k-points
0
gamma
4 4 4
0 0 0
```

## Calculation

- The total magnetic moment should be 0 in the **OSZICAR** file:

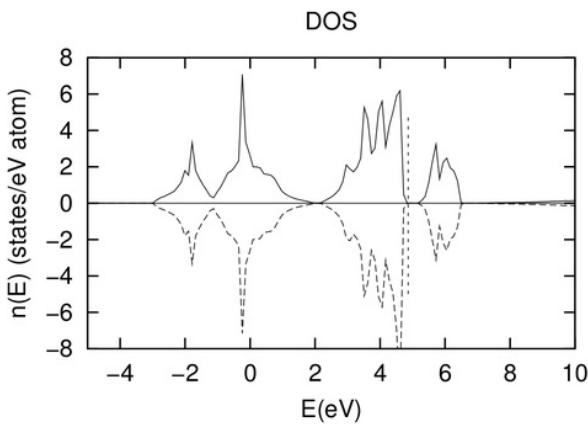
```
DAV: 13 -0.267936242334E+02 0.12794E-03 -0.12638E-04 552 0.298E-01 0.169E-02
DAV: 14 -0.267936352231E+02 -0.10990E-04 -0.21775E-05 520 0.107E-01
  1 F= -.26793635E+02 E= -.26793635E+02 d E = 0.000000E+00 mag= 0.0000
```

- The partial and integrated magnetic moments within the PAW spheres are given in the **OUTCAR** file:

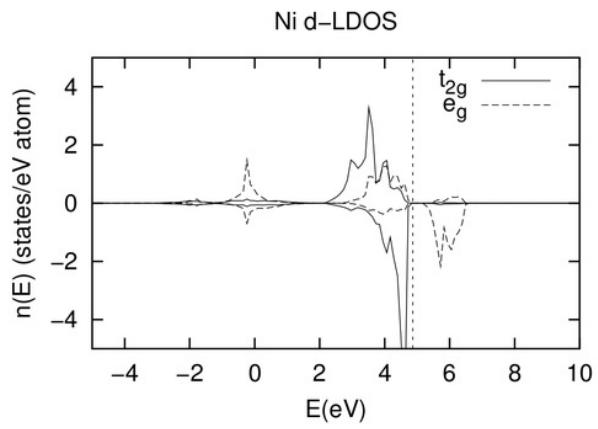
## magnetization (x)

# of ion	s	p	d	tot
1	-0.012	-0.014	1.245	1.219
2	0.012	0.014	-1.242	-1.216
3	0.000	-0.001	0.000	-0.001
4	0.000	-0.001	0.000	-0.001
tot	0.000	-0.003	0.003	0.000

- The example total DOS and the partial l-decomposed DOS for the d orbitals of Ni should look like the following:



$$|m_{\text{Ni}}| = 1.21 \mu_B \text{ (exp. } 1.70 \mu_B)$$



$$E_{\text{gap}} = 0.44 \text{ eV (exp. } 4.0 \text{ eV)}$$

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## NiO GGA

*Exercise :* Determine the most stable magnetic order between the antiferromagnetic (AFM) and ferromagnetic (FM) configurations. Compare the both DOS.

### ■ INCAR

NiO GGA AFM  
SYSTEM = "NiO"

Electronic minimization  
ENCUT = 450  
EDIFF = 1E-5  
LORBIT = 11  
LREAL = .False.  
ISTART = 0  
NELMIN = 6

DOS  
ISMEAR = -5

Magnetism  
ISPIN = 2  
MAGMOM = 2.0 -2.0 2\*0 # AFM order  
# MAGMOM = 2.0 2.0 2\*0 # FM order

Mixer  
AMIX = 0.2  
BMIX = 0.00001  
AMIX\_MAG = 0.8  
BMIX\_MAG = 0.00001

### ■ KPOINTS

k-points  
0  
gamma  
4 4 4  
0 0 0

### ■ POSCAR

NiO  
4.17  
1.0 0.5 0.5  
0.5 1.0 0.5  
0.5 0.5 1.0  
2 2  
Cartesian  
0.0 0.0 0.0  
1.0 1.0 1.0  
0.5 0.5 0.5  
1.5 1.5 1.5

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## NiO GGA+U

Description: Antiferromagnetic (AFM) configuration for NiO in the GGA+U<sub>eff</sub> (Dudarev's) approach ; PBE functional

In the Dudarev method, a Hubbard effective parameter U<sub>eff</sub> = U - J is used. Concretely, the J value is considered equal to 0, and U<sub>eff</sub> = U. For more details read the page on the [LDAUTYPE](#)-tag .

**Exercise :** Study the change of the magnetic moment of Ni atoms and the DOS by varying the U<sub>eff</sub> value.

### ■ INCAR

NiO GGA+U AFM  
SYSTEM = "NiO"

Electronic minimization  
ENCUT = 450  
EDIFF = 1E-5  
LORBIT = 11  
LREAL = .False.  
ISTART = 0  
NELMIN = 6

DOS  
ISMEAR = -5

Magnetism  
ISPIN = 2  
MAGMOM = 2.0 -2.0 2\*0.0

Mixer  
AMIX = 0.2  
BMIX = 0.00001  
AMIX\_MAG = 0.8  
BMIX\_MAG = 0.00001

GGA+U  
LDAU = .TRUE.  
LDAUTYPE = 2  
LDAUL = 2 -1  
LDAUU = 5.00 0.00  
LDAUJ = 0.00 0.00  
LDAUPRINT = 2  
LMAXMIX = 4

### ■ KPOINTS

k-points  
0  
gamma  
4 4 4  
0 0 0

### ■ POSCAR

NiO  
4.17  
1.0 0.5 0.5  
0.5 1.0 0.5  
0.5 0.5 1.0  
2 2  
Cartesian  
0.0 0.0 0.0  
1.0 1.0 1.0  
0.5 0.5 0.5  
1.5 1.5 1.5

To check the results obtained with this approach, they can be compared to those determined with a [hybrid](#) approach. The magnetic moment for the Ni atoms and the E<sub>g</sub> calculated using this approach are 1.67 μ<sub>B</sub> and 3.97 eV respectively.

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## NiO HSE06

Description: Hybrid functional calculation using the HSE06 functional.

It is strongly recommended to start from a converged PBE calculation (**ISTART** = 1) before beginning with a DFT+HF method. For other [hybrid functionals](#)

Exercise : Check the values presented [here](#).

### ■ INCAR

```
NiO HSE06 AFM  
SYSTEM = "NiO"
```

```
Electronic minimization  
ENCUT = 450  
EDIFF = 1E-5  
LORBIT = 11  
LREAL = .False.  
ISTART = 0  
NELMIN = 6
```

#### DOS

```
ISMEAR = -5
```

#### Magnetism

```
ISPIN = 2  
MAGMOM = 2.0 -2.0 2*0.0
```

#### Mixer

```
AMIX = 0.2  
BMIX = 0.00001  
AMIX_MAG = 0.8  
BMIX_MAG = 0.00001
```

#### Hybrid functional

```
#LHFCAUC = .TRUE.  
#HFSSCREEN = 0.2  
#ALGO = D  
#TIME = 0.4
```

### ■ KPOINTS

```
k-points  
0  
gamma  
4 4 4  
0 0 0
```

### ■ POSCAR

```
NiO  
4.17  
1.0 0.5 0.5  
0.5 1.0 0.5  
0.5 0.5 1.0  
2 2  
Cartesian  
0.0 0.0 0.0  
1.0 1.0 1.0  
0.5 0.5 0.5  
1.5 1.5 1.5
```

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# NiO L(S)DA+U

Description: AFM NiO in the L(S)DA+U (Dudarev's approach).

## ■ INCAR

NiO LSDA AFM  
SYSTEM = "NiO"

Electronic minimization  
ENCUT = 300  
EDIFF = 1E-4  
LORBIT = 11  
LREAL = .False.  
ISTART = 0  
NELMIN = 6

DOS  
ISMEAR = -5

Magnetism  
ISPIN = 2  
MAGMOM = 2.0 -2.0 2\*0

Mixer  
AMIX = 0.2  
BMIX = 0.00001  
AMIX\_MAG = 0.8  
BMIX\_MAG = 0.00001

LSDA+U  
LDAU = .TRUE.  
LDAUTYPE = 2  
LDAUL = 2 -1  
LDAUU = 8.00 0.00  
LDAUJ = 0.95 0.00  
LDAUPRINT = 2  
LMAXMIX = 4

## ■ KPOINTS

k-points  
0  
gamma  
4 4 4  
0 0 0

## ■ POSCAR

NiO  
4.17  
1.0 0.5 0.5  
0.5 1.0 0.5  
0.5 0.5 1.0  
2 2  
Cartesian  
0.0 0.0 0.0  
1.0 1.0 1.0  
0.5 0.5 0.5  
1.5 1.5 1.5

## Download

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# NiO LSDA

## ■ INCAR

NiO LSDA AFM  
SYSTEM = "NiO"

Electronic minimization  
ENCUT = 300  
EDIFF = 1E-4  
LORBIT = 11  
LREAL = .False.  
ISTART = 0  
NELMIN = 6

DOS  
ISMEAR = -5

Magnetism  
ISPIN = 2  
MAGMOM = 2.0 -2.0 2\*0

Mixer

AMIX = 0.2  
BMIX = 0.00001  
AMIX\_MAG = 0.8  
BMIX\_MAG = 0.00001

## ■ KPOINTS

k-points  
0  
gamma  
4 4 4  
0 0 0

## ■ POSCAR

NiO  
4.17  
1.0 0.5 0.5  
0.5 1.0 0.5  
0.5 0.5 1.0  
2 2  
Cartesian  
0.0 0.0 0.0  
1.0 1.0 1.0  
0.5 0.5 0.5  
1.5 1.5 1.5

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# NiO LSDA+U

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## Task

Calculation of antiferromagnetic NiO in the LSDA+U (Dudarev's approach).

## Input

### POSCAR

```
AFM NiO
4.17
1.0 0.5 0.5
0.5 1.0 0.5
0.5 0.5 1.0
2 2
Cartesian
0.0 0.0 0.0
1.0 1.0 1.0
0.5 0.5 0.5
1.5 1.5 1.5
```

### INCAR

```
SYSTEM = NiO
ISTART = 0
ISPIN = 2
MAGMOM = 2.0 -2.0 2*0
ENMAX = 250.0
EDIFF = 1E-3
ISMEAR = -5
AMIX = 0.2
BMIX = 0.00001
AMIX_MAG = 0.8
BMIX_MAG = 0.00001
LORBIT = 11
LDAU = .TRUE.
LDAUTYPE = 2
LDAUL = 2 -1
LDAUU = 8.00 0.00
LDAUJ = 0.95 0.00
LDAUPRINT = 2
LMAXMIX = 4 ! Important: mix paw occupancies up to L=4
```

- Switching on LSDA+U using Dudarev's approach ([LDAUTYPE=2](#)).
- [LDAUL](#) selects the I quantum number for which on site interaction is added (-1 = no on site interaction).
- The U and J parameters have to be specified.
- Print occupation matrices in the [OUTCAR](#) file ([LDAUPRINT=2](#)).
- L, U, and J must be specified for all atomic types!

### KPOINTS

```
k-points
0
gamma
4 4 4
0 0 0
```

## Calculation

### On site occupancies

- The sample output for the on site occupancies in the [OUTCAR](#) file should look like the following (the meaning of the columns after the second equality sign is given below):

```
atom = 1 type = 1 1 = 2
```

onsite density matrix  
...  
occupancies and eigenvectors

```

o = 0.1696 v = 0.0000 0.0000 0.0000 0.0000 0.0000 0.0013 -0.0006 -0.9999 -0.0007 -0.0104
o = 0.1696 v = 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000 -0.0011 -0.0104 0.0011 0.9999
o = 0.9770 v = 0.0000 0.0000 0.0000 0.0000 0.0000 0.7787 -0.1766 0.0015 -0.6020 0.0005
o = 0.9770 v = 0.0000 0.0000 0.0000 0.0000 0.0000 0.2456 -0.7972 0.0005 0.5516 -0.0015
o = 0.9770 v = 0.0000 0.0000 0.0000 0.0000 0.0000 0.5774 0.5774 0.0000 0.5774 0.0000
o = 0.9803 v = -0.0193 0.7166 0.0001 -0.6972 -0.0039 0.0000 0.0000 0.0000 0.0000 0.0000
o = 0.9803 v = 0.8163 -0.3914 -0.0039 -0.4249 -0.0001 0.0000 0.0000 0.0000 0.0000 0.0000
o = 0.9803 v = 0.5774 0.5774 0.0000 0.5774 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000
o = 1.0248 v = -0.0032 0.0016 -1.0000 0.0016 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000
o = 1.0248 v = 0.0000 0.0027 0.0000 -0.0027 1.0000 0.0000 0.0000 0.0000 0.0000 0.0000

```

$d_{xy}^\dagger \quad d_{yz}^\dagger \quad d_{z^2-r^2}^\dagger \quad d_{xz}^\dagger \quad d_{z^2-y^2}^\dagger \quad d_{xy}^\dagger \quad d_{yz}^\dagger \quad d_{z^2-r^2}^\dagger \quad d_{xz}^\dagger \quad d_{z^2-y^2}^\dagger$

■ Just for comparison when U=0 and J=0 (i.e. just LSDA) the on site occupancies are as follows:

```

o = 0.3462 v = 0.0000 0.0000 0.0000 0.0000 0.0000 -0.0048 0.0028 0.9951 0.0020 -0.0986
o = 0.3462 v = 0.0000 0.0000 0.0000 0.0000 0.0000 0.0005 0.0039 -0.0986 -0.0044 -0.9951
o = 0.9491 v = 0.0000 0.0000 0.0000 0.0000 0.0000 0.5774 0.5774 0.0000 0.5774 0.0000
o = 0.9495 v = 0.0000 0.0000 0.0000 0.0000 0.0000 -0.0588 0.7347 -0.0004 -0.6759 0.0059
o = 0.9495 v = 0.0000 0.0000 0.0000 0.0000 0.0000 0.8144 -0.3563 0.0059 -0.4581 0.0004
o = 0.9527 v = 0.0477 -0.0256 0.9974 -0.0221 -0.0420 0.0000 0.0000 0.0000 0.0000 0.0000
o = 0.9527 v = 0.0020 0.0403 0.0420 -0.0423 0.9974 0.0000 0.0000 0.0000 0.0000 0.0000
o = 0.9598 v = 0.5774 0.5774 0.0000 0.5774 0.0000 0.0000 0.0000 0.0000 0.0000 0.0000
o = 0.9599 v = -0.1186 0.7577 0.0085 -0.6391 -0.0579 0.0000 0.0000 0.0000 0.0000 0.0000
o = 0.9599 v = 0.8064 -0.3005 -0.0570 -0.5059 -0.0085 0.0000 0.0000 0.0000 0.0000 0.0000

```

$d_{xy}^\dagger \quad d_{yz}^\dagger \quad d_{z^2-r^2}^\dagger \quad d_{xz}^\dagger \quad d_{z^2-y^2}^\dagger \quad d_{xy}^\dagger \quad d_{yz}^\dagger \quad d_{z^2-r^2}^\dagger \quad d_{xz}^\dagger \quad d_{z^2-y^2}^\dagger$

## Magnetic moments

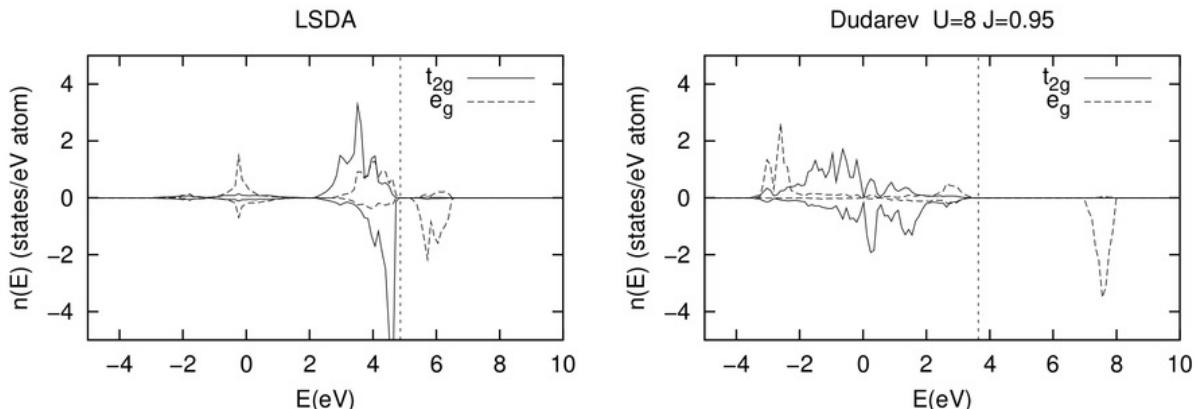
■ The sample output for the I dependent local magnetic moments is given in the **OUTCAR** file:

magnetization (x)

# of ion	s	p	d	tot
1	-0.003	-0.006	1.721	1.711
2	0.003	0.006	-1.719	-1.710
3	0.000	-0.001	0.000	-0.001
4	0.000	-0.001	0.000	-0.001
tot	0.000	-0.002	0.002	0.000

## DOS

■ The Ni lm decomposed DOS for the d states should look like the following:



## Total energy

■ The on site occupy matrix is not idempotent, hence the total energy contains a penalty contribution.  
■ The sample output for the total energy in the **OSZICAR** file should look like the following:

```

DAV: 15 -0.229633055256E+02 -0.11057E-03 -0.50020E-05 520 0.104E-01 0.118E-02
DAV: 16 -0.229633263321E+02 -0.20806E-04 -0.16650E-05 520 0.492E-02
1 F= -.22963326E+02 E0= -.22963326E+02 d E =0.000000E+00 mag= 0.0000

```

■ The sample output for a calculation using just LSDA is given below:

```

DAV: 13 -0.267936242334E+02 0.12794E-03 -0.12638E-04 552 0.298E-01 0.169E-02
DAV: 14 -0.267936352231E+02 -0.10990E-04 -0.21775E-05 520 0.107E-01
1 F= -.26793635E+02 E0= -.26793635E+02 d E =0.000000E+00 mag= 0.0000

```

■ The total energy for (U-J)>0 is always higher than for (U-J)=0.  
■ Comparing the total energies from calculations with different (U-J) is meaningless!

## Download

[4\\_3\\_NiO\\_LSDA+U.tgz](#)

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# O atom

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## Task

Performing a standard calculation for a single oxygen atom in a box. Getting to know the main input and output files of VASP.

## Input

### POSCAR

```
O atom in a box
1.0      ! universal scaling parameters
8.0 0.0 0.0 ! lattice vector a(1)
0.0 8.0 0.0 ! lattice vector a(2)
0.0 0.0 8.0 ! lattice vector a(3)
1          ! number of atoms
cart       ! positions in cartesian coordinates
0 0 0
```

We are using a POSCAR file with a single atom. Sufficiently large lattice parameters are selected so that no (significant) interactions between atoms in neighbouring cells is present.

### INCAR

```
SYSTEM = O atom in a box
ISMEAR = 0 ! Gaussian smearing
```

### KPOINTS

```
Gamma-point only
0
Monkhorst Pack
1 1 1
0 0 0
```

For atoms or molecules a single k point is sufficient. When more k points are used only the interaction between atoms (which should be zero) is described more accurately.

## Calculation

### stdout

```
running on 8 total cores
distrk: each k-point on 8 cores, 1 groups
distr: one band on 1 cores, 8 groups
using from now: INCAR
vasp.5.4.1 05Feb16 (build Aug 22 2016 16:46:23) complex
POSCAR found : 1 types and 1 ions
scaLAPACK will be used
LDA part: xc-table for Pade appr. of Perdew
POSCAR, INCAR and KPOINTS ok, starting setup
WARNING: small aliasing (wrap around) errors must be expected
FFT: planning ...
WAVECAR not read
entering main loop
```

N	E	dE	d eps	ncg	rms	rms(c)
DAV: 1	0.384469664751E+02	0.38447E+02	-0.96726E+02	16	0.293E+02	
DAV: 2	0.345965628955E+01	-0.34987E+02	-0.34942E+02	32	0.450E+01	
DAV: 3	-0.244485866931E+00	-0.37041E+01	-0.34307E+01	16	0.308E+01	
DAV: 4	-0.312557021227E+00	-0.68071E-01	-0.66914E-01	16	0.508E+00	
DAV: 5	-0.313520305300E+00	-0.96328E-03	-0.96311E-03	32	0.506E-01	0.286E-01
DAV: 6	-0.314540466589E+00	-0.10202E-02	-0.17853E-03	16	0.332E-01	0.142E-01
DAV: 7	-0.314637222361E+00	-0.96756E-04	-0.22710E-04	16	0.134E-01	
1 F=	-0.31463722E+00	E= -0.16037490E+00	d E = -0.308525E+00			
writing wavefunctions						

The example output (stdout) for the O atom was obtained using VASP version 5.4.1. The initial charge corresponds to the charge of isolated overlapping atoms ([POTCAR](#) file). For the first 4 steps the charge remains fixed, then the charge is updated (*rms(c)* column)

Short explanation of the symbols in the [OSZICAR](#) and stdout file:

N	iteration count
E	total energy
dE	change of total energy
d	eps change of the eigenvalues (fixed potential)
ncg	number of optimisation steps $\mathbf{H}\psi$
rms	total residual vector $\sum_{nk} w_k f_{nk} (\mathbf{H} - \epsilon_{nk}) \psi_{nk}$
rms(c)	charge density residual vector

## OUTCAR

The individual parts of the [OUTCAR](#) file are separated by lines.

The [OUTCAR](#) file is divided into the following parts:

- Reading [INCAR](#), [POTCAR](#), [POSCAR](#)
- Nearest neighbor distances and analysis of symmetry
- Verbose job information
- Information on lattice, k points and positions
- Information on the basis set (number of plane waves)
- Non-local pseudo potential information
- Information for each electronic step (one line in [OSZICAR](#))
- Timing and energy information

```
POTLOK: cpu time 0.0878: real time 0.0877
SETDIJ: cpu time 0.0015: real time 0.0014
EDDAV: cpu time 0.0267: real time 0.0434
DOS: cpu time 0.0001: real time 0.0001
-----
LOOP: cpu time 0.1165: real time 0.1346
```

eigenvalue-minimisations : 16  
 total energy-change (2. order) : 0.3844697E+02 (-0.9672571E+02)  
 number of electron 6.0000000 magnetization  
 augmentation part 6.0000000 magnetization

Free energy of the ion-electron system (eV)

```
alpha Z PSCENC = 0.27135287
Ewald energy TEWEN = -91.92708002
-Hartree energ DENC = -281.84385691
-exchange EXHF = 0.00000000
-V(xc)+E(xc) XCENC = 26.11948841
PAW double counting = 245.99840262 -247.84808825
entropy T'S EENTRO = -0.08636665
eigenvalues EBANDS = -44.50008162
atomic energy EATOM = 432.26319604
Solvation Ediel_sol = 0.00000000
-----
free energy TOTEN = 38.44696648 eV
energy without entropy = 38.53333313 energy(sigma->0) = 38.49014980
```

- Information on the Eigenvalues

```
E-fermi : -8.8431 XC(G=0): -0.8043 alpha+bet : -0.1463
k-point 1 : 0.0000 0.0000 0.0000
band No. band energies occupation
```

```

1 -23.8439  2.00000
2 -8.9040  1.33333
3 -8.9040  1.33333
4 -8.9040  1.33333
5 -0.4676  0.00000
6  1.8633  0.00000
7  1.8633  0.00000
8  1.8633  0.00000

```

■ Information on stress tensor

```

The O atom (Example: Oatom)
FORCE on cell =-STRESS in cart. coord. units (eV):
Direction XX YY ZZ XY YZ ZX
-----
Alpha Z  0.27135  0.27135  0.27135
Ewald   -30.64236 -30.64236 -30.64236  0.00000  0.00000  0.00000
Hartree  93.90244  93.90244  93.90244 -0.00000 -0.00000 -0.00000
E(xc)   -27.93035 -27.93035 -27.93035 -0.00000 -0.00000 -0.00000
Local   -147.86211 -147.86211 -147.86211  0.00000  0.00000  0.00000
n-local -20.54942 -20.54942 -20.54942 -0.00000 -0.00000 -0.00000
augment  5.55366  5.55366  5.55366  0.00000 -0.00000  0.00000
Kinetic  126.50998 126.50998 126.50997 -0.00000  0.00000 -0.00000
Fock    0.00000  0.00000  0.00000  0.00000  0.00000  0.00000
-----
Total   -0.74681 -0.74681 -0.74681  0.00000 -0.00000 -0.00000
in kB   -2.33695 -2.33695 -2.33695  0.00000 -0.00000 -0.00000
external pressure =      -2.34 kB Pullay stress =  0.00 kB

```

■ Information on the energy

FREE ENERGIE OF THE ION-ELECTRON SYSTEM (eV)

```

free energy TOTEN = -0.31463722 eV
energy without entropy= -0.00611258 energy(sigma>0) = -0.16037490

```

The relevant energy for molecules and atoms is energy without entropy.

```
energy without entropy= -0.00611258 energy(sigma>0) = -0.16037490
```

Three degenerate p orbitals are occupied by 2/3 electrons causing an unphysical electronic entropy

```
entropy T*S EENTRO = -0.30852464
```

A tiny value of **SIGMA**=0.01 would reduce the entropy but might slow convergence (default is **SIGMA**=0.2). **SIGMA** controls the electronic temperature, which is not a very meaningful quantity for molecules and atoms.

The total energy is found to be essentially zero. VASP subtracts from any calculated energy the energy of the atom in the configuration for which the pseudo potential was generated. All pseudo potentials were generated using non spin-polarized reference atoms.

### Restart of the calculation

When VASP is restarted the **WAVECAR** file is read and the run is continued from the previous wave functions (converging rapidly).

```

running on 8 total cores
distrk: each k-point on 8 cores, 1 groups
distr: one band on 1 cores, 8 groups
using from now: INCAR
vasp.5.4.1 05Feb16 (build Aug 22 2016 16:46:23) complex

POSCAR found : 1 types and 1 ions
scaLAPACK will be used
LDA part: xc-table for Pade appr. of Perdew
found WAVECAR, reading the header
POSCAR, INCAR and KPOINTS ok, starting setup
WARNING: small aliasing (wrap around) errors must be expected
FFT: planning ...
reading WAVECAR
the WAVECAR file was read successfully
initial charge from wavefunction
entering main loop
      N   E          dE        d eps      ncg      rms      rms(c)
DAV: 1 -0.314680766875E+00 -0.31468E+00 -0.83090E-05 16 0.564E-02 0.107E-02
DAV: 2 -0.314677281013E+00 0.34859E-05 -0.10030E-05 16 0.198E-02
1 F= -.31467728E+00 E0= -.16041496E+00 d E =-.308525E+00
writing wavefunctions

```

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# O atom spinpolarized

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## Task

Performing a spin polarized calculation for a single oxygen atom in a cubic box to get the correct magnetic moment of the atom.

## Input

### POSCAR

```
O atom in a box
1.0      ! universal scaling parameters
8.0 0.0 0.0 ! lattice vector a(1)
0.0 8.0 0.0 ! lattice vector a(2)
0.0 0.0 8.0 ! lattice vector a(3)
1          ! number of atoms
cart      ! positions in cartesian coordinates
0 0 0
```

### INCAR

```
SYSTEM = O atom in a box
ISMEAR = 0 ! Gaussian smearing
ISPIN = 2 ! spin polarized calculation
```

### KPOINTS

```
Gamma-point only
0
Monkhorst Pack
1 1 1
0 0 0
```

## Calculation

- The O atom is an open shell system with 2 unpaired electrons.
- Starting from the previous chapter add **ISPIN=2** to the **INCAR** file remove the **WAVECAR** file and restart VASP.
- The following example output is obtained (stdout):

```
running on 8 total cores
distrk: each k-point on 8 cores, 1 groups
distr: one band on 1 cores, 8 groups
using from now: INCAR
vasp.5.4.1 05Feb16 (build Aug 22 2016 16:46:23) complex
POSCAR found : 1 types and 1 ions
scaLAPACK will be used
LDA part: xc-table for Pade appr. of Perdew
POSCAR, INCAR and KPOINTS ok, starting setup
WARNING: small aliasing (wrap around) errors must be expected
FFT: planning ...
WAVECAR not read
entering main loop
N   E       dE      d eps    ncg    rms      rms(c)
DAV: 1   0.389725012498E+02  0.38973E+02  -0.10098E+03  32  0.259E+02
DAV: 2   0.317912429240E+01  -0.35793E+02  -0.35786E+02  64  0.438E+01
DAV: 3  -0.119085682530E+01  -0.43700E+01  -0.36686E+01  32  0.328E+01
DAV: 4  -0.126198272139E+01  -0.71126E-01  -0.69189E-01  32  0.508E+00
DAV: 5  -0.126284205021E+01  -0.85933E-03  -0.85925E-03  48  0.504E-01  0.653E+00
DAV: 6   0.164008071667E+00   0.14269E+01  -0.32208E+00  32  0.894E+00  0.151E+00
...  ...  ...
DAV: 13  -0.167302579657E+01  -0.25698E-03  -0.13177E-05  32  0.203E-02  0.956E-03
```

```
DAV: 14 -0.167302926747E+01 -0.34709E-05 -0.34771E-06 32 0.116E-02
1 F= -1.16730293E+01 E0= -.15958981E+01 d E =-.154262E+00 mag= 1.9999
writing wavefunctions
E-fermi : -7.1152 XC(G=0): -0.7730 alpha+bet : -0.1463
```

- Eigenstates for spin up and spin down are calculated "separately". In LSDA they interact only via the effective local potential spin-up and spin-down potential.
- In the **OUTCAR** file one can see two spin components:

#### spin component 1

```
k-point 1 : 0.0000 0.0000 0.0000
band No. band energies occupation
 1 -25.0878 1.00000
 2 -10.0830 1.00000
 3 -10.0830 1.00000
 4 -10.0830 1.00000
 5 -0.4932 0.00000
 6 1.8213 0.00000
 7 1.8303 0.00000
 8 1.8303 0.00000
```

#### spin component 2

```
k-point 1 : 0.0000 0.0000 0.0000
band No. band energies occupation
 1 -21.8396 1.00000
 2 -7.0543 0.33333
 3 -7.0543 0.33333
 4 -7.0543 0.33333
 5 -0.3594 0.00000
 6 1.9830 0.00000
 7 1.9830 0.00000
 8 1.9830 0.00000
```

The spin component 1 has two more electrons corresponding to a magnetization of  $2\mu_B$ .

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# O atom spinpolarized low symmetry

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## Task

Performing a spin-polarized low symmetry calculation of a single oxygen atom in a non cubic box to get the right energy minimum.

## Input

### POSCAR

```
O atom in a box
1.0      ! universal scaling parameters
7.0 0.0 0.0 ! lattice vector a(1)
0.0 7.5 0.0 ! lattice vector a(2)
0.0 0.0 8.0 ! lattice vector a(3)
1          ! number of atoms
cart       ! positions in cartesian coordinates
0 0 0
```

### INCAR

```
SYSTEM = O atom in a box
ISMEAR = 0 ! Gaussian smearing
SIGMA = 0.01
ISPIN = 2 ! spin polarized calculation
```

### KPOINTS

```
Gamma-point only
0
Monkhorst Pack
1 1 1
0 0 0
```

## Calculation

- In the GGA most atoms are characterized by a symmetry broken solution. VASP, however, symmetrizes the charge density according to the determined symmetry of the cell. Check the [OUTCAR](#) file, to see what symmetry VASP is using.
- To lower the symmetry, simply change the lattice parameters to 7.0, 7.5 and 8.0 in the [POSCAR](#) file (see the example file above) and reduce [SIGMA](#) to [SIGMA](#)=0.01 in the [INCAR](#) file.
- By rerunning VASP one finds a much lower energy:

```
vasp.5.4.1 05Feb16 (build Aug 22 2016 16:46:23) complex
... ...
DAV: 15 -0.189071145737E+01 -0.29321E-03 -0.39183E-05 48 0.478E-02 0.995E-03
DAV: 16 -0.189071145737E+01 -0.27775E-03 -0.39294E-05 40 0.290E-02 0.541E-03
DAV: 17 -0.189104076616E+01 -0.51555E-04 -0.34087E-06 48 0.132E-02
1 F= -.18910408E+01 E0= -.18910408E+01 d E =-.309633E-20 mag= 1.9998
```

## Further things to try

- How does the energy change when one decreases [SIGMA](#) to [SIGMA](#)=0.01 in the [INCAR](#) file? Why?

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# O dimer

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## Task

Relaxation of the bond length of an oxygen dimer.

## Input

### POSCAR

```
O dimer in a box
1.0      ! universal scaling parameters
8.0 0.0 0.0 ! lattice vector a(1)
0.0 8.0 0.0 ! lattice vector a(2)
0.0 0.0 8.0 ! lattice vector a(3)
2          ! number of atoms
cart       ! positions in cartesian coordinates
0 0 0      ! first atom
0 0 1.22   ! second atom
```

### INCAR

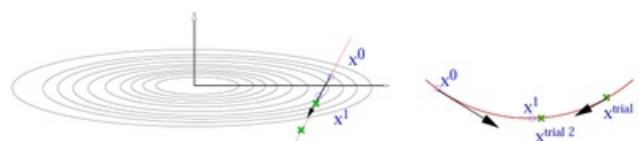
```
SYSTEM = O2 dimer in a box
ISMEAR = 0 ! Gaussian smearing
ISPIN = 2 ! spin polarized calculation
NSW = 5   ! 5 ionic steps
IBRION = 2 ! use the conjugate gradient algorithm
```

### KPOINTS

```
Gamma-point only
0
Monkhorst Pack
1 1 1
0 0 0
```

## Calculation

- We have selected in the **INCAR** file that geometry relaxation should be performed. In this case 5 ionic steps (**NSW**=5) should be done at most. For the relaxation a conjugate gradient (CG) algorithm is used (**IBRION**=2).
- The CG algorithm requires line minimizations along the search direction. This is done using a variant of Brent's algorithm. (Picture missing)
  - Trial step along search direction (gradient scaled by **POTIM**)
  - Quadratic or cubic interpolation using energies and forces at  $x_0$  and  $x_1$  allows to determine the approximate minimum
  - Continue minimization, if app. minimum is not accurate enough



## stdout

```

DAV: 1  0.517118590134E+02  0.51712E+02 -0.31393E+03  80  0.366E+02
...
...
DAV: 14 -0.985349953776E+01 -0.15177E-03 -0.57546E-06  64  0.125E-02  0.371E-03
DAV: 15 -0.985357023804E+01 -0.70700E-04 -0.22439E-06  64  0.741E-03
  1 F= -.98535702E+01 E0= -.98535702E+01 d E =-.985357E+01 mag= 2.0000
curvature: 0.00 expect dE= 0.000E+00 dE for cont linesearch 0.000E+00
trial: gam= 0.00000 g(F)= 0.113E+00 g(S)= 0.000E+00 ort = 0.000E+00 (trialstep = 0.100E+01)
search vector abs. value= 0.113E+00
bond charge predicted
...
...
  2 F= -.96234585E+01 E0= -.96234585E+01 d E =0.230112E+00 mag= 2.0000
trial-energy change: 0.230112 1 .order 0.190722 -0.113406 0.494850
step: 0.1397(harm= 0.1864) dis= 0.00731 next Energy= -9.861386 (dE=-0.782E-02)
bond charge predicted
...
...
  3 F= -.98607735E+01 E0= -.98607735E+01 d E =-.720327E-02 mag= 2.0000
curvature: -0.09 expect dE=-0.900E-05 dE for cont linesearch -0.900E-05
trial: gam= 0.00000 g(F)= 0.969E-04 g(S)= 0.000E+00 ort =-0.331E-02 (trialstep = 0.828E+00)
search vector abs. value= 0.969E-04
reached required accuracy - stopping structural energy minimisation

```

Explanation of the output:

- The quantity *trial-energy change* is the change of the energy in the trial step.
- The first value after 1. order is the expected energy change calculated from the forces  $((\mathbf{F}(\text{start}) + \mathbf{F}(\text{trial}))/2 \times \text{change of positions} - \text{central difference})$ .
- The second and third value correspond to  $\mathbf{F}(\text{start}) \times \text{change of positions}$  and  $\mathbf{F}(\text{trial}) \times \text{change of position}$ .
- The value *step* is the estimated size of the step leading to a line minimization along the current search direction. *harm* is the optimal step using a second order (or harmonic) interpolation.
- The trial step size can be controlled by the parameter **POTIM**.
- The final positions after the optimization are stored in the **CONTCAR** file. One can copy **CONTCAR** to **POSCAR** and continue the relaxation.

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# Output

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VASP gives several different output files, depending on which task is performed. The most important files that are produced in (almost) every calculation are described in the following:

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## OUTCAR

- The **OUTCAR** file gives detailed output of a VASP run, including:
  - A summary of the used input parameters.
  - Information about the electronic steps:  $E_{\text{Fermi}}$ , KS-eigenvalues.
  - Stress tensors.
  - Forces on the atoms.
  - Local charges and magnetic moments.
  - Dielectric properties
- The amount of output written onto the **OUTCAR** file can be chosen by modifying the **NWRITE** tag in the **INCAR** file.

## OSZICAR, job.stdout

- The **OSZICAR** file gives a short summary of the results:
  - Chosen scf algorithm.
  - Convergence of the total energy, charge- and spin densities.
  - Free energies.
  - Magnetic moments of the cell.

## CONTCAR

- The **CONTCAR** file gives the updated geometry data at the end of a run:
  - Lattice parameter.
  - Bravais matrix.
  - Ionic positions.
  - (Optionally velocities).
- The format of the **CONTCAR** file is the same as of the **POSCAR** file, hence it can be used directly for continuation runs after having been copied to the **POSCAR** file.

## XDATCAR

- The **XDATCAR** file contains updated ionic positions of each ionic step.

## DOSCAR

- The **DOSCAR** file contains the total and integrated DOS and optionally the local partial DOS.

## CHGCAR

- The **CHGCAR** file contains the charges  $\rho * V$ .

## WAVECAR

- The **WAVECAR** file contains the wave function coefficients. This file can be used to continue from a previous rung.

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# Partial DOS of CO on Ni 111 surface

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## Task

Calculation of the work function and partial DOS of a CO@Ni (111) surface, adsorbed on top.

## Input

### POSCAR

```
Ni - (111) + CO ontop
3.530000000000000
 0.7071067800000000  0.0000000000000000  0.0000000000000000
 -0.3535533900000000  0.6123724000000000  0.0000000000000000
  0.0000000000000000  0.0000000000000000  5.1961523999999998
 5 1 1
Selective dynamics
Direct
 0.0000000000000000  0.0000000000000000  0.0000000000000000  F  F  F
 0.3333333300000021  0.666666669999979  0.111111100000031  F  F  F
 0.666666669999979  0.3333333300000021  0.222222219999990  F  F  F
 0.0000000000000000  0.0000000000000000  0.3330391292438326  T  T  T
 0.3333333300000021  0.666666669999979  0.4445422014835692  T  T  T
 0.3333333300000021  0.666666669999979  0.5402025044116211  T  T  T
 0.3333333300000021  0.666666669999979  0.6031536532245922  T  T  T

 0.00000000E+00  0.00000000E+00  0.00000000E+00
 0.00000000E+00  0.00000000E+00  0.00000000E+00
```

### INCAR

```
general:
ENMAX = 400
SYSTEM = CO adsorption on Ni(111)
ISMEAR = -5
ALGO = Fast
```

```
LDOS:
LORBIT = 11
```

```
workfunction:
IDIPOL = 3
LDIPOL = .TRUE.
LVHAR = .TRUE.
# LVTOT = .TRUE.
```

- For the calculation of the DOS we use a tetrahedron method with Blöchl corrections (**ISMEAR**=-5).
- By setting **LVHAR=.TRUE.** the Hartree part of the local potential is written to the file **LOCPUT**.
- By setting **LVTOT=.TRUE.** the total local potential is written tot the file **LOCPUT**.
- By setting **IDIPOL=3** dipole corrections in the direction of the third lattice vector are enabled.
- We have active dipole corrections to potential (=dipole layer).

### KPOINTS

k-points

```

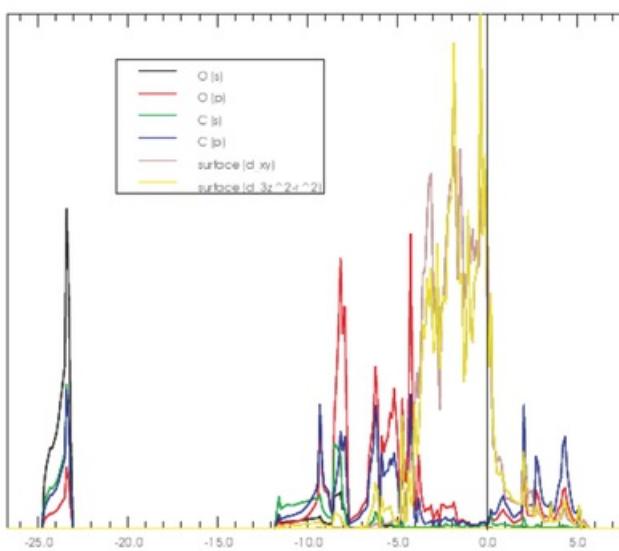
0
Monkhorst-Pack
9 9 1
0 0 0

```

## Calculation

### DOS

- The Im-decomposed DOS helps to analyze the bonding:

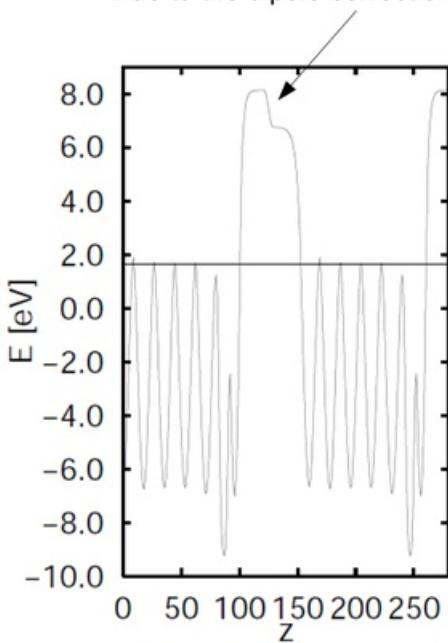


- CO  $5\sigma, 1\pi, 2\pi^*$  bonds.
- From comparison with substrate LDOS:
  - Hybridization with Ni-  $d_{3z^2-r^2}$ .
  - No interaction with  $d_{xy}$  due to symmetry.

### Work function

- The planar average of the potential for this example should look like the following:

Due to the dipole corrections!



- $\epsilon_F = 1.65$  eV (from OUTCAR file).
- Vacuum-potential at 8.24/677 eV:  $\Phi_{CO} = 6.58, \Phi_{clean} = 5.11$  eV.
- Too small result for clean surface due to too small vacuum ...

### Download

[COonNi111\\_LDOS.tgz](#)

Overview > Ni 100 surface relaxation > Ni 100 surface DOS > Ni 100 surface bandstructure > Ni 111 surface relaxation > CO on Ni 111 surface > Ni 111 surface high precision > **partial DOS of CO on Ni 111 surface** > vibrational frequencies of CO on Ni 111 surface > STM of graphite > STM of graphene > collective jumps of a Pt adatom on fcc-Pt (001):

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# Plotting the BSE fatband structure of Si

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## Task

Visualization of the BSE eigenvectors using fatbands.

## Input

```
Si
5.4300
0.5 0.5 0.0
0.0 0.5 0.5
0.5 0.0 0.5
2
cart
0.00 0.00 0.00
0.25 0.25 0.25
```

## INCAR

- This is the [INCAR](#) file for the basic DFT calculation:

```
System = Si
PREC = Normal ; ENCUT = 250.0
ISMEAR = 0 ; SIGMA = 0.01
KPAR = 2

EDIFF = 1.E-8
NBANDS = 16
LOPTICS = .TRUE. # needed for WAVEDER file
LPEAD = .TRUE.
OMEGAMAX = 40
```

## KPOINTS

The [KPOINTS](#) file will be automatically generated in this example.

## Calculation

- In this example we will calculate and plot the first "bright" BSE eigenstates of silicon, also called fatbands<sup>[1]</sup>. In this tutorial the modelBSE setup from the previous tutorial is used in combination with a 10x10x10 gamma centered k-point grid (Note: This calculation takes ~ 50 min. on 16 cores, if you don't want to wait that long, a 4x4x4 grid requires only a minute.) In principle the standard BSE method can also be used instead.

## Step 1 DFT calculation

We run a standard DFT calculation with the input files given above.

## Step 2 BSE calculation with fatbands

- The [INCAR](#) file for the modelBSE calculation looks like the following:

```
System = Si
PREC = Normal ; ENCUT = 250.0
#ALGO = BSE
ANTIRES = 0
ISMEAR = 0 ; SIGMA = 0.01
```

```

ENCUTGW = 150
EDIFF = 1.E-8 # default 1.E-4
NBANDS = 16 # only bands that are used are required, prepare the same set in a forgoing DFT run
NBANDSO = 4
NBANDSV = 8
OMEGAMAX = 20
PRECFOCK = Normal
ALGO = TDHF
LMODELHF = .TRUE. #Turn model on
HFSCREEN = 1.26 # Screening lenght
AEXX = 0.088 #Inverse of epsilon_infinity
SCISSOR = 0.69 # Difference GW-DFT band gap
NBSEEIG = 10 # number of BSE eigenvectors written out in BSEFATBAND

```

- The important tag for fatband calculations is **NBSEEIG**. In this example this will write the 10 energetically lowest BSE eigenvectors to the output file **BSEFATBAND**.
- After the (model)BSE calculation we first look into the **vasprun.xml** file to have a look at the BSE eigenvalues and the oscillator strengths (exact numbers can of course differ depending on the method you use and the density of your k-point grid):

```

<varray name="opticaltransitions" >
<v> 3.148 0.000 </v>
<v> 3.148 0.000 </v>
<v> 3.148 0.000 </v>
<v> 3.149 25654.244 </v>
<v> 3.149 25660.601 </v>
<v> 3.149 25665.652 </v>
<v> 3.151 0.001 </v>
<v> 3.151 0.001 </v>
<v> 3.152 423.751 </v>
<v> 3.310 216931.963 </v>
<v> 3.310 216916.814 </v>
<v> 3.310 216935.593 </v>

```

The first number column shows the BSE eigenvalue and the second one the oscillator strength. We are going to plot the first "bright" state, that means in this case number 4.

- We inspect the fourth band in the **BSEFATBAND** output file:

```

28428          10
 1BSE eigenvalue 3.14798542   IP-eigenvalue: 3.25790292
 0.00000 0.00000 0.00000 -6.1302666  9.0994773  0.0000001  1  5  -0.000000+i*  -0.000000
 0.00000 0.00000 0.00000  5.8415744  9.0994773  0.0876503  2  5  0.000076+i*  0.000043
 0.00000 0.00000 0.00000  5.8415744  9.0994773  341.0850802 3  5  0.088630+i*  -0.329369
 0.00000 0.00000 0.00000  5.8415744  9.0994773  543.1678695 4  5  0.361803+i*  -0.405130
 0.00000 0.00000 0.00000 -6.1302666  9.0994773  0.0000004  1  6  -0.000000+i*  0.000000
...(28428-6 more lines till 2BSE eigenvalue ...)
 4BSE eigenvalue 3.14855812   IP-eigenvalue: 3.25790292
 0.00000 0.00000 0.00000 -6.1302666  9.0994773  0.0024165  1  5  0.000002+i*  0.000001
 0.00000 0.00000 0.00000  5.8415744  9.0994773  31.4738813 2  5  -0.027821+i*  -0.014718
 0.00000 0.00000 0.00000  5.8415744  9.0994773  187.8684774 3  5  0.049093+i*  -0.181341
 0.00000 0.00000 0.00000  5.8415744  9.0994773  360.1697144 4  5  0.239775+i*  -0.268757
 0.00000 0.00000 0.00000 -6.1302666  9.0994773  0.0289534  1  6  0.000019+i*  -0.000022
...

```

The description of the values is given as follows:

1. line: Number of e-h pairs in the BSE basis and value for **NBSEEIG**.
2. line: BSE eigenvalue and minimum band gap before BSE.
3. line: Columns 1-3 k-point coordinates, column 4 hole eigenvalue, column 5 electron eigenvalue, column 6 absolute value of coupling coefficient (radius of circles), column 7 hole orbitalnumber, column 8 electron orbitalnumber, column 9 real part of coupling coefficient, column 10 imaginary part of coupling coefficient.

Columns 1-6 are used to plot the fatbands.

- Plotting of data:

1. Choose the BSE eigenstate from the **BSEFATBAND** file that you want to plot.
2. Filter out all e-h pairs that lie on the high symmetry k-lines along which you want to plot the fat bandstructure:

```

#!/bin/bash
NBSE=1 #Select the BSE eigenvector of interest.
BSIZE=$(head -n 1 BSEFATBAND|awk '{print $1}') # The BSE product basis size.
i= echo "($BSIZE+1)*$NBSE+1"\|bc
head -n $i BSEFATBAND | tail -n $BSIZE > BSE-$NBSE.dat #Cut out the selected eigenstate.
awk <BSE-$NBSE.dat ' { if ($1==$2 && $3==$2) print sqrt($1*$1+$2*$2+$3*$3), $4, $5, $6 }' >bands-GL.dat
awk <BSE-$NBSE.dat ' { if ($1==$3 && $2==0.0) print sqrt($1*$1+$2*$2+$3*$3), $4, $5, $6 }' >bands-GX.dat

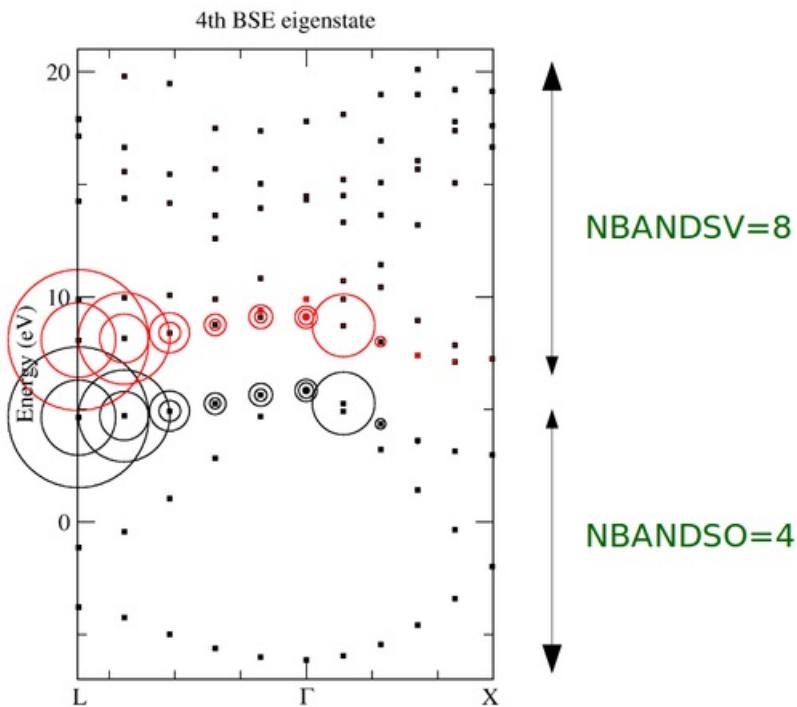
```

1. Use a plotting program to plot the output in the following manner:

k-point	electron eigenvalue	hole eigenvalue	A
---------	---------------------	-----------------	---

x	y1	y2	radius
---	----	----	--------

- The sample output for this tutorial should look like the following:



The fat band picture allows you to visually inspect which e-h pairs contribute the most to a particular BSE eigenstate. When k-point convergence is important, you can use it to truncate your e-h product basisset by choosing smarter NBANDSO/NBANDSV and/or OMEGAMAX values. Try **NBANDSO=NBANDSV=2** and check how much this effects the BSE results.

## Download

[Si\\_BSEfatbands.tgz](#)

## References

- ↑ M.Bokdam et al., Scientific Reports 6, 28618 (2016). [🔗](#)

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## Relaxed geometry

Description: calculate the relaxed geometry of NH<sub>3</sub>: the total energy is the energy of the initial state of the flipping reaction

### ■ INCAR

```
SYSTEM = Ammonia flipping
IBRION = 2
NSW = 10
ALGO = N
POTIM = 0.5
EDIFF = 1e-6
EDIFFG = -0.01
NELMIN = 5
```

### ■ KPOINTS

```
k-points
0
G
1 1 1
```

### ■ POSCAR

```
ammonia flipping
1.0000000000000000
 6.000000  0.000000  0.000000
 0.000000  7.000000  0.000000
 0.000000  0.000000  8.000000
H  N
3  1
Selective dynamics
Direct
0.636429  0.567446  0.549205  T  T  T
0.500000  0.364896  0.549205  T  T  T
0.363571  0.567446  0.549205  T  T  T
0.500000  0.500000  0.500000  F  F  F
```

## Download

[ammonia\\_flipping.tgz, sub-folder scf](#) 

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# Si bandstructure

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  - 4.4 Obtain bandstructure (Wannier interpolation) and plot using XMGRACE or GNUPLOT
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## Task

Calculation of the bandstructure for Si within DFT+HF.

The bandstructure in VASP can be obtained following three different procedures. The standard procedure (procedure 1), applicable at PBE level, is also described in [Fcc Si bandstructure example](#).

Within Hybrid functional theory it is possible to plot bandstructure using procedure 2 or 3.

## Procedure 1: Standard procedure (DFT)

Only possible within DFT. Described in [Fcc Si bandstructure example](#):

### Standard self-consistent (SC) run

- POSCAR

```
system Si
5.430
0.5 0.5 0.0
0.0 0.5 0.5
0.5 0.0 0.5
2
cart
0.00 0.00 0.00
0.25 0.25 0.25
```

- INCAR

```
System = fcc Si
ISMEAR = 0; SIGMA = 0.1;
```

- KPOINTS

```
4x4x4
0
G
4 4 4
0 0 0
```

### Non-SC calculation (ICHARG=11)

Use preconverged [CHGCAR](#) file and a suitable [KPOINTS](#) file (KPOINTS\_PBE\_bands)

- INCAR

```
System = fcc Si
ICHARG = 11 #charge read file
ISMEAR = 0; SIGMA = 0.1;
LORBIT = 11
```

## ■ KPOINTS

```
k-points for bandstructure L-G-X-U K-G
10
line
reciprocal
 0.50000 0.50000 0.50000 1
  0.00000 0.00000 0.00000 1

  0.00000 0.00000 0.00000 1
  0.00000 0.50000 0.50000 1

  0.00000 0.50000 0.50000 1
  0.25000 0.62500 0.62500 1

  0.37500 0.7500 0.37500 1
  0.00000 0.00000 0.00000 1
```

## Plot using p4v

P4VASP: [p4v](#) ↗

## Procedure 2: 0-weight (Fake) SC procedure (PBE & Hybrids)

---

This procedure can be applied to compute bandstructure at Hybrid functionals and DFT level.

### Standard DFT run

#### ■ INCAR

```
## Default
ISMEAR = 0
SIGMA = 0.01
GGA = PE

## HSE
#LHFCALC = .TRUE. ; HFSCREEN = 0.2 ; AEXX = 0.25
#ALGO = D ; TIME = 0.4 ; LDIAG = .TRUE.
```

#### ■ KPOINTS

```
Automatically generated mesh
0
G
4 4 4
0 0 0
```

## Hybrid calculation using a suitably modified KPOINTS file

#### ■ INCAR

```
## Default
ISMEAR = 0
SIGMA = 0.01
GGA = PE

## HSE
LHFCALC = .TRUE. ; HFSCREEN = 0.2 ; AEXX = 0.25
ALGO = D ; TIME = 0.4 ; LDIAG = .TRUE.
```

#### ■ KPOINTS\_HSE\_bands (see README.txt)

```
Explicit k-points list
18
Reciprocal lattice
  0.000000000000000 0.000000000000000 0.000000000000000 1
  0.250000000000000 0.000000000000000 0.000000000000000 8
  0.500000000000000 0.000000000000000 0.000000000000000 4
  0.250000000000000 0.250000000000000 0.000000000000000 6
  0.500000000000000 0.250000000000000 0.000000000000000 24
 -0.250000000000000 0.250000000000000 0.000000000000000 12
  0.500000000000000 0.500000000000000 0.000000000000000 3
 -0.250000000000000 0.500000000000000 0.250000000000000 6
  0.00000000 0.00000000 0.00000000 0.000
  0.00000000 0.05555556 0.05555556 0.000
  0.00000000 0.11111111 0.11111111 0.000
  0.00000000 0.16666667 0.16666667 0.000
  0.00000000 0.22222222 0.22222222 0.000
  0.00000000 0.27777778 0.27777778 0.000
  0.00000000 0.33333333 0.33333333 0.000
  0.00000000 0.38888889 0.38888889 0.000
  0.00000000 0.44444444 0.44444444 0.000
  0.00000000 0.50000000 0.50000000 0.000
```

## Plot using p4v

**Mind:** Remove from the bandstructure plot the eigenvalues corresponding to the the regular k-points mesh.

### Procedure 3: VASP2WANNIER90 (GW, Hybrids, PBE)

Wannier function interpolation using the VASP2WANNIER90 interface. Applicable in all cases (here applied for hybrids; for GW see [Bandstructure\\_of\\_Si\\_in\\_GW\\_\(VASP2WANNIER90\) example](#)).

#### Standard DFT run

- INCAR

```
## Default
ISMEAR = 0
SIGMA = 0.01
GGA = PE

## HSE
#LHFCALC = .TRUE. ; HFSCREEN = 0.2 ; AEXX = 0.25
#ALGO = D ; TIME = 0.4 ; LDIAG = .TRUE.

##VASP2WANNIER
#LWANNIER90=.TRUE.
```

- KPOINTS

```
Automatically generated mesh
0
G
4 4 4
0 0 0
```

#### HSE + LWANNIER90 run

- INCAR

```
## Default
ISMEAR = 0
SIGMA = 0.01
GGA = PE

## HSE
LHFCALC = .TRUE. ; HFSCREEN = 0.2 ; AEXX = 0.25
ALGO = D ; TIME = 0.4 ; LDIAG = .TRUE.

##VASP2WANNIER
LWANNIER90=.TRUE.
```

Use the wannier90.win file given below which contains all instructions needed to generate the necessary input files for the WANNIER90 runs (wannier90.amn, wannier90.mmn, wannier90.eig).

**Mind:** If the wannier90.win file does not exist VASP will create a default wannier90.win compatible with the POSCAR and INCAR files, which needs to be suitably modified by including the proper instruction required to generate the maximally localized wannier functions (refer to the [WANNIER90 manual](#) □).

- wannier90.win

```
num_wann=8
num_bands=8

Begin Projections
Si:sp3
End Projections

dis_froz_max=9
dis_num_iter=1000

guiding_centres=true

#restart      = plot
#bands_plot   = true
#begin kpoint_path
#L 0.50000  0.50000  0.50000 G 0.00000  0.00000  0.00000
#G 0.00000  0.00000  0.00000 X 0.50000  0.00000  0.50000
#X 0.50000  0.00000  0.50000 K 0.37500 -0.37500  0.00000
#K 0.37500 -0.37500  0.00000 G 0.00000  0.00000  0.00000
#end kpoint_path
#bands_num_points 40
#bands_plot_format gnuplot xmgrace

begin unit_cell_cart
    2.7150000  2.7150000  0.0000000
    0.0000000  2.7150000  2.7150000
    2.7150000  0.0000000  2.7150000
end unit_cell_cart

begin atoms_cart
```

## Compute Wannier functions

run wannier90

wannier90.x wannier90

This run generates the wannier90 standard output (wannier90.wout) and the file wannier90.chk needed for the wannier interpolation (next step)

**Obtain bandstructure (Wannier interpolation) and plot using XMGRACE or GNUPLOT**

Uncomment the bandstructure plot flags in wannier90.win and rerun (restart) wannier90:

wannier90.x wannier90

This run generates the following bandstructure files which can be visualized using xmgrace or gnuplot:

## wannier90 band.agr

wannier90\_band.dat

wannier90 band.gnu

## ■ README.txt

Bandstructure plot in VASP (Three different ways)

- 1) Standard way: PBE (Fcc Si bandstructure example).
  - 1.1 Standard self-consistent (SC) run
  - 1.2 non-SC calculation ( $\{\{TAGBL\|ICHARG\}\}=11$ ) using preconverged  $\{\{TAGBL\|CHGCAR\}\}$  file and KPOINTS\_PBE\_bands
  - 1.3 Plot using p4v
- 2) Fake SC procedure: PBE & HSE
  - 2.1 Standard self-consistent (SC) run
  - 2.2 Additional SC-run using KPOINTS\_HSE\_bands
  - 2.3 Plot using p4v

---  
The file KPOINTS\_HSE\_bands is constructed by copying the  $\{\{TAG\|IBZKPT\}\}$  file from run 2.1 to the  $\{\{TAG\|KPOINTS\}\}$  file:

IBZKPT

Automatically generated mesh

8

Reciprocal lattice

0.00000000000000	0.00000000000000	0.00000000000000	1
0.25000000000000	0.00000000000000	0.00000000000000	8
0.50000000000000	0.00000000000000	0.00000000000000	4
0.25000000000000	0.25000000000000	0.00000000000000	6
0.50000000000000	0.25000000000000	0.00000000000000	24
-0.25000000000000	0.25000000000000	0.00000000000000	12
0.50000000000000	0.50000000000000	0.00000000000000	3
-0.25000000000000	0.50000000000000	0.25000000000000	6

Then add the desired additional k-points with zero weight and change the total number of k-points

Explicit k-points list

18 <--- CHANGE TOTAL NUMBER OF K-POINTS !!

Reciprocal lattice

0.00000000000000	0.00000000000000	0.00000000000000	1
0.25000000000000	0.00000000000000	0.00000000000000	8
0.50000000000000	0.00000000000000	0.00000000000000	4
0.25000000000000	0.25000000000000	0.00000000000000	6
0.50000000000000	0.25000000000000	0.00000000000000	24
-0.25000000000000	0.25000000000000	0.00000000000000	12
0.50000000000000	0.50000000000000	0.00000000000000	3
-0.25000000000000	0.50000000000000	0.25000000000000	6
0.00000000000000	0.00000000000000	0.00000000000000	<--- ZERO WEIGHT !!
0.00000000 0.05555556	0.05555556 0.000		
0.00000000 0.11111111	0.11111111 0.000		
0.00000000 0.16666667	0.16666667 0.000		
0.00000000 0.22222222	0.22222222 0.000		
0.00000000 0.27777778	0.27777778 0.000		
0.00000000 0.33333333	0.33333333 0.000		
0.00000000 0.38888889	0.38888889 0.000		
0.00000000 0.44444444	0.44444444 0.000		
0.00000000 0.50000000	0.50000000 0.000		

---

3) VASP2WANNIER90: PBE, HSE & GW

- 3.1 Standard SC run using the existing wannier.win file
- 3.2 run wannier90 (wannier90.x wannier90) to generate MLWFs
- 3.3 uncomment bandstructure plot flags in wannier90.win and restart wannier90

---  
If the wannier90.win file does not exist VASP will create a default wannier90.win compatible with the  $\{\{TAG\|POSCAR\}\}$  and  $\{\{TAG\|INCAR\}\}$ , which need to be suitably modify by including the proper instruction required to generate the MLWFs (refer to the wannier90 manual):

```
default wannier90.win
num_wann = 8 ! set to NBANDS by VASP

use_bloch_phases = .T.

begin unit_cell_cart
  2.7150000 2.7150000 0.0000000
  0.0000000 2.7150000 2.7150000
  2.7150000 0.0000000 2.7150000
end unit_cell_cart

begin atoms_cart
Si 0.0000000 0.0000000 0.0000000
Si 1.3575000 1.3575000 1.3575000
end atoms_cart

mp_grid = 4 4 4

begin kpoints
  0.0000000 0.0000000 0.0000000
  0.2500000 0.0000000 0.0000000
  0.5000000 0.0000000 0.0000000
  0.2500000 0.2500000 0.0000000
  0.5000000 0.2500000 0.0000000
  -0.2500000 0.2500000 0.0000000
  0.5000000 0.5000000 0.0000000
  -0.2500000 0.5000000 0.2500000
  0.0000000 0.2500000 0.0000000
  0.0000000 0.0000000 0.2500000
  -0.2500000 -0.2500000 -0.2500000
  -0.2500000 0.0000000 0.0000000
  0.0000000 -0.2500000 0.0000000
  0.0000000 0.0000000 -0.2500000
  0.2500000 0.2500000 0.2500000
```

Wannier90 Manual: [WANNIER90 manual](#)

LWANNIER90 in the VASP Manual: [LWANNIER90](#).

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5\_4\_Si\_bandstructure.tgz 

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# Si HSE bandstructure

Description: Bandstructure for Si within DFT+HF

Bandstructure in VASP can be obtained following three different procedures. The standard procedure (procedure 1), applicable at PBE level, is also described in [Fcc Si bandstructure example](#).

Within Hybrid functional theory it is possible to plot bandstructure using procedure 2 or 3.

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- 1 Procedure 1: Standard procedure (suitable for DFT calculations)
  - 1.1 Standard self-consistent (SC) run
  - 1.2 Non-SC calculation (ICHARG=11)
  - 1.3 Plot using p4v
- 2 Procedure 2: 0-weight (Fake) SC procedure (works DFT & hybrid functionals)
  - 2.1 Standard DFT run
  - 2.2 Hybrid calculation using a suitably modified KPOINTS file
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## Procedure 1: Standard procedure (suitable for DFT calculations)

Only possible within DFT. Described in [Fcc Si bandstructure example](#):

### Standard self-consistent (SC) run

- [POSCAR](#)

```
system Si
5.430
0.5 0.5 0.0
0.0 0.5 0.5
0.5 0.0 0.5
2
cart
0.00 0.00 0.00
0.25 0.25 0.25
```

- [INCAR \(see INCAR.dft\)](#)

```
ISMEAR = 0
SIGMA = 0.01
NBANDS = 8
```

- [KPOINTS \(see KPOINTS.6\)](#)

```
6x6x6
0
G
6 6 6
0 0 0
```

### Non-SC calculation (ICHARG=11)

Use preconverged [CHGCAR](#) file and a suitable [KPOINTS](#) file

- [INCAR](#)

```
ISMEAR = 0
SIGMA = 0.01
NBANDS = 8

ICHARG = 11 #read charge from CHGCAR and keep fixed
LORBIT = 11
```

- [KPOINTS \(see KPOINTS\\_PBE\\_bands\)](#)

```
k-points for bandstructure L-G-X-U K-G
10
line
```

```

reciprocal
0.50000 0.50000 0.50000 1
0.00000 0.00000 0.00000 1

0.00000 0.00000 0.00000 1
0.00000 0.50000 0.50000 1

0.00000 0.50000 0.50000 1
0.25000 0.62500 0.62500 1

0.37500 0.7500 0.37500 1
0.00000 0.00000 0.00000 1

```

## Plot using p4v

P4VASP: [p4v](#)

### Procedure 2: 0-weight (Fake) SC procedure (works DFT & hybrid functionals)

This procedure can be applied to compute bandstructure at hybrid functionals and DFT level (see the HSE\_bandstructure.sh script).

#### Standard DFT run

Just as before

- [INCAR](#) (see INCAR.dft)

```

ISMEAR = 0
SIGMA = 0.01
NBANDS = 8

```

- [KPOINTS](#) (see KPOINTST.6)

```

6x6x6
0
G
6 6 6
0 0 0

```

#### Hybrid calculation using a suitably modified KPOINTS file

- [INCAR](#) (see INCAR.hse)

```

ISMEAR = 0
SIGMA = 0.01

LHFALC = .TRUE. ; HFSCREEN = 0.2 ; AEXX = 0.25
ALGO = D ; TIME = 0.4 ; LDIAG = .TRUE.

EDIFF = 1.E-6
NBANDS = 8

```

- [KPOINTS](#) (see KPOINTS\_HSE\_bands.6 and README.txt)

```

Automatically generated mesh
26
Reciprocal lattice
0.000000000000000 0.000000000000000 0.000000000000000 1
0.166666666666667 0.000000000000000 0.000000000000000 8
0.333333333333333 0.000000000000000 0.000000000000000 8
0.500000000000000 0.000000000000000 0.000000000000000 4
0.166666666666667 0.166666666666667 0.000000000000000 6
0.333333333333333 0.166666666666667 0.000000000000000 24
0.500000000000000 0.166666666666667 0.000000000000000 24
-0.333333333333333 0.166666666666667 0.000000000000000 24
-0.166666666666667 0.166666666666667 0.000000000000000 12
0.333333333333333 0.333333333333333 0.000000000000000 6
0.500000000000000 0.333333333333333 0.000000000000000 24
-0.333333333333333 0.333333333333333 0.000000000000000 12
0.500000000000000 0.500000000000000 0.000000000000000 3
0.500000000000000 0.333333333333333 0.166666666666667 24
-0.333333333333333 0.333333333333333 0.166666666666667 24
-0.333333333333333 0.500000000000000 0.166666666666667 12
0.00000000 0.00000000 0.00000000 0.000
0.00000000 0.05555556 0.05555556 0.000
0.00000000 0.11111111 0.11111111 0.000
0.00000000 0.166666667 0.166666667 0.000
0.00000000 0.22222222 0.22222222 0.000
0.00000000 0.27777778 0.27777778 0.000
0.00000000 0.33333333 0.33333333 0.000
0.00000000 0.38888889 0.38888889 0.000
0.00000000 0.44444444 0.44444444 0.000
0.00000000 0.50000000 0.50000000 0.000

```

Please note that step two requires a WAVECAR obtained from a standard DFT run (not an HSE calculation), otherwise the resulting conduction bands often have a zig-zag structure.

## Plot using p4v

P4VASP: [p4v](#)

**Mind:** Zoom in on the right-side part of the bandstructure plot.

## Procedure 3: VASP2WANNIER90 (works for DFT, hybrid functionals, and GW)

Wannier function interpolation using the VASP2WANNIER90 interface: this procedure is applicable to DFT, hybrid functionals, and GW bandstructure calculations. Here we apply it for a hybrid functional. For GW see the [Bandstructure of Si in GW \(VASP2WANNIER90\)](#) and [bandstructure of SrVO<sub>3</sub> in GW](#) examples.

To see a summary of the workflow below, have a look at the `HSE_bandstructure_with_wannier90.sh`.

### Standard DFT run

Just as before

- [INCAR](#) (see INCAR.dft)

```
ISMEAR = 0
SIGMA = 0.01
NBANDS = 8
```

- [KPOINTS](#) (see KPOINTST.6)

```
6x6x6
0
G
6 6 6
0 0 0
```

### Increase the number of states to 24

This step is optional.

- [INCAR](#) (see INCAR.diag)

```
ISMEAR = 0
SIGMA = 0.01
ALGO = Exact
NELM = 1
NBANDS = 24
```

### HSE + LWANNIER90 run

Run the hybrid functional calculation and call wannier90 (see [LWANNIER90\\_RUN](#)) . . .

- [INCAR](#) (see INCAR.hse\_with\_wannier90)

```
ISMEAR = 0
SIGMA = 0.01
LHFALC = .TRUE. ; HFSCREEN = 0.2 ; AEXX = 0.25
ALGO = D ; TIME = 0.4 ; LDIAG = .TRUE.
NKRED = 2
EDIFF = 1.E-6
NBANDS = 24
LWANNIER90_RUN = .TRUE.
```

You will have to provide some instructions for wannier90 as well:

- [wannier90.win](#) (see wannier90.win\_start)

```
num_wann=18
num_bands=24

Begin Projections
Si:s ; p ; d
End Projections

#dis_froz_max=9
dis_num_iter=100

#guiding_centres=true
```

```
bands_plot = true
begin kpoint_path
L 0.50000 0.50000 0.5000 G 0.00000 0.00000 0.0000
G 0.00000 0.00000 0.0000 X 0.50000 0.00000 0.5000
X 0.50000 0.00000 0.5000 K 0.37500 -0.37500 0.0000
K 0.37500 -0.37500 0.0000 G 0.00000 0.00000 0.0000
end kpoint_path
bands_num_points 40
bands_plot_format gnuplot xmgrace
```

**Mind:** If the wannier90.win file does not exist VASP will create a default wannier90.win compatible with the POSCAR and INCAR files, which needs to be suitably modified by including the proper instruction required to generate the maximally localized wannier functions (refer to the [WANNIER90 manual](#)).

## Plot bandstructure (Wannier interpolation) using XMGRACE or GNUPLOT

If all went well, wannier90 will have generated the following bandstructure files which can be visualized using xmgrace or gnuplot:

- wannier90\_band.agr

```
xmgrace ./wannier90_band.agr
```

- wannier90\_band.dat
- wannier90\_band.gnu

```
gnuplot -persist ./wannier90_band.gnu
```

**N.B.:** Most modern versions of gnuplot will respond with an error message unless you remove the first line of wannier90\_band.gnu (some deprecated syntax issue).

## Download

[Si\\_HSE\\_band.tgz](#)

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# Spin-orbit coupling in a Fe monolayer

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- 3 Calculation
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## Task

Spin-orbit coupling (SOC) in a freestanding Fe monolayer. This example is carried out in total analogy to [Spin-orbit coupling in a Ni monolayer](#).

## Input

### POSCAR

```
fcc Fe 100 surface
3.45
.50000 .50000 .00000
-.50000 .50000 .00000
.00000 .00000 5.00000
1
Cartesian
.00000 .00000 .00000
```

### INCAR

```
SYSTEM      = Fe (100) monolayer
ISTART     = 0
ENCUT      = 270.00
LNONCOLLINEAR = .TRUE.
MAGMOM     = 0.0 0.0 3.0
VOSKOWN    = 1
LSORBIT    = .TRUE.
LMAXMIX    = 4
```

■ For the second calculation, switch to in-plane magnetization by setting **MAGMOM= 3.0 0.0 0.0**.

### KPOINTS

```
k-points
0
Monkhorst-Pack
9 9 1
0 0 0
```

## Calculation

■ From the energy differences of the calculations using in plane and out of plane magnetization we see that the easy axis lies (in contrast to Ni) out of plane:

$$E_{\text{MAE}} = E(m_{\perp}) - E(m_{\parallel}) = -0.2 \text{ meV}$$

## Download

[4\\_4\\_SOI\\_Fe.tgz](#)

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# Spin-orbit coupling in a Ni monolayer

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## Task

Spin-orbit coupling (SOC) in a freestanding Ni monolayer.

## Input

### POSCAR

```
fcc Ni 100 surface
3.53
.50000 .50000 .00000
-.50000 .50000 .00000
.00000 .00000 5.00000
1
Cartesian
.00000 .00000 .00000
```

### INCAR

```
SYSTEM      = Ni (100) monolayer
ISTART     = 0
ENCUT      = 270.00
LNONCOLLINEAR = .TRUE.
MAGMOM     = 0.0 0.0 1.0
VOSKOWN    = 1
LSORBIT    = .TRUE.
LMAXMIX   = 4
```

- Initialization of moment along z-direction (out of plane) (**MAGMOM** = 0.0 0.0 1.0).
- Spin-orbit interaction switched on (**LSORBIT**=.TRUE.).
- For the second calculation, switch to in-plane magnetization by setting **MAGMOM** = 1.0 0.0 0.0 in the **INCAR** file.

## KPOINTS

```
k-points
0
Monkhorst-Pack
9 9 1
0 0 0
```

## Calculation

- The sample output for the total energy using out of plane magnetization is given in the **OSZICAR** file:

```
...
DAV: 20 -0.371322930070E+01 0.15852E-03 -0.11632E-03 636 0.235E-01 0.225E-02
DAV: 21 -0.371323204989E+01 -0.27492E-05 -0.13047E-05 500 0.184E-02
1 F= -.37132320E+01 E0= -.37139803E+01 d E =0.224478E-02 mag= 0.0000 0.0000 0.9035
```

- The sample output for the total energy using in plane magnetization looks like the following:

```
...
DAV: 19 -0.371443443024E+01 -0.80757E-04 -0.35822E-03 1084 0.323E-01 0.119E-02
DAV: 20 -0.371446032472E+01 -0.25894E-04 -0.42423E-05 916 0.263E-02
1 F= -.37144603E+01 E0= -.37150300E+01 d E =0.170900E-02 mag= 0.9049 0.0000 0.0000
```

- From the energy difference of these calculations we see that the easy axis lies in plane:

$$E_{\text{MAE}} = E(m_{\perp}) - E(m_{\parallel}) = 1.2 \text{ meV}$$

## Download

[4\\_4\\_SOI\\_Ni.tgz](#) 

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# Standard relaxation

## Used INCAR Tags

[ANDERSEN\\_PROB](#), [EDIFF](#), [EDIFFG](#), [ENMAX](#), [IBRION](#), [ISMEAR](#), [MDALGO](#), [NSW](#), [POTIM](#), [SIGMA](#), [SYSTEM](#), [TEBEG](#), [TEEND](#)

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[h2o\\_on\\_tio2.tgz](#), sub-folder std\_relaxation 

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# STM of graphene

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## Task

Generation of an STM image of a graphene surface.

## Input

### POSCAR

```
C: Graphite Lattice
1.0
+2.4410462393 +0.0000000000 +0.0000000000
-1.2205231197 +2.1140080551 +0.0000000000
+0.0000000000 +0.0000000000 +10.0000000000
2
Cartesian
+0.0000000000 +0.0000000000 +0.0000000000
+0.0000000000 +1.4093387034 +0.0000000000
```

### INCAR

```
general:
  SYSTEM = Graphite surface slap
  ENMAX = 400
  ISMEAR = 2 ; SIGMA = 0.2
  ALGO = Fast

partial charge densities:
  LPARD = .TRUE.
  LSEPK = .FALSE.
  LSEPB = .FALSE.
  NBMOD = -3
  EINT = -0.1 0.1

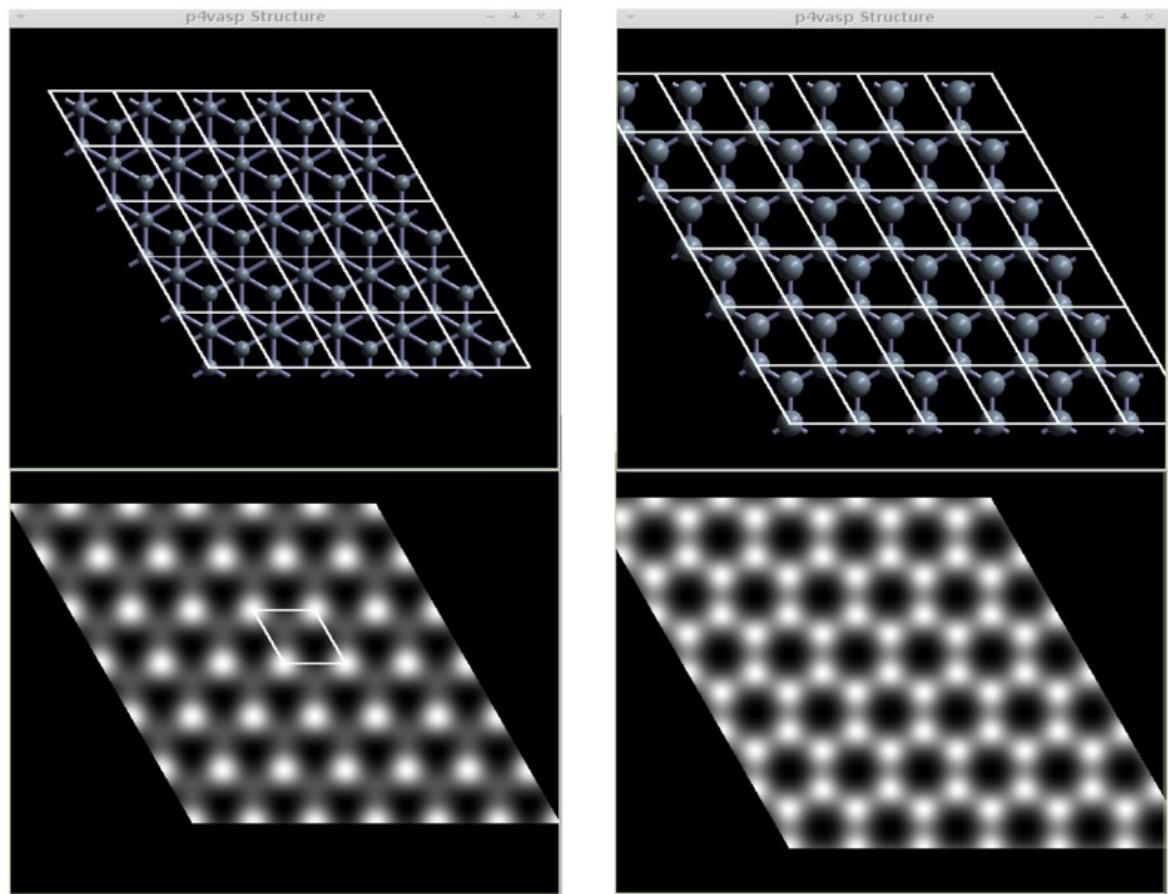
#DOS:
  #ISTART = 0
  #ICHARG = 2
  #LORBIT = 11
```

### KPOINTS

```
K-Points
0
Monkhorst-Pack
9 9 1
0 0 0
```

## Calculation

- This example is carried out in complete analogy to the example [STM of graphite](#).
- The sample output for the graphite (left) and graphene (right) STM images should look like the following:



## Download

[Graphene\\_STM.tgz](#)

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## Task

Generation of an STM image of a graphite surface.

## Input

## POSCAR

```
C: Graphite Lattice
1.0
+2.4410462393 +0.0000000000 +0.0000000000
-1.2205231197 +2.1140080551 +0.0000000000
+0.0000000000 +0.0000000000 +22.0000000000
10
Cartesian
+0.0000000000 +0.0000000000 +0.0000000000
+0.0000000000 +1.4093387034 +0.0000000000
+0.0000000000 +1.4093387034 +3.3070243927
+1.2205231197 +0.7046693517 +3.3070243927
+0.0000000000 +0.0000000000 +6.6140487854
+0.0000000000 +1.4093387034 +6.6140487854
+0.0000000000 +1.4093387034 +9.9210731781
+1.2205231197 +0.7046693517 +9.9210731781
+0.0000000000 +0.0000000000 +13.2280975708
+0.0000000000 +1.4093387034 +13.2280975708
```

## INCAR

```
general:
SYSTEM = Graphite surface slap
ENMAX = 400
ISMEAR = 2 ; SIGMA = 0.2
ALGO = Fast
```

```
partial charge densities:
LPARD = .TRUE.
LSEPK = .FALSE.
LSEPB = .FALSE.
NBMOD = -3
EINT = -0.1 0.1

# DOS:
# ISTART = 0
# ICHARG = 2
# LORBIT = 11
```

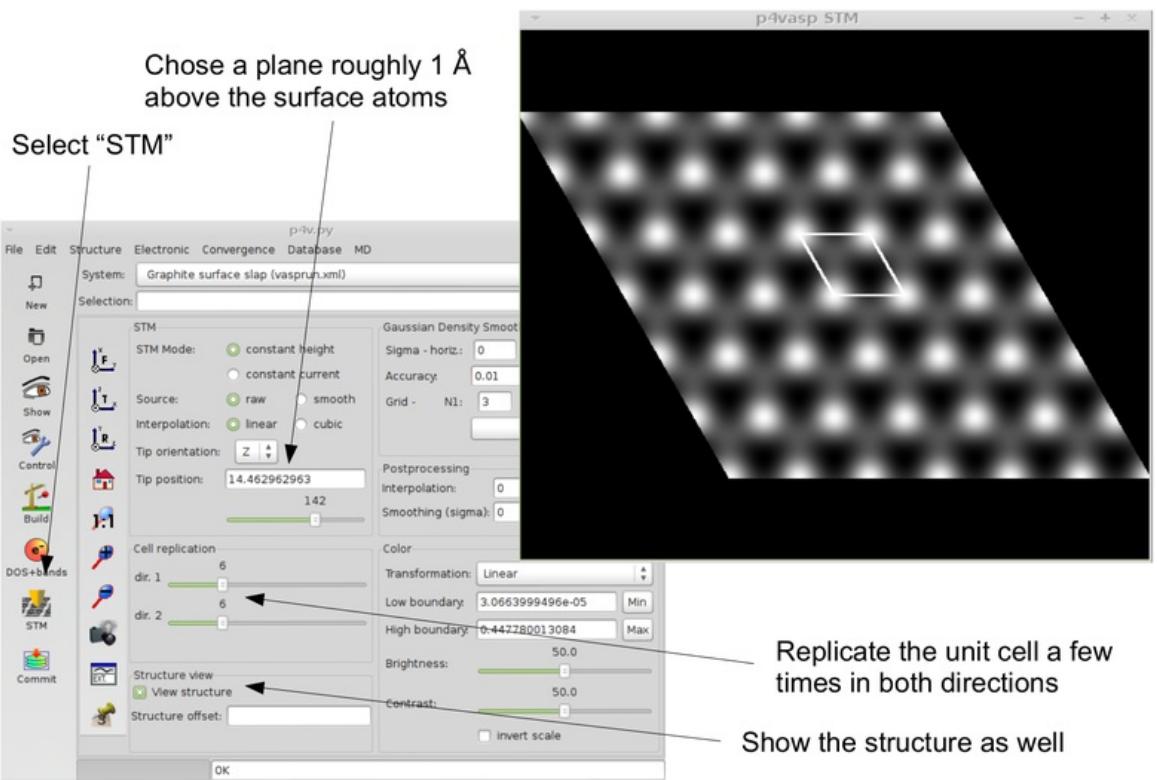
## KPOINTS

```
K-Points
0
Monkhorst-Pack
9 9 1
0 0 0
```

- Only one k point in z direction since we have a surface.

## Calculation

- First copy INCAR.par to [INCAR](#) and run VASP for the preliminary calculation.
- Second copy INCAR.DOS to [INCAR](#) to get the Im-decomposed DOS.
- To get an STM image use p4vasp:



## Download

[Graphite\\_STM.tgz](#)

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# TS search using the Improved Dimer Method

## Description:

### ■ INCAR

```
SYSTEM = Ammonia flipping
IBRION = 44
NSW = 100
EDIFF = 1e-6
EDIFFG = -0.01
```

### ■ KPOINTS

```
k-points
0
G
1 1 1
```

### ■ POSCAR

```
ammonia flipping
1.000000000000000
 6.000000 0.000000 0.000000
 0.000000 7.000000 0.000000
 0.000000 0.000000 8.000000
H N
 3 1
Direct
 0.6462 0.5736 0.5000
 0.5000 0.3547 0.5000
 0.3538 0.5736 0.5000
 0.5000 0.5000 0.5000
! decay direction
 0.000004 -0.000001 0.511990
 0.000000 -0.000003 0.547859
-0.000004 -0.000001 0.511988
 0.000000 0.000000 -0.111986
```

## Download

[ammonia\\_flipping.tgz, sub-folder improved\\_dimer](#)

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## TS search using the NEB Method

Description: the Nudged Elastic Band Method generates an energy profile along a reaction path, using equidistant IMAGES along the path. The input geometries of the IMAGES are interpolated between the geometries of the initial and the final states, e.g. using the script interpolatePOSCAR, which processes the con-catenated POSCAR files of the initial and the final state of the reaction (POSCAR\_if). in the case of ammonia flipping the final state is a mirror of the initial state and need not be calculated explicitly. For each IMAGE, a separate sub-directory 00 ... (IMAGES+1) is needed, which contains all output of the respective IMAGE. The number of cores on which VASP is run has to be an integer multiple of the number of IMAGES.

### ■ INCAR

```
SYSTEM = Ammonia flipping
IMAGES = 6
SPRING = -5
IBRION = 2
NSW = 50
ALGO = N
POTIM = 1.0
EDIFF = 1e-6
```

### ■ KPOINTS

```
k-points
0
G
1 1 1
```

### ■ POSCAR\_if

```
ammonia flipping
1.000000000000000
 6.000000  0.000000  0.000000
 0.000000  7.000000  0.000000
 0.000000  0.000000  8.000000
 3 1
Direct
0.636428  0.567457  0.5491645
0.500000  0.364985  0.5491330
0.363572  0.567457  0.5491645
0.500000  0.500000  0.5000000
ammonia flipping
1.000000000000000
 6.000000  0.000000  0.000000
 0.000000  7.000000  0.000000
 0.000000  0.000000  8.000000
 3 1
Direct
0.636428  0.567457  0.4508355
0.500000  0.364985  0.4508670
0.363572  0.567457  0.4508355
0.500000  0.500000  0.5000000
```

## Download

[ammonia\\_flipping.tgz, sub-folder NEB](#) 

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# Vibrational Analysis of the TS

Description: the [Improved Dimer Method](#) needs an educated guess of the decay path, which is estimated from the hardest vibration mode with imaginary frequency of the TS geometry (which is a planar NH<sub>3</sub> molecule):

## ■ INCAR

```
SYSTEM = Ammonia flipping
IBRION = 5
NSW = 1
ALGO = F
POTIM = 0.015
EDIFF = 1e-8
EDIFFG = -0.01
NWRITE = 3
```

## ■ KPOINTS

```
k-points
0
G
1 1 1
```

## ■ POSCAR

```
ammonia flipping
1.000000000000000
 6.000000  0.000000  0.000000
 0.000000  7.000000  0.000000
 0.000000  0.000000  8.000000
H   N
 3   1
Direct
 0.6462  0.5736  0.5000
 0.5000  0.3547  0.5000
 0.3538  0.5736  0.5000
 0.5000  0.5000  0.5000
```

## Download

[ammonia\\_flipping.tgz, sub-folder TS\\_vib](#)

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# Vibrational frequencies of CO on Ni 111 surface

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## Task

Calculation of the vibrational frequencies of CO@Ni(111) (on top).

## Input

### POSCAR

```
Ni - (111) + CO on-top
3.530000000000000
 0.7071067800000000  0.0000000000000000  0.0000000000000000
 -0.3535533900000000  0.6123724000000000  0.0000000000000000
 0.0000000000000000  0.0000000000000000  5.1961523999999999
Ni C O
 5 1 1
Selective dynamics
Direct
 0.0000000000000000  0.0000000000000000  0.0000000000000000  F F F
 0.3333333300000021  0.6666666699999979  0.1111111100000031  F F F
 0.6666666699999979  0.3333333300000021  0.2222222199999990  F F F
-0.0000000000000000  0.0000000000000000  0.3326227833039623  F F F
 0.3333333300000021  0.6666666699999979  0.4445699380869117  F F F
 0.3333333300000021  0.6666666699999979  0.5403264650180125  F F T
 0.3333333300000021  0.6666666699999979  0.6032949698060487  F F T

 0.0000000E+00  0.0000000E+00  0.0000000E+00
 0.0000000E+00  0.0000000E+00  0.0000000E+00
```

- Frequencies only for CO molecule and z-direction (z- and (x,y) are independent).

### INCAR

SYSTEM = CO on Ni111 - frequencies

general:

```
ENMAX = 400
ISMEAR = 2 ; SIGMA = 0.2
ALGO = Fast
EDIFF = 1E-6
MAXMIX = 60 # reuse the mixer between ionic steps, saves time
```

dynamic:

```
NSW = 100
IBRION = 5
NFREE = 2
```

- Small termination criterion (EDIFF).
- Automatic frequency calculation (displacement 0.04 ).
- Reuse of the mixer between ionic steps (MAXMIX) to save time.

### KPOINTS

```
k-points
0
Monkhorst-Pack
9 9 1
0 0 0
```

## Calculation

- Finite differences give the following additional output in the **OUTCAR** file for frequency calculations:

Finite differences progress:  
Degree of freedom: 1/ 2  
Displacement: 1/ 2  
Total: 1/ 4

- After the first calculation for the equilibrium geometry, **NFREE** displacements ( $\pm$  **POTIM**) are performed for each degree of freedom. From these displacements the dynamical matrix is set up and diagonalized.
- At the end of the **OUTCAR** file the following are listed:
  - Forces.
  - The dynamical matrix and finally.
  - The eigenfrequencies.
  - Eigenvectors (first normalized and then mass-weighted).
- The example output for the eigenvectors and eigenvalues of the dynamical matrix from the **OUTCAR** file should look like the following:

### Eigenvectors and eigenvalues of the dynamical matrix

```
1 f = 63.914144 THz 401.584411 2PiTHz 2131.946301 cm-1 264.327748 meV
      X   Y   Z   dx   dy   dz
0.000000 0.000000 0.000000 0   0   0
0.000000 1.441116 2.038046 0   0   0
1.248043 0.720558 4.076093 0   0   0
0.000000 0.000000 6.108743 0   0   0
0.000000 1.441116 8.153979 0   0   0
0.000000 1.441116 9.908620 0   0   -0.761748
0.000000 1.441116 11.063296 0   0   0.623594

2 f = 12.467410 THz 78.335050 2PiTHz 415.868035 cm-1 51.561083 meV
      X   Y   Z   dx   dy   dz
0.000000 0.000000 0.000000 0   0   0
0.000000 1.441116 2.038046 0   0   0
1.248043 0.720558 4.076093 0   0   0
0.000000 0.000000 6.108743 0   0   0
0.000000 1.441116 8.153979 0   0   0
0.000000 1.441116 9.908620 0   0   -0.623594
0.000000 1.441116 11.063296 0   0   -0.781748
```

- Try to change the selective dynamics tag such that displacements in x and y direction are allowed as well for CO (note that the selective dynamics flags always refer to cartesian coordinates), i.e,

```
0.3333333300000021 0.6666666699999979 0.5403264650180125 F F T
0.3333333300000021 0.6666666699999979 0.6032949698060487 F F T
```

to

```
0.3333333300000021 0.6666666699999979 0.5403264650180125 T T T
0.3333333300000021 0.6666666699999979 0.6032949698060487 T T T
```

Also test whether you need to decrease **EDIFF** to 1E-8.

## Download

[COonNi111\\_freq.tgz](#)

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# XANES in Diamond

(UNDER CONSTRUCTION)

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## Task

Calculation of the XANES K-edge in diamond using the supercell core-hole method.

## Input

### POSCAR

```
cubic diamond
3.567
0.5 0.5 0.0
0.0 0.5 0.5
0.5 0.0 0.5
2
direct
0.0 0.0 0.0
0.25 0.25 0.25
```

- We will not use this structure as input but rather use it to construct a super cell from it that is actually used in the calculations.

### INCAR

```
System = DIAMOND
ALGO = FAST
ISMEAR = 0; SIGMA = 0.1;
ICORELEVEL = 2
CLNT = 1
CLN = 1
CLL = 0
CLZ = 1.0
CH_LSPEC = .TRUE.
CH_SIGMA = 0.5
NBANDS = 300
LREAL = A
```

- To promote a core electron into the conduction bands and hence create the core-hole **ICORELEVEL**=2 has to be set. This corresponds to the final state approximation
- **CLNT**=1 selects the first atom species in the **POSCAR** file.
- **CLN**=1 selects main quantum number 1 (hence K-edge).
- **CLL**=0 selects angular quantum number 0 (s).
- **CLZ**=1.0 selects the charge of the core hole. By setting this number to a fractional value we can mimick different screening of the electrons.. Since this purely exploits error cancellation and the physical background of non-integer charges is not defined well, it should be only used with caution.
- By setting **CH\_LSPEC=.TRUE.** we enable the calculation of matrix elements between core and conduction states and the calculation of the core electron absorption spectrum.
- The broadening of the core electron absorption spectrum is controlled by the tag **CH\_SIGMA**. Usually it is good practice to set this value low and broaden the spectrum in post processing.
- We have to set **NBANDS** to a larger value to consider enough conduction band states in the calculation.
- Since super cells are used the calculation of the projection operators in real space is much faster, hence **LREAL=A** is set.

## Calculation

### Step 1 build a supercell

To perform calculations with a core~/VASP\_WIKI/WIKI\_TUTORIALS/CORE\_HOLES/Diamond/S3x3x3/FCH/P4V-hole we need

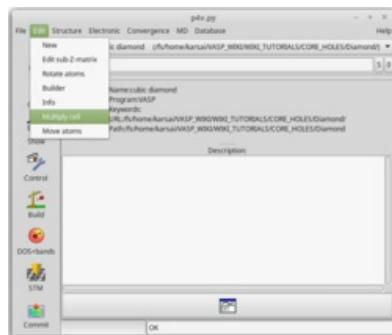
sufficiently large super cells to reduce the interaction of neighbouring core-holes. Usually the obtained spectrum with respect to the size of the super cell has to be converged. This means calculations are done with successively larger cells until no significant change is visible in the spectrum anymore. To save computational time we chose a  $3 \times 3 \times 3$  cell for this tutorial, although for converged values one should use at least  $4 \times 4 \times 4$ .

The super cell can be obtained either by taking the file POSCAR.3x3x3 provided with this tutorial. In the following we show how to get the super cell from the primitive cell using p4vasp:

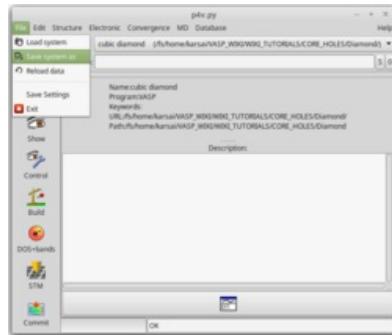
- Open p4vasp by typing *p4v* on the terminal.
- Load the primitive cell by clicking on **File → Load system**:



- Multiply cell in each direction (enter 3 for each direction) by clicking on **Edit → Multiply Cell**:



- Save new system by clicking on **File → Save system as**:



## Step 2 Prepare input files

The first few lines of the [POSCAR](#) file for the super cell should look like the following

```
cubic diamond
3.567
+1.5000000000 +1.5000000000 +0.0000000000
+0.0000000000 +1.5000000000 +1.~//VASP_WIKI/WIKI_TUTORIALS/CORE_HOLES/Diamond/S3x3x3/FCH/P4V5000000000
+1.5000000000 +0.0000000000 +1.5000000000
54
Cartesian
+0.0000000000 +0.0000000000 +0.0000000000
+0.2500000000 +0.2500000000 +0.2500000000
+0.5000000000 +0.0000000000 +0.5000000000
...
```

Here we have only one atom species with 54 atoms (line 6). To construct a core hole on a single atom we have to, take one of these atoms and treat it as a different species. We choose the first atom and we end up with 1 and 53 in the 6th line of the modified [POSCAR](#) file

```
cubic diamond
3.567
+1.5000000000 +1.5000000000 +0.0000000000
+0.0000000000 +1.5000000000 +1.5000000000
+1.5000000000 +0.0000000000 +1.5000000000
1 53
Cartesian
+0.0000000000 +0.0000000000 +0.0000000000
+0.2500000000 +0.2500000000 +0.2500000000
```

```
+0.5000000000 +0.0000000000 +0.5000000000
...

```

Accordingly we have to set CLNT=1 in the [INCAR](#) file which selects the first atom species in [POSCAR](#) to carry the core-hole. Also one has to create a [POTCAR](#) file with the PAW/PS information for both species. Since the two species are both diamond this can be simply done by concatenation of the [POTCAR](#) file for diamond by using the command `cat POT_C POT_C > POTCAR`. Alternatively the [POTCAR](#) appropriate for core-hole calculations in diamond is provided in the tar file.

The number of used bands in the calculation have to be set manually. Usually one needs to select enough bands, depending on how far one wants to calculate the spectrum and on the number of electrons in the system, to have enough conduction states available in the calculation. Selecting too high numbers a priori is also not good, since it drastically increases the computation time. Hence want has to test the optimal number of bands. In our example we set [NBANDS](#)=300.

The rest of the [INCAR](#) file is described above.

**Mind:** The multiplicity of the species carrying the core hole has to be 1 otherwise the code will not work correctly. Also mind that the selected species (CLNT in the [INCAR](#) file) is consistent with the order of the species specified in the [POSCAR](#) and [POTCAR](#) files.

### Step 3 Running Calculation

The SCF calculation with the core-hole and afterwards the calculation dielectric matrix (spectrum) is done in a single calculation. Usually the command to run the calculation looks like this: `mpirun -np $np vasp_version`, where `$np` corresponds to the number of processes and `_version` in the executable usually stands for `std`, `gam`, `nci` namely standard, gamma-point only and non-collinear version, respectively. Since we have to use super cells in the calculation, which are large enough to minimize the interaction between core-holes on neighbouring cells, parallel execution with many computational cores is necessary to achieve good results within reasonable time. Hence for this example we use a **3 × 3 × 3** cell, which gives sufficiently accurate results but more importantly finishes fast using only a few number of cores. For accurate results one should use at least a **4 × 4 × 4** cell.

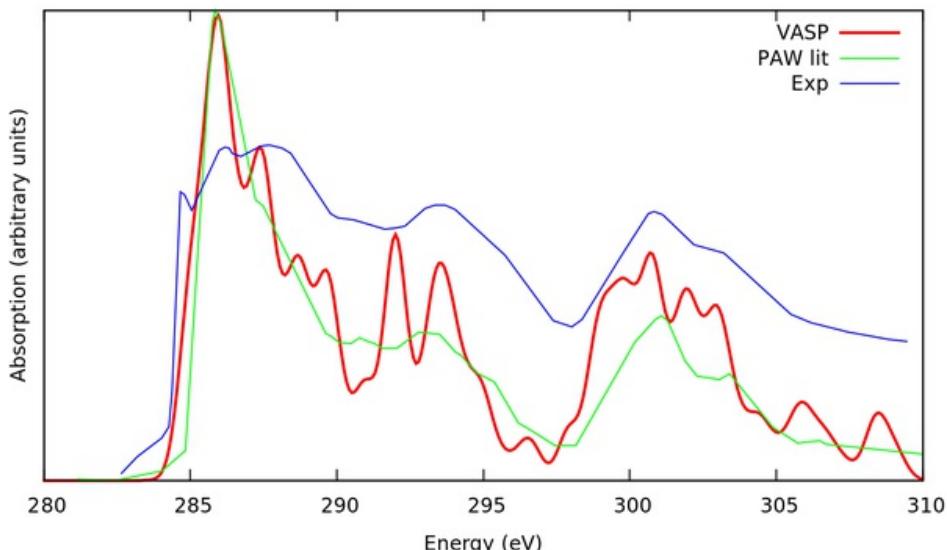
### Step 4 Extraction of XAS Spectrum

To get the spectrum we want to plot the imaginary part of the frequency dependent dielectric function. This is written out in the [OUTCAR](#) file

E(eV)	X	Y	Z	XY	YZ	ZX	
243.589609	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	density-density
243.677325	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	
243.765042	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	
...							

Usually we are interested in the sum of all components of the dielectric matrix. You can either obtain this by your script or you use the script provided in this example. If you decide for the latter use the command `perl ./plot_core_imdil.pl`. This will create the file `CORE_DIELECTRIC_IMAG.dat` which contains the summed up imaginary part of the dielectric matrix.

For this example we want to compare with experimental<sup>[1]</sup> and theoretical<sup>[2]</sup> XAS spectra from literature. They are provided in the files `C_XAS_aligned_to_VASP.dat` and `C_PARATEC_aligned_to_VASP.dat`. The literature calculations were obtained using the PARATEC code, which is also a PAW/Pseudopotential code. Both spectra are shifted to coincide with the VASP at the first peak. One can either plot these two spectra together with the VASP spectrum using his own preferred method of choice or using the script provided with this tutorial and invoking the command `gnuplot gnuplot.script`. One can also type `plot.sh` which does all the plotting steps together. The output should hopefully look like the this:



The experimental offset of the spectrum (absolute value of the first peak) is rather impossible to reproduce, since the calculated core energies are very different compared to experiment. Usually there is even a noticeable deviation between calculations using different codes. It is accepted in literature to look at the relative peak positions in the spectra and the

spectra can be scaled arbitrarily . In this example we scaled the experiment to VASP, since in this way the obtained results can be very easily compared to the experiment using a script. Usually one would either scale the first peak to 0 or would scale the calculated value to the experiment. Additionally the intensity of the spectrum can be scaled arbitrarily. So in this example we align the position and the height of the first peak for the calculations. The experiment is a little bit more tricky. It's a matter of taste what to consider as the first peak, but we decided that most likely the second peak corresponds to the first peak in the calculations and the first peak in experiment is a shoulder that is simply not pronounced in experiment.

Another important issue is the broadening. Many factors contribute to the experimental broadening depending totally on the experimental setup and hence it is impossible to reproduce the broadening exactly. We can choose a broadening that gives approximately the same width as experiment, but the choice of broadening parameters is rather arbitrary than systematic. For simplicity in this example we choose to use a 0.5 eV constant Lorentzian broadening (this is the only type of broadening built in for the calculation of XAS spectra in VASP). For more elaborate spectra we strongly advise users to choose a 0.05 eV broadening and apply the desired broadening in post-processing.

Apart from the obviously lower broadening width, we get quite reasonable agreement with theoretical literature calculations. We stress again that we used a **3 × 3 × 3** cell in this example and that our results with respect to cell size are not fully converged. The interested user can repeat the calculations for the **4 × 4 × 4** cell, which can be done in complete analogy to the **3 × 3 × 3** cell (set **NBANDS** carefully since we have many more atoms in the **4 × 4 × 4** cell). The files for this example are also given in the tar file.

## Download

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[XANES\\_in\\_Diamond.tgz](#)

## References

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1. ↑ Y.Ma et al., Phys. Rev. Lett 69, 2598 (1992). [\[1\]](#)
2. ↑ M.Tallefumier et al., Phys. Rev. B 66, 195107 (2002). [\[2\]](#)

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