Introduction to VASP

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Outlines

- Introduction
- Input files
  - INCAR
  - POTCAR
  - POSCAR
  - KPOINTS
- Output files
  - OUTCAR and CHGCAR
  - DOSCAR and EIGENVAL
  - PROCAR
- Examples
  - Si
  - NiO and MnO
  - $NdNiO_2$

Introduction

- Perform *ab initio* quantum-mechanical molecular dynamics (MD) simulations.
- It is based on the local-density approximation with the free energy as variational quantity and an exact evaluation of the instantaneous electronic ground state at each MD time step.
- The interaction between ions and electrons is described by ultra-soft Vanderbilt pseudopotentials (US-PP) or by the projector-augmented wave (PAW) method and a plane wave basis set.
- Highlights:
  - VASP provides well-tested pseudopotentials for almost every element.
  - Algorithms are efficient and stable.
  - VASP includes a full featured symmetry code which determines the symmetry of arbitrary configurations automatically.
  - VASP can conduct various calculation.
  - VASP runs equally well on super-scalar processors, vector computers and parallel computers.

Input Files

Main input files:

- INCAR: determines 'what to do and how to do' and contains a relatively large number of parameters.
- POTCAR: contains the pseudopotential for each atmoic species used in the calculation.
- POSCAR: contains the lattice geometry and the ionic positions.
- KPOINTS: create the k-point grid with k-point coordinates and weights or the mesh size.

INCAR

```
SYSTEM = Si
ISTART = 0
ICHARG = 2
ENCUT = 240
ISMEAR = 0
SIGMA = 0.1
```

Frequently used parameters:

- SYSTEM: notation of system
- ISTART: restart from the previous calculation or not
- ICHARG: initial guess for charge density
  - ICHARG = 0: Calculate charge density from initial orbitals
  - ICHARG = 2: Take superposition of atomic charge densities
  - ICHARG = 11: To obtain the eigenvalues or the DOS for a given charge density read from CHGCAR (non-self consistent calculation).
- ENCUT: cut-off energy for plane wave basis set in eV.
- ISMEAR, SIGMA: parameters for smearing.
  - ISMEAR = -1 (Fermi-smearing); 0 (Gaussian smearing), -2 (partial occupancies from WAVEVAR), -5 (tetrahedron method with Blochl corrections)
  - SIGMA: determines the width of the smearing in eV for the finite temperature LDA.

INCAR

- ISPIN = 1 (non spin polarized); 2 (spin polarized)
- MAGMOM: specifies the initial magnetic moment for each atom.
- EDIFF: accuracy for electronic minimization
- PREC:
- NELM: the maximum number of electronic self-consistency steps
- AMIX, BMIX, LMAXMIX: charge density mixer
  - LMAXMIX: which *l* quantum number are passed through mixer (for s and p, set to 2; for d, set to 4; for f, set to 6)
- LORBIT: create output files at certain level
  - LORBIT = 11 (work for PAW method and produce DOSCAR and PROCAR)
- IBRION: determines how the ions are updated and moved
  - IBRION = 2: conjugate gradient algorithm (recommended for difficult relaxation problem)

```
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
```

POTCAR

- The ordering corresponds to the species ordering on the POSCAR and INCAR.
- POTCAR files contains
  - Information about the atoms (mass, valence, etc.)
  - Default energy cutoff (the value of ENCUT in the INCAR file overwrites the default in the POTCAR)
- Supplied pseudopotentials
  - Methods: US-PP and PAW
  - Exchange correlation function: LDA and GGA (PW91 or PBE)
  - Semi-core states: X, X_sv (with s semi-core states), X_pv (with p semi-core states), X_d (with f semi-core states)
  - ENMAX: X, X_s, X_h (with harder pseudopotential)
- NOTES
  - Use PAW for transition metal 3d elements, lanthanides and actinides.
  - For 3d elements, recommend to use X_pv.

POSCAR

- A comment line
- A universal scaling factor (‘lattice constant’)
  - If this value is negative, it is interpreted as the total volume of the cell.
- Three lattice vectors defining the unit cell of the system
- The number of atoms per atomic species
  - The ordering must be consistent with the POTCAR and INCAR
- Whether the atomic positions are provided in cartesian coordinates or in direct coordinates
  - If the first character is ‘C’, ‘c’, ‘K’ or ‘k’, switch to the cartesian mode.
- The three coordinates for each atom.

```
NdNiO2
1.0
3.920000 0.000000 0.000000
0.000000 3.920000 0.000000
0.000000 0.000000 3.280000
Nd Ni O
1 1 2
direct
0.500000 0.500000 0.500000
0.000000 0.000000 0.000000
0.000000 0.500000 0.000000
0.500000 0.000000 0.000000
```

Direct

$$\vec{R} = x_1\vec{a}_1 + x_2\vec{a}_2 + x_3\vec{a}_3$$

Cartesian

$$\vec{R} = s\begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix}$$

KPOINTS

- Automatic k-mesh generation
  - 0 means number of k-points = 0 -> automatic generation scheme
  - Three formats
    - Auto: fully automatic with length l

$$N_1 = \max(1, l * |\vec{b}_1| + 0.5)$$
$$N_2 = \max(1, l * |\vec{b}_2| + 0.5)$$
$$N_3 = \max(1, l * |\vec{b}_3| + 0.5)$$

$$\vec{k} = \vec{b}_1 \frac{n_1}{N_1} + \vec{b}_2 \frac{n_2}{N_2} + \vec{b}_3 \frac{n_3}{N_3}$$

```
Automatic mesh
0
Auto
  10
```

    - Gamma-centered or Monkhorst-Pack case

$$\vec{k} = \vec{b}_1 \frac{n_1 + s_1}{N_1} + \vec{b}_2 \frac{n_2 + s_2}{N_2} + \vec{b}_3 \frac{n_3 + s_3}{N_3}$$

$$\vec{k} = \vec{b}_1 \frac{n_1 + s_1 + 1/2}{N_1} + \vec{b}_2 \frac{n_2 + s_2 + 1/2}{N_2} + \vec{b}_3 \frac{n_3 + s_3 + 1/2}{N_3}$$

```
Automatic generation
0
Monhkorst-Pack
9     9     9
0.0   0.0    0.0
```

    - Cartesian or reciprocal coordinates

```
Automatic generation
0
Cartesian
0.25 0.00 0.00
0.00 0.25 0.00
0.00 0.00 0.25
0.00 0.00 0.00
```

KPOINTS

- Strings of k-points for band structure calculations

```
k-points along high symmetry lines
 10  ! 10 intersections
Line-mode
rec
  0   0   0   ! gamma
  0.5 0.5 0   ! X

  0.5 0.5 0   ! X
  0.5 0.75 0.25  ! W

  0.5 0.75 0.25  ! W
  0   0   0   ! gamma
```

Output files

Main output files

- OUTCAR: contains most of the results and information for each iteration.
- CHGCAR: contains the lattice vectors, atomic coordinates, the total charge density multiplied by the volume $\rho(r) * V_{\text{cell}}$ on the fine FFT-grid.
- DOSCAR: contains the DOS and integrated DOS.
- EIGENVAL: contains the Kohn-Sham-eigenvalues for all k-points.
- PROCAR: contains the spd- and site projected wave function character of each band.

OUTCAR and CHGCAR

- Useful information in OUTCAR
  - volume of the system: *grep 'volume' OUTCAR*
  - total energy of the system: *grep 'TOTEN' OUTCAR*
  - the Fermi energy: *grep 'Fermi' OUTCAR | tail -1*
  - reciprocal lattice vectors: *g/reciprocal lattice vectors*
  - the difference between the free energy and the total energy: *grep "EENTRO" OUTCAR*
- CHGCAR
  - lattice parameters
  - NGX, NGY, NGZ

```
Au-Zn_zig
 1.00000000000000
    15.000000     0.000000     0.000000
     0.000000    15.000000     0.000000
     0.000000     0.000000     6.600000
   1   1
Direct
0.000000  0.000000  0.000000
0.000000  0.000079  0.500000

160  160   72
0.18441120499E+05 0.17909524567E+05 0.16406959292E+05 0.14179806898E+05 0.11554638997E+05
0.88581841033E+04 0.63620171557E+04 0.42583169365E+04 0.26537018923E+04 0.15676950926E+04
..................................
```

DOSCAR and EIGENVAL

```
   4    4    1    2
 0.1260045E+02  0.3920000E-09  0.3920000E-09  0.3280000E-09  0.5000000E-15
 1.000000000000000E-004
 CAR
unknown system
    39    105     48

 0.0000000E+00  0.0000000E+00  0.0000000E+00  0.9523810E-02
   1      -57.428443    -56.757701   1.000000   1.000000
   2      -57.428443    -56.757701   1.000000   1.000000
   3      -56.919609    -56.623246   1.000000   1.000000
   4      -32.016976    -32.020730   1.000000   1.000000
   5      -13.527106    -13.474671   1.000000   1.000000
   6      -13.094556    -13.100395   1.000000   1.000000
   7      -13.094556    -13.100395   1.000000   1.000000
   8      -12.626410    -12.608481   1.000000   1.000000
   9      -12.605169    -12.563061   1.000000   1.000000
```

PROCAR

```
PROCAR lm decomposed
# of k-points:  105         # of bands:  48         # of ions:   4

 k-point    1 :    0.00000000 0.00000000 0.00000000     weight = 0.00952381

band   1 # energy  -57.42844285 # occ.  1.00000000

ion      s     py     pz     px    dxy    dyz    dz2    dxz    dx2    tot
  1  0.000  0.000  0.000  0.000  0.000  0.000  0.000  0.000  0.000  0.000
  2  0.000  0.508  0.000  0.489  0.000  0.000  0.000  0.000  0.000  0.996
  3  0.000  0.000  0.000  0.000  0.000  0.000  0.000  0.000  0.000  0.000
  4  0.000  0.000  0.000  0.000  0.000  0.000  0.000  0.000  0.000  0.000
tot  0.000  0.508  0.000  0.489  0.000  0.000  0.000  0.000  0.000  0.997

band   2 # energy  -57.42844276 # occ.  1.00000000

ion      s     py     pz     px    dxy    dyz    dz2    dxz    dx2    tot
  1  0.000  0.000  0.000  0.000  0.000  0.000  0.000  0.000  0.000  0.000
  2  0.000  0.489  0.000  0.508  0.000  0.000  0.000  0.000  0.000  0.996
  3  0.000  0.000  0.000  0.000  0.000  0.000  0.000  0.000  0.000  0.000
  4  0.000  0.000  0.000  0.000  0.000  0.000  0.000  0.000  0.000  0.000
tot  0.000  0.489  0.000  0.508  0.000  0.000  0.000  0.000  0.000  0.997
```

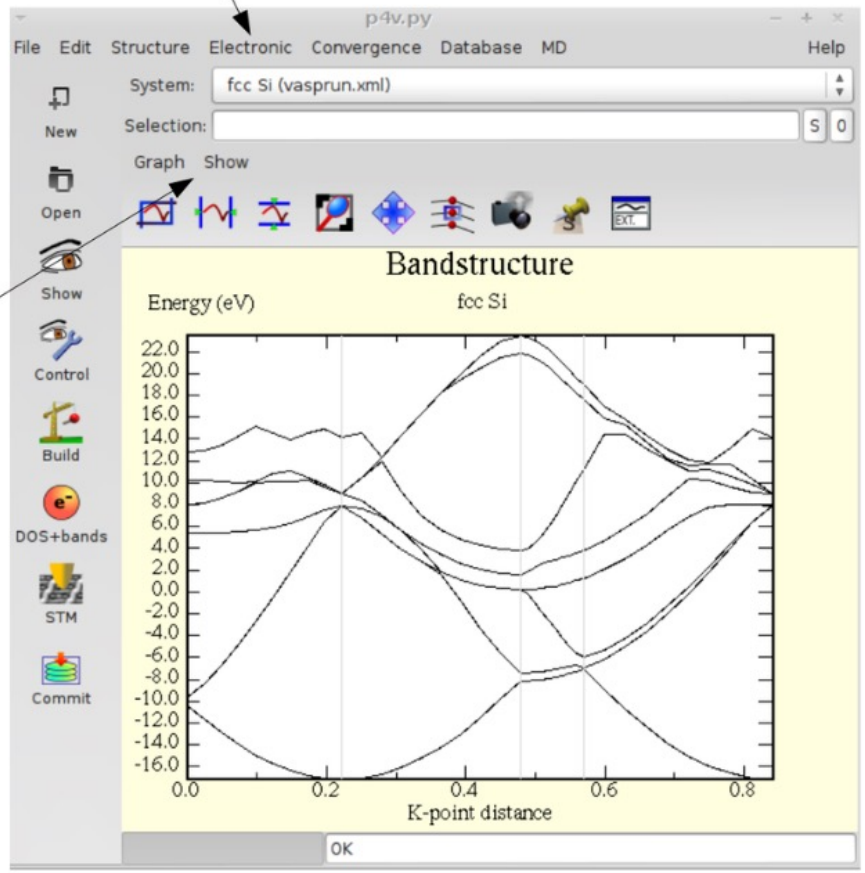
p4vasp: DOS and band

- p4v vasprun.xml

Start p4vasp:
> p4v [vasprun.xml]

Step 1.) Go to: Electronic/DOS+bands

Step 2.) Go to: Show/Bands



Example: Si

self-consistency calculation

POSCAR

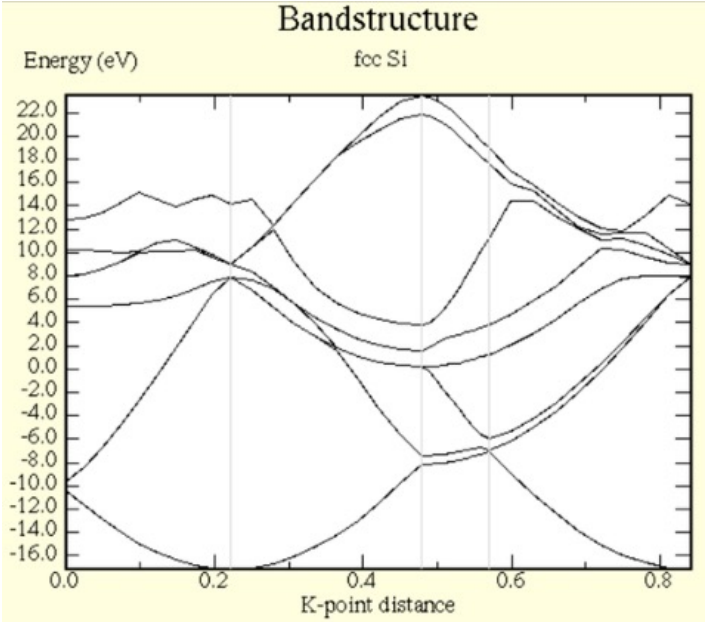
```
fcc Si:
 3.9
 0.5 0.5 0.0
 0.0 0.5 0.5
 0.5 0.0 0.5
   1
cartesian
0 0 0
```

INCAR

```
SYSTEM = Si
ISTART = 0
ICHARG = 2
ENCUT = 240
ISMEAR = 0
SIGMA = 0.1
```

KPOINTS

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



non self-consistency calculation
for band structure

POTCAR

```
PAW_PBE Si
```

INCAR

```
System = fcc Si
ICHARG = 11
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
  0.00000  0.00000  0.00000

  0.00000  0.00000  0.00000
  0.00000  0.50000  0.50000

  0.00000  0.50000  0.50000
  0.25000  0.62500  0.62500

  0.37500  0.7500   0.37500
  0.00000  0.00000  0.00000
```

Example: NiO

self-consistency calculation

non self-consistency calculation
for band structure

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
```

KPOINTS

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

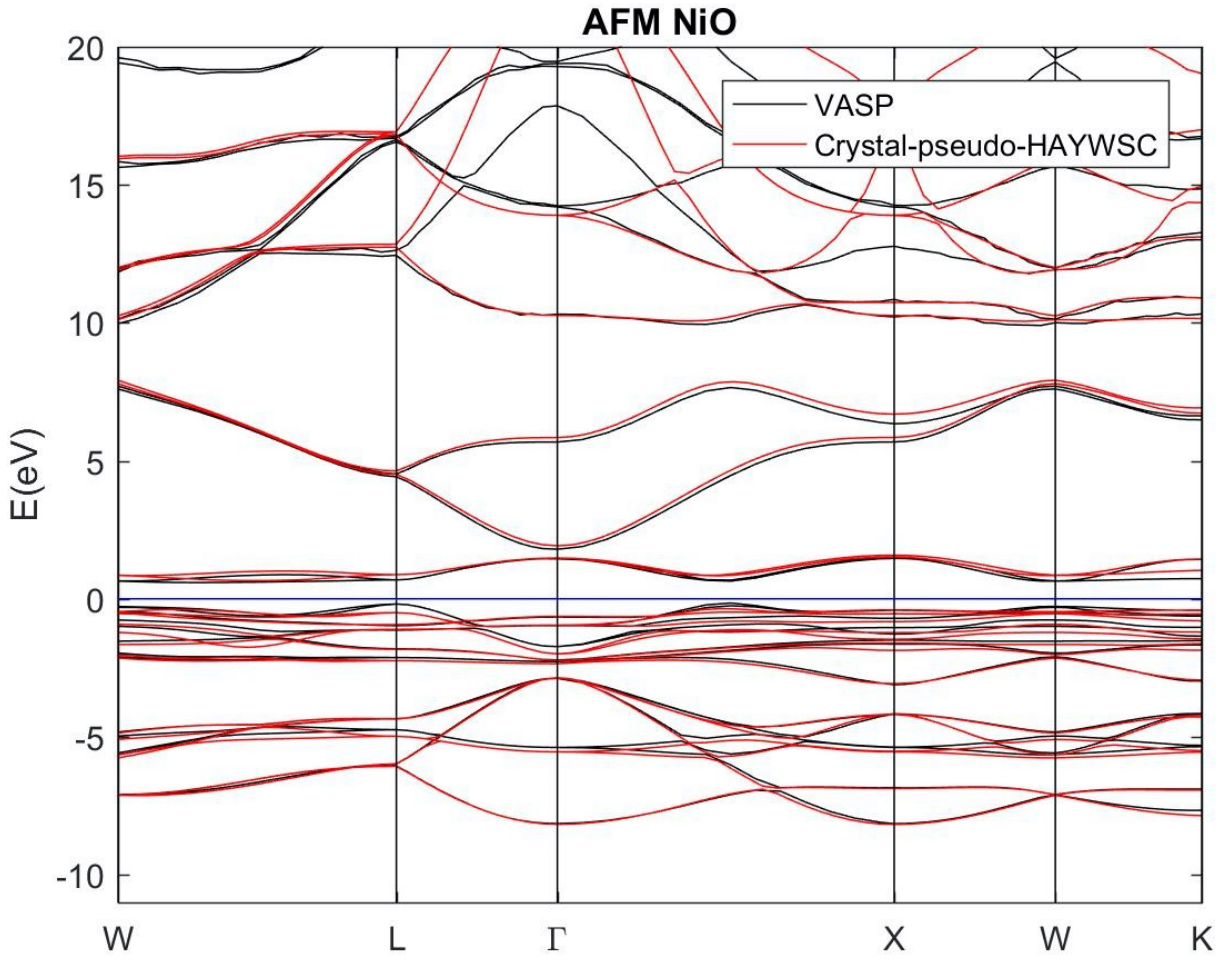
INCAR

```
SYSTEM    = NiO

ISTART    = 1
ICHARG    = 11
NBANDS    = 96

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
```

KPOINTS

```
k-points along hign symmetry
15
Line-mode
rec
0.500 0.250 0.750  ! W
0.500 0.500 0.500  ! L

0.500 0.500 0.500  ! L
0.000 0.000 0.000  ! GAMMA

0.000 0.000 0.000  ! GAMMA
0.500 0.000 0.500  ! X

0.500 0.000 0.500  ! X
0.500 0.250 0.750  ! W

0.500 0.250 0.750  ! W
0.375 0.375 0.000  ! K
```

Example: NiO



Example: $NdNiO_2$

POSCAR

```
NdNiO2
1.0
3.920000 0.000000 0.000000
0.000000 3.920000 0.000000
0.000000 0.000000 3.280000
Nd Ni O
1 1 2
direct
0.500000 0.500000 0.500000
0.000000 0.000000 0.000000
0.000000 0.500000 0.000000
0.500000 0.000000 0.000000
```

POTCAR

```
PAW_PBE Nd_3
```

```
PAW_PBE Ni_pv
```

```
PAW_PBE O
```

self-consistency calculation

INCAR

```
ALGO = Fast
EDIFF = 0.0002
ENCUT = 520
IBRION = 2
ICHARG = 1
ISIF = 3
ISMEAR = -5
ISPIN = 2

LMAXMIX = 6
LORBIT = 11
LREAL = Auto
LWAVE = False
MAGMOM = 1*0.6 1*5.0 2*0.6
NELM = 100
NSW = 99
PREC = Accurate
SIGMA = 0.05
```

KPOINTS

```
automatic mesh
0
Gamma
6 6 6
```

non self-consistency calculation for band structure

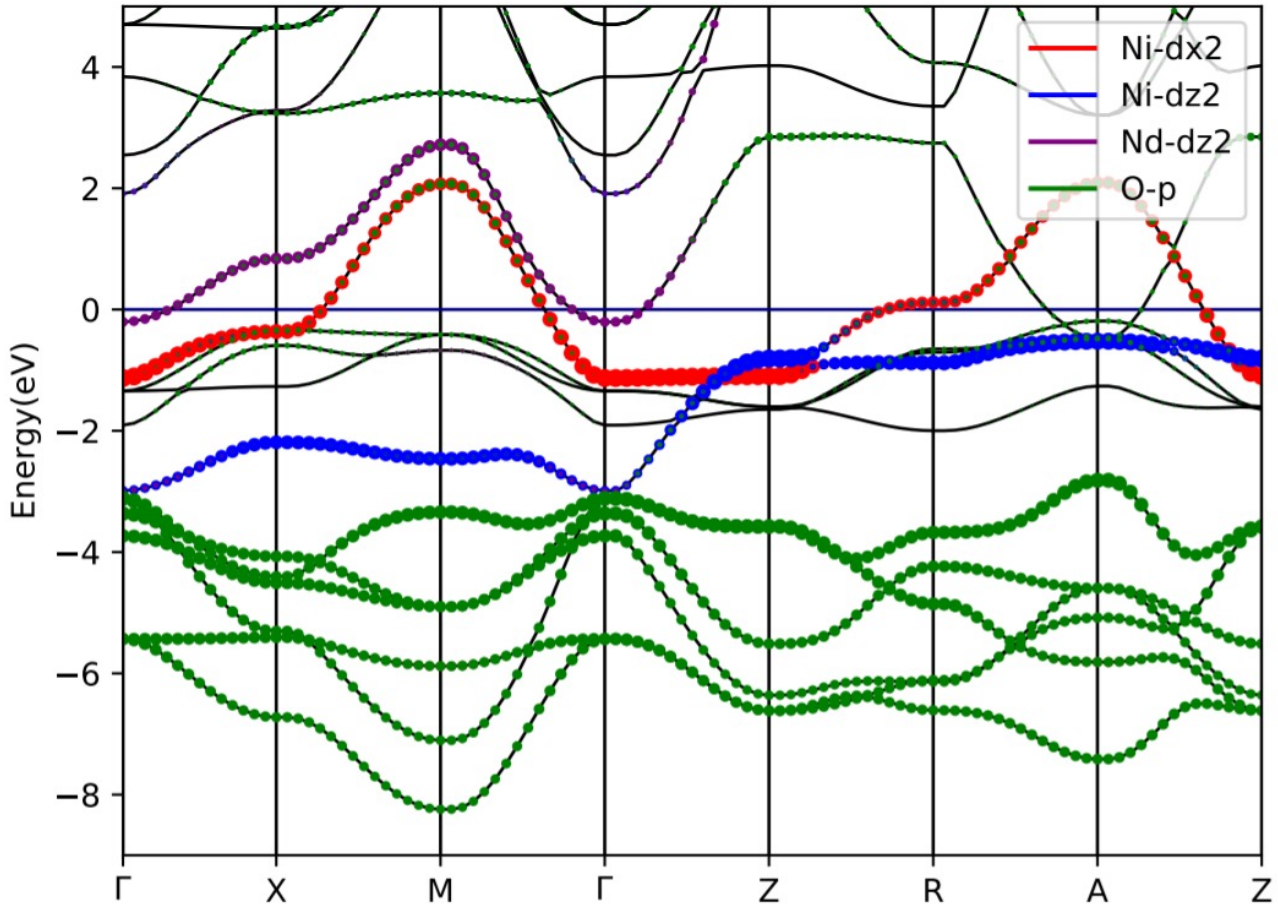
KPOINTS

```
k-points along hign symmetry
15
Line-mode
rec
0.0  0.0  0.0   ! GAMMA
0.0  0.5  0.0   ! X

0.0  0.5  0.0   ! X
0.5  0.5  0.0   ! M

0.5  0.5  0.0   ! M
0.0  0.0  0.0   ! GAMMA

0.0  0.0  0.0   ! GAMMA
0.0  0.0  0.5   ! Z

0.0  0.0  0.5   ! Z
0.0  0.5  0.5   ! R

0.0  0.5  0.5   ! R
0.5  0.5  0.5   ! A

0.5  0.5  0.5   ! A
0.0  0.0  0.5   ! Z
```

INCAR

```
ALGO = Fast
EDIFF = 0.0002
ENCUT = 520
IBRION = 2
ICHARG = 11
ISIF = 3
ISMEAR = 0
ISPIN = 2
LMAXMIX = 6
LORBIT = 11
LREAL = Auto
LWAVE = False
MAGMOM = 1*0.6 1*5.0 2*0.6
NELM = 100
NSW = 0
PREC = Accurate
SIGMA = 0.05
```

Example: $NdNiO_2$



Reference

[1] Kresse G. VASP the Guide[J]. http://cms. mpi. univie. ac. at/vasp/, 2001.

[2] VASP wiki: https://www.vasp.at/wiki/index.php/The_VASP_Manual