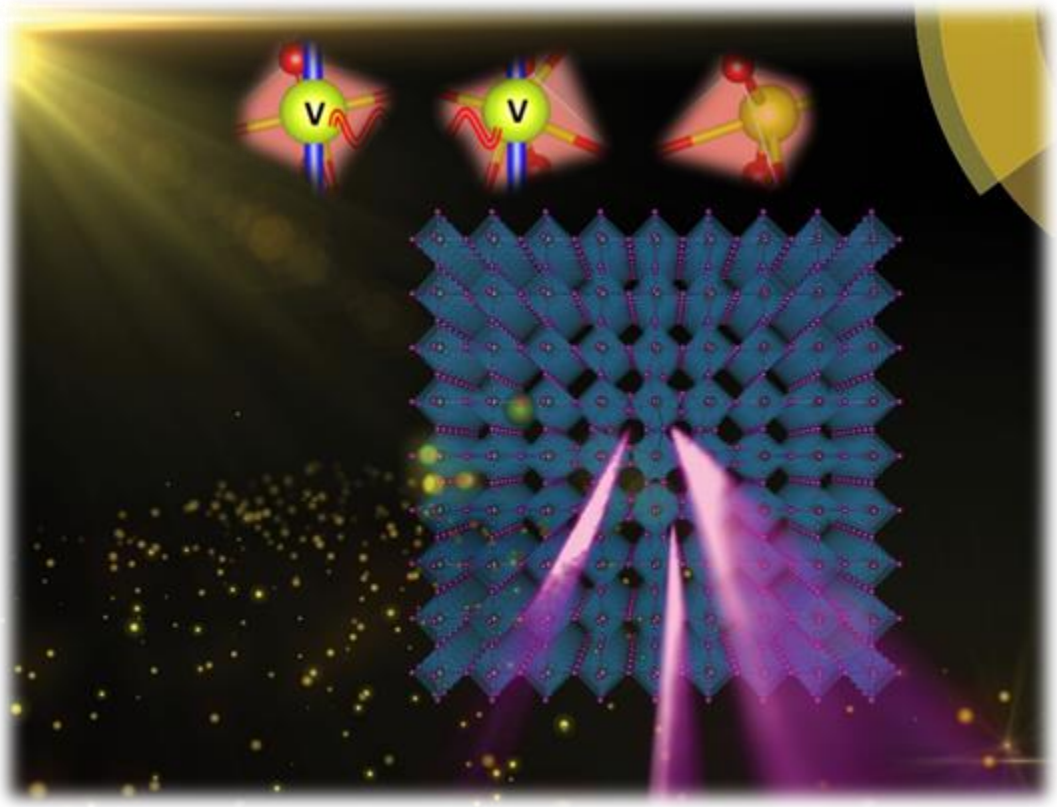
DFT Hands-on NiO



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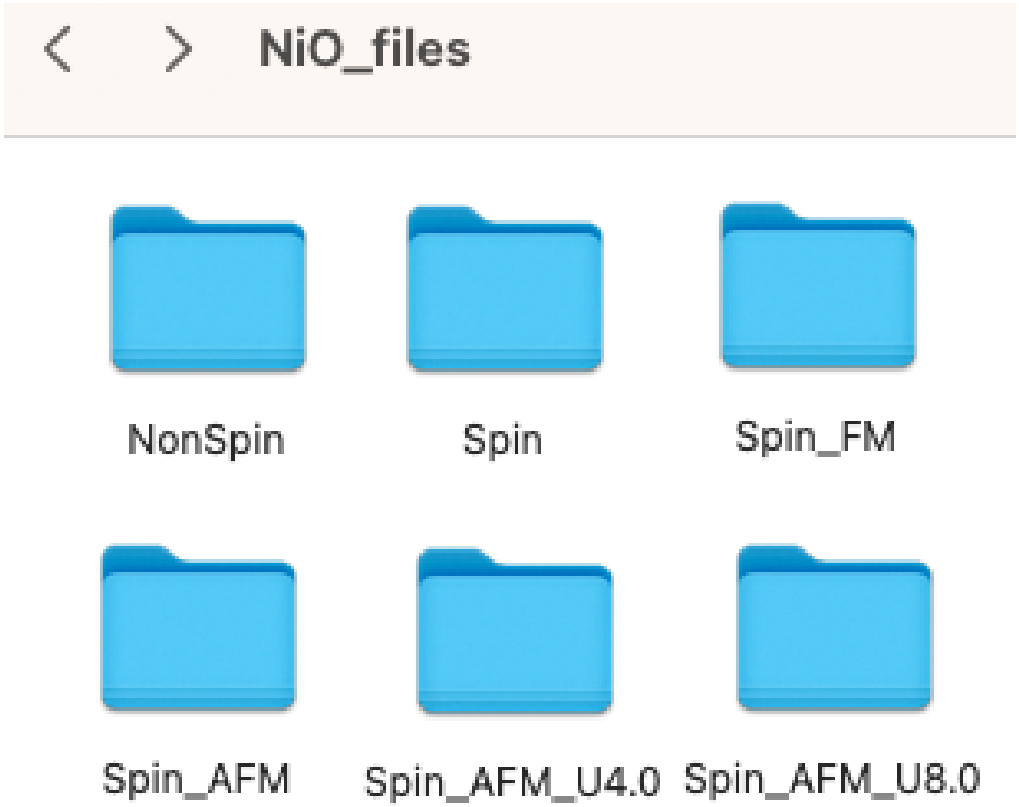
Computational Materials Physics Bootcamp at UD August 2024

Prepare input files

Download NiO_files into desktop



Use WinScp to copy NiO_files into Keldysh (XXX@keldysh.physics.udel.edu)

Go to work directory (XXX/NiO/NonSpin) using ssh

ssh XXX@keldysh.physics.udel.edu

Open only one putty

../NiO$ **module load vasp**

Only use one core => **mpirun -n 1 vasp_std**

Only run one job

NonSpin

Check files

NonSpin$ nano INCAR

```
  GNU nano 2.9.8                          INCAR

SYSTEM = NiO
#ISPIN = 2
#MAGMOM = 2.0 -2.0 2*0
ENMAX = 250
EDIFF = 1E-3
ISMEAR = 0
AMIX = 0.2
BMIX = 0.00001
AMIX_MAG = 0.8
BMIX_MAG = 0.00001
LORBIT = 11

ISIF = 3
IBRION = 2
EDIFFG = -0.03

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

#LDAU = True
#LDAUJ = 0.95 0
#LDAUL = 2 -1
#LDAUPRINT = 2
#LDAUTYPE = 2
#LDAUU = 8.0 0


^G Get Help  ^O Write Out ^W Where Is  ^K Cut Text  ^J Justify   ^C Cur Pos
^X Exit      ^R Read File ^\ Replace   ^U Uncut Text^T To Spell  ^_ Go To Line
```

Check files

POTCAR

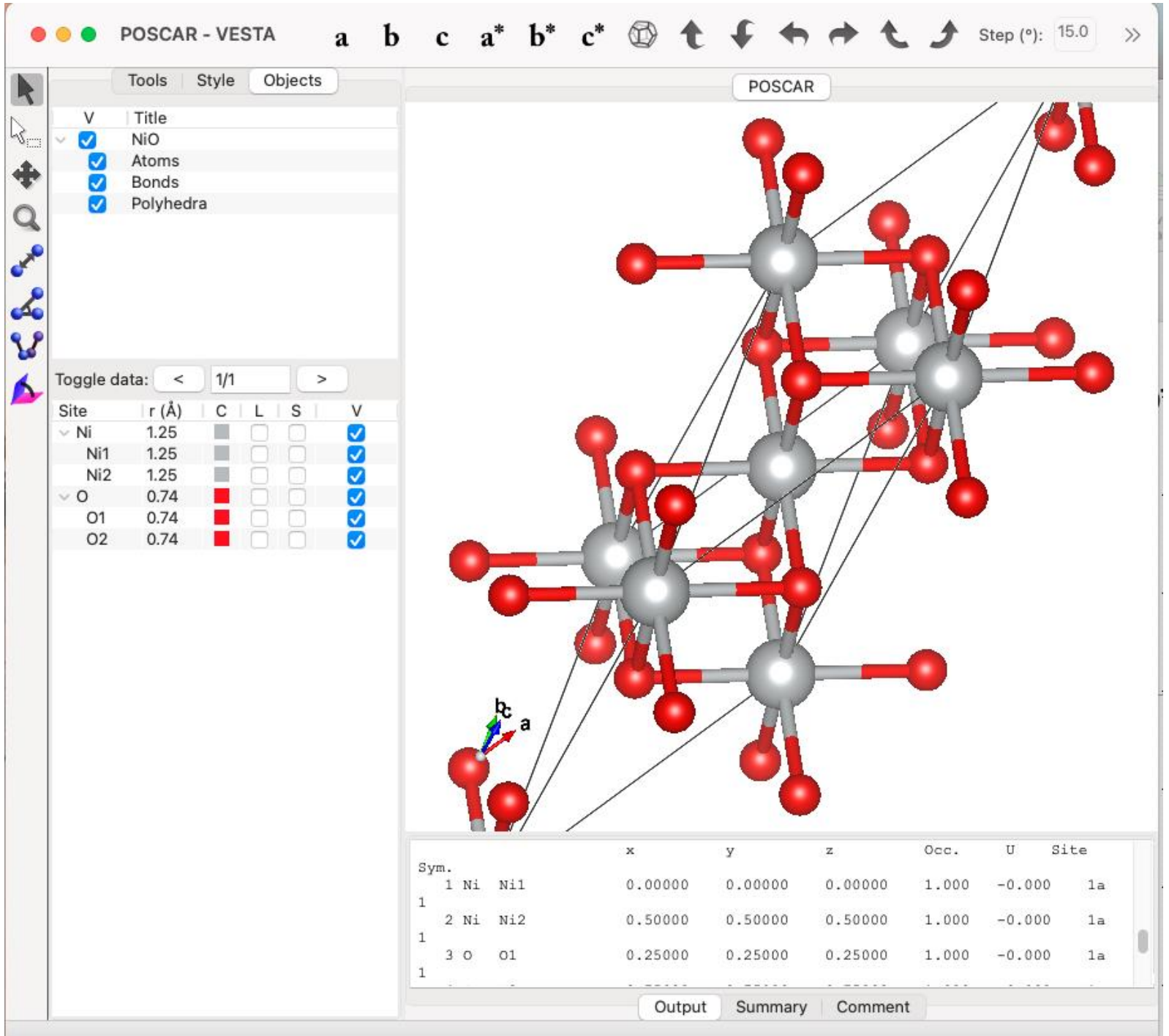
KPOINT

pymatgen with grid density =
1470 / number of atoms
0
Gamma
4 4 4

Try to open using VESTA on Desktop

POSCAR

NiO
4.17
1.0 0.5 0.5
0.5 1.0 0.5
0.5 0.5 1.0
Ni O
2 2
cart
0.0 0.0 0.0
1.0 1.0 1.0
0.5 0.5 0.5
1.5 1.5 1.5



Run job: NonSpin$ **mpirun -n 1 vasp_std**

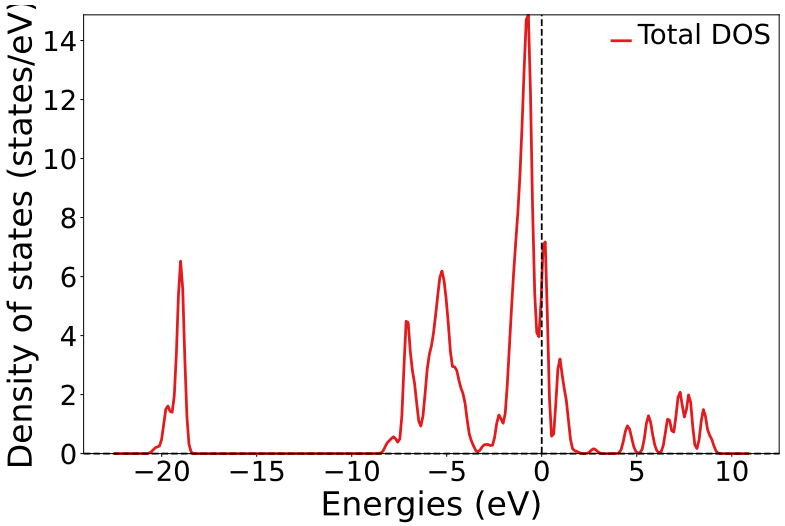
Check output: tail OSZICAR

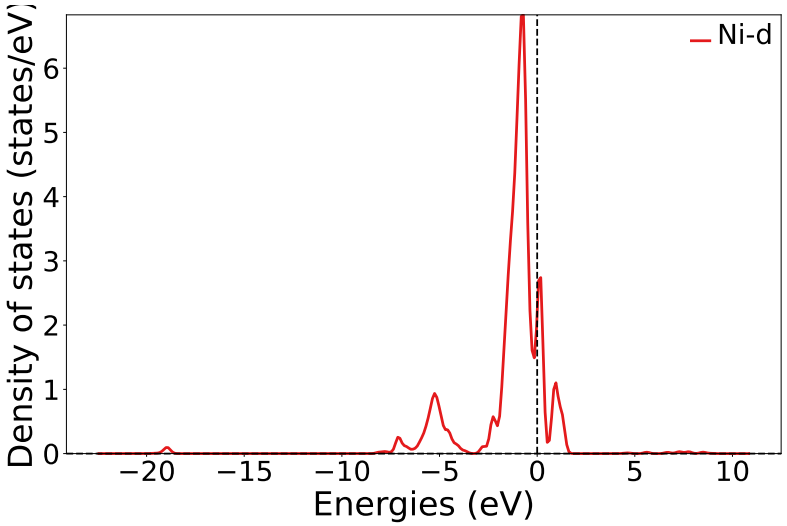
```
DAV:  10    -0.226171176158E+02   -0.61918E-03   -0.13003E-
02   700   0.218E+00    0.430E-01
DAV:  11    -0.226148211865E+02    0.22964E-02   -0.47544E-
03   460   0.156E+00    0.115E-01
DAV:  12    -0.226149642841E+02   -0.14310E-03   -0.14655E-03   316   0.285E-01
   1 F= -.22614964E+02 E0= -.22545036E+02  d E =-.139857E+00
```

Transfer vasprun.xml to XXX/NiO_files/NonSpin

XXX/NiO_files/NonSpin/python dos_tot.py

XXX/NiO_files/NonSpin/python dos_pdos.py





Spin

Check fils

Spin$ nano INCAR

```
SYSTEM = NiO
ISPIN = 2
#MAGMOM = 2.0 -2.0 2*0
ENMAX = 250
EDIFF = 1E-3
ISMEAR = 0
AMIX = 0.2
BMIX = 0.00001
AMIX_MAG = 0.8
BMIX_MAG = 0.00001
LORBIT = 11
ISIF = 3
IBRION = 2
EDIFFG = -0.03
AMIX = 0.2
BMIX = 0.00001
AMIX_MAG = 0.8
BMIX_MAG = 0.00001
#LDAU = True
#LDAUJ = 0.95 0
#LDAUL = 2 -1
#LDAUPRINT = 2
#LDAUTYPE = 2
#LDAUU = 8.0 0
```

1.Run job: NonSpin$ **mpirun -n 1 vasp_std**

2.Check output: tail OSZICAR

```
   1 F= -.22842210E+02 E0= -.22812270E+02
d E =-.598805E-01  mag=     2.3079
```

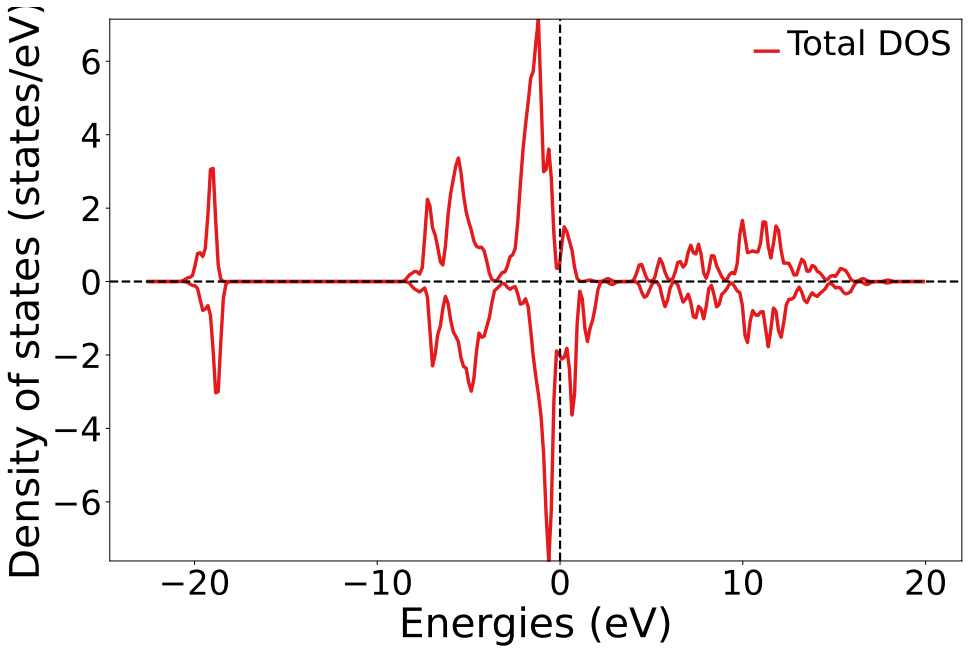
3.Check OUTCAR

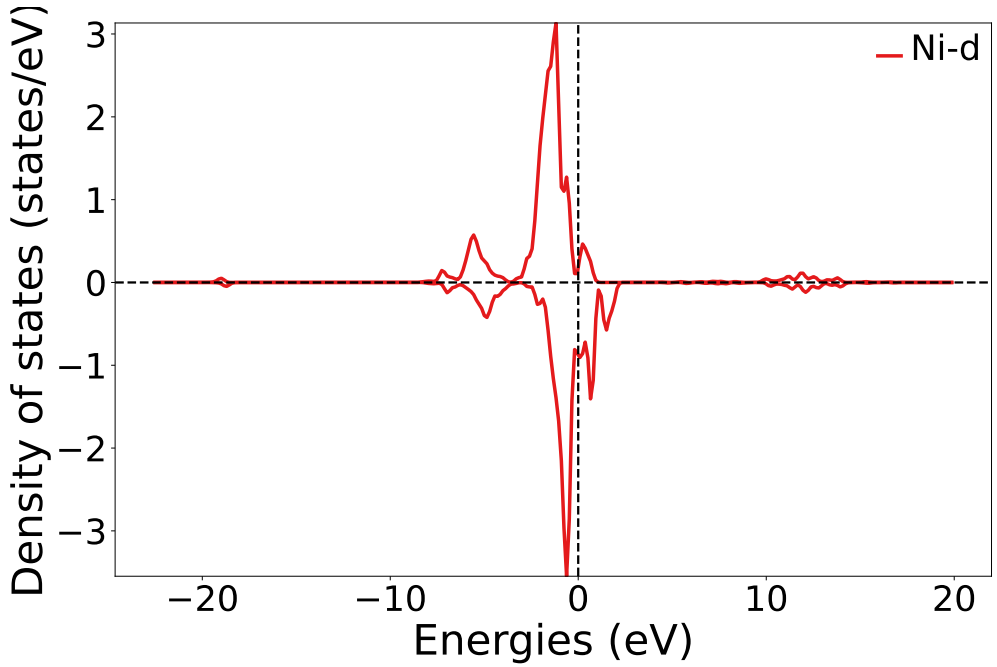
```
 magnetization (x)
# of ion       s       p       d       tot
--------------------------------------------
     1        0.012   0.013   0.953   0.977
     2        0.012   0.013   0.953   0.977
     3        0.019   0.133   0.000   0.152
     4        0.019   0.133   0.000   0.152
--------------------------------------------
-----
tot           0.062   0.291   1.906   2.259
```

4.Transfer vasprun.xml to XXX/NiO_files/Spin

5.XXX/NiO_files/Spin/python dos_tot.py

6.XXX/NiO_files/Spin/python dos_pdos.py





Spin_AFM

Check fils

Spin_AFM$ nano INCAR

```
SYSTEM = NiO
ISPIN = 2
MAGMOM = 2.0 -2.0 2*0
ENMAX = 250
EDIFF = 1E-3
ISMEAR = 0
AMIX = 0.2
BMIX = 0.00001
AMIX_MAG = 0.8
BMIX_MAG = 0.00001
LORBIT = 11
ISIF = 3
IBRION = 2
EDIFFG = -0.03
AMIX = 0.2
BMIX = 0.00001
AMIX_MAG = 0.8
BMIX_MAG = 0.00001
#LDAU = True
#LDAUJ = 0.95 0
#LDAUL = 2 -1
#LDAUPRINT = 2
#LDAUTYPE = 2
#LDAUU = 8.0 0
```

1.Run job: Spin_AFM$ **mpirun -n 1 vasp_std**

2.Check output: tail OSZICAR

```
1 F= -.23239827E+02 E0= -.23239422E+02  d
E =-.810958E-03  mag=     -0.0000
```

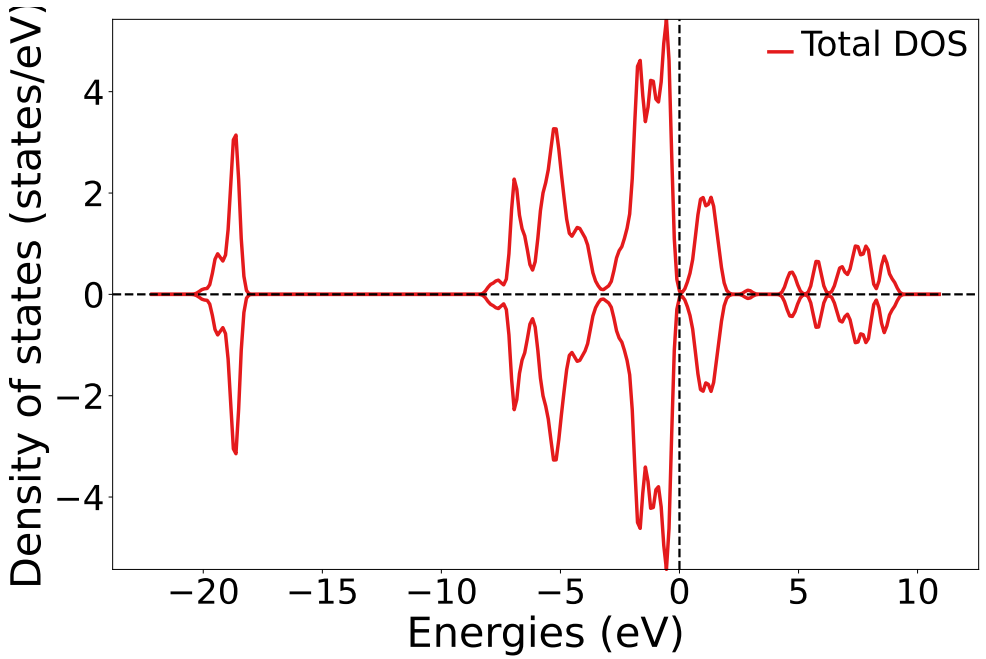
3.Check OUTCAR

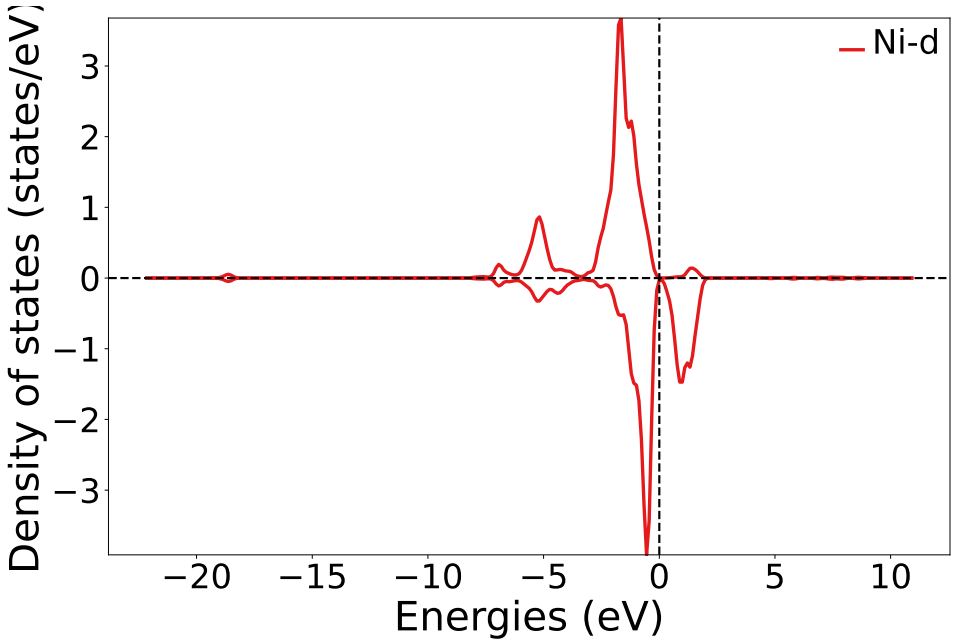
```
 magnetization (x)
# of ion       s       p       d       tot
--------------------------------------------
    1        -0.011  -0.015   1.357   1.331
    2         0.011   0.015  -1.357  -1.331
    3         0.000   0.000   0.000   0.000
    4         0.000   0.000   0.000   0.000
--------------------------------------------
tot           0.000   0.000   0.000   0.000
```

4.Transfer vasprun.xml to XXX/NiO_files/Spin_AFM

5.XXX/NiO_files/Spin_AFM/python dos_tot.py

6.XXX/NiO_files/Spin_AFM/python dos_pdos.py





Spin_FM

Check fils

Spin_FM$ nano INCAR

```
SYSTEM = NiO
ISPIN = 2
MAGMOM = 2.0 2.0 2*0
ENMAX = 250
EDIFF = 1E-3
ISMEAR = 0
AMIX = 0.2
BMIX = 0.00001
AMIX_MAG = 0.8
BMIX_MAG = 0.00001
LORBIT = 11
ISIF = 3
IBRION = 2
EDIFFG = -0.03
AMIX = 0.2
BMIX = 0.00001
AMIX_MAG = 0.8
BMIX_MAG = 0.00001
#LDAU = True
#LDAUJ = 0.95 0
#LDAUL = 2 -1
#LDAUPRINT = 2
#LDAUTYPE = 2
#LDAUU = 8.0 0
```

1.Run job: Spin_FM$ **mpirun -n 1 vasp_std**

2.Check output: tail OSZICAR

```
1 F= -.22842210E+02 E0= -.22811754E+02  d
E =-.609116E-01  mag=     2.3236
```

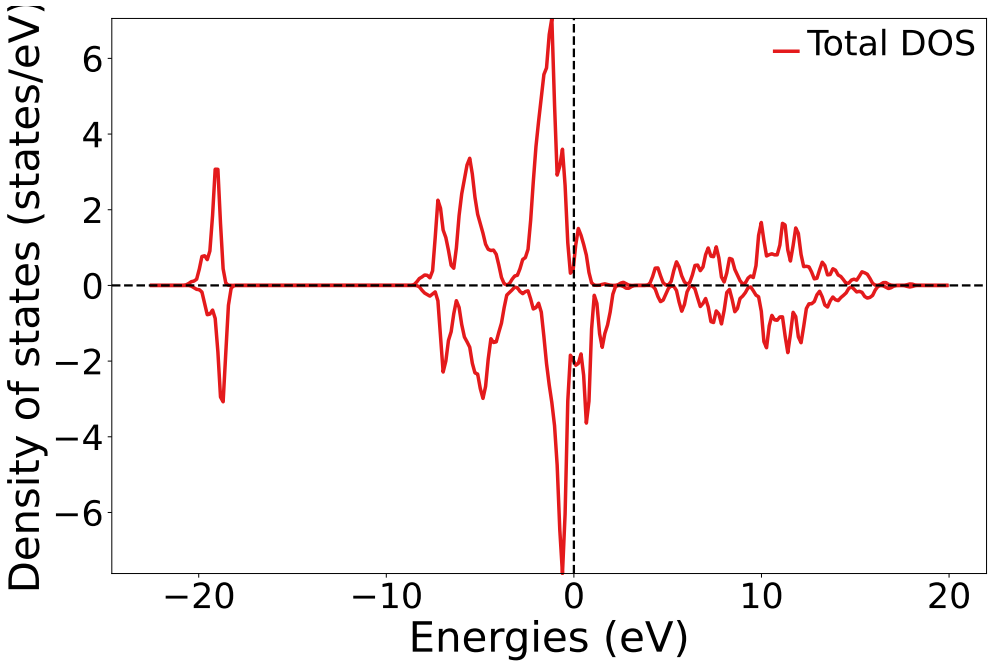
3.Check OUTCAR

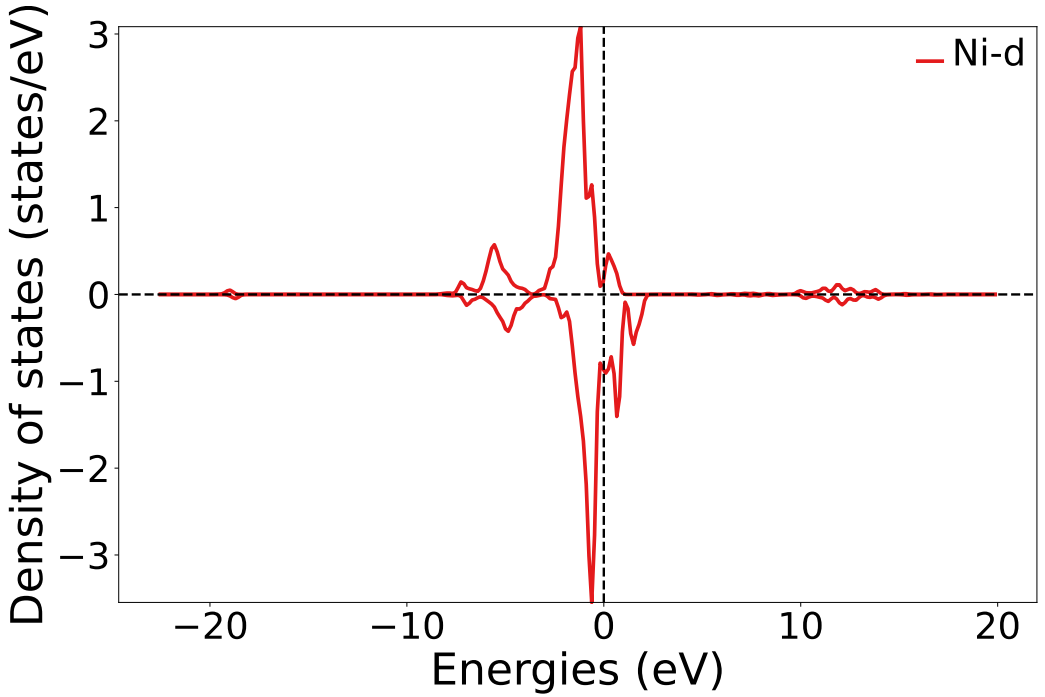
```
 magnetization (x)
# of ion       s       p       d       tot
------------------------------------------
    1        0.011   0.012   0.959   0.983
    2        0.011   0.012   0.959   0.983
    3        0.020   0.136   0.000   0.156
    4        0.020   0.136   0.000   0.156
------------------------------------------
-------
tot          0.062   0.297   1.919   2.278
```

4.Transfer vasprun.xml to XXX/NiO_files/Spin_FM

5.XXX/NiO_files/Spin_FM/python dos_tot.py

6.XXX/NiO_files/Spin_FM/python dos_pdos.py





Total energy difference between Spin_AFM and Spin_FM ?

Spin_AFM_U4.0

Check fils

Spin_AFM_U4.0$ nano INCAR

```
SYSTEM = NiO
ISPIN = 2
MAGMOM = 2.0 -2.0 2*0
ENMAX = 250
EDIFF = 1E-3
ISMEAR = 0
AMIX = 0.2
BMIX = 0.00001
AMIX_MAG = 0.8
BMIX_MAG = 0.00001
LORBIT = 11
ISIF = 3
IBRION = 2
EDIFFG = -0.03
AMIX = 0.2
BMIX = 0.00001
AMIX_MAG = 0.8
BMIX_MAG = 0.00001
LDAU = True
LDAUJ = 0.95 0
LDAUL = 2 -1
LDAUPRINT = 2
LDAUTYPE = 2
LDAUU = 4.0 0
```

1.Run job: Spin_AFM_U4.0$ **mpirun -n 1 vasp_std**

2.Check output: tail OSZICAR

```
1 F= -.21430196E+02 E0= -.21430196E+02  d
E =-.463674E-11  mag=     0.0000
```

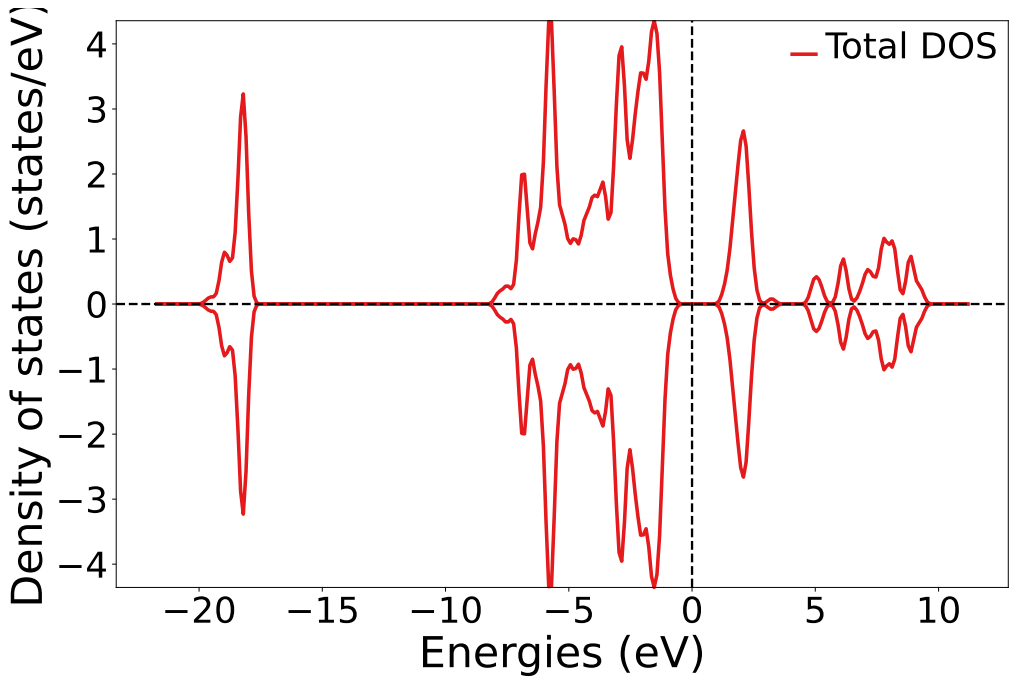
3.Check OUTCAR

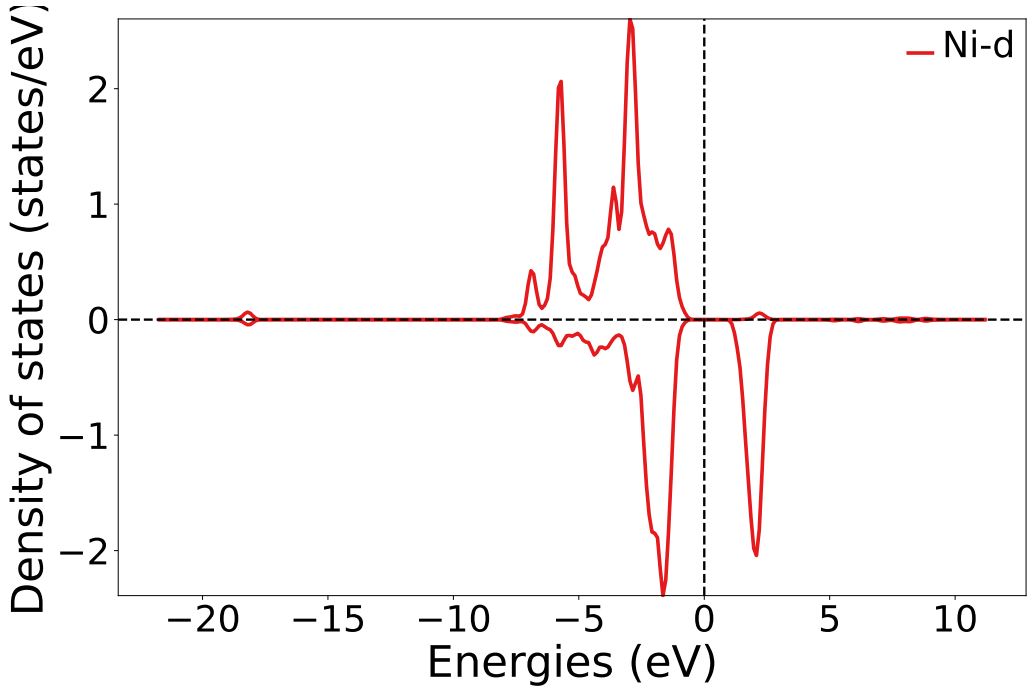
```
 magnetization (x)
# of ion       s       p       d       tot
------------------------------------------------
    1        -0.007  -0.012   1.587   1.568
    2         0.007   0.012  -1.587  -1.568
    3         0.000   0.000   0.000   0.000
    4         0.000   0.000   0.000   0.000
------------------------------------------------
tot           0.000   0.000   0.000   0.000
```

4.Transfer vasprun.xml to XXX/NiO_files/Spin_AFM_U4.0

5.XXX/NiO_files/Spin_AFM_U4.0/python dos_tot.py

6.XXX/NiO_files/Spin_AFM_U4.0/python dos_pdos.py





Spin_AFM_U8.0

Check fils

Spin_AFM_U8.0$ nano INCAR

```
SYSTEM = NiO
ISPIN = 2
MAGMOM = 2.0 -2.0 2*0
ENMAX = 250
EDIFF = 1E-3
ISMEAR = 0
AMIX = 0.2
BMIX = 0.00001
AMIX_MAG = 0.8
BMIX_MAG = 0.00001
LORBIT = 11
ISIF = 3
IBRION = 2
EDIFFG = -0.03
AMIX = 0.2
BMIX = 0.00001
AMIX_MAG = 0.8
BMIX_MAG = 0.00001
LDAU = True
LDAUJ = 0.95 0
LDAUL = 2 -1
LDAUPRINT = 2
LDAUTYPE = 2
LDAUU = 8.0 0
```

1.Run job: Spin_AFM_U8.0$ **mpirun -n 1 vasp_std**

2.Check output: tail OSZICAR

```
1 F= -.19847651E+02 E0= -.19847651E+02  d
E =-.216936E-10  mag=     0.0000
```

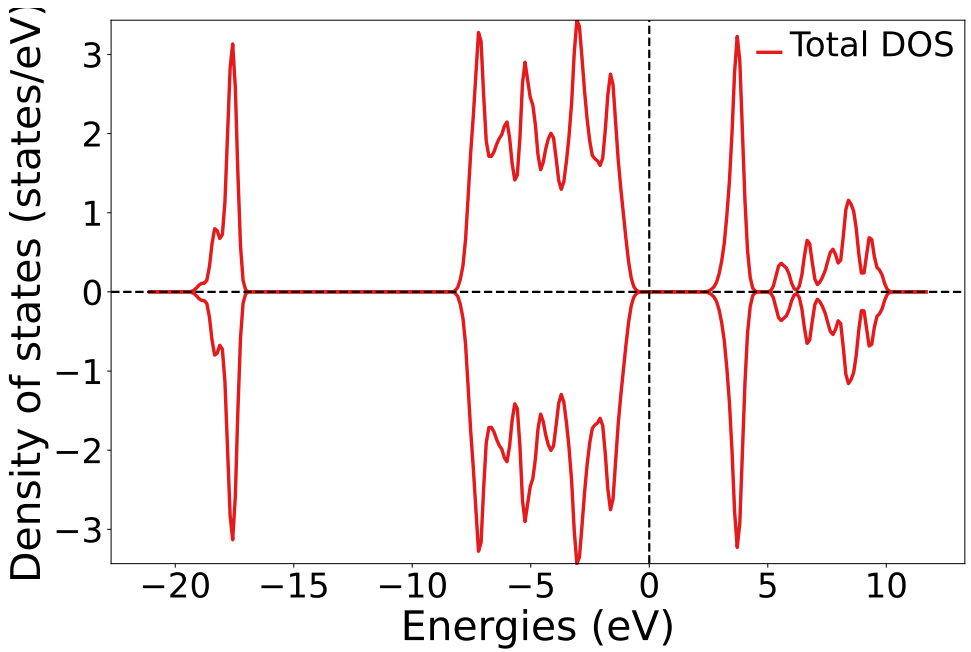
3.Check OUTCAR

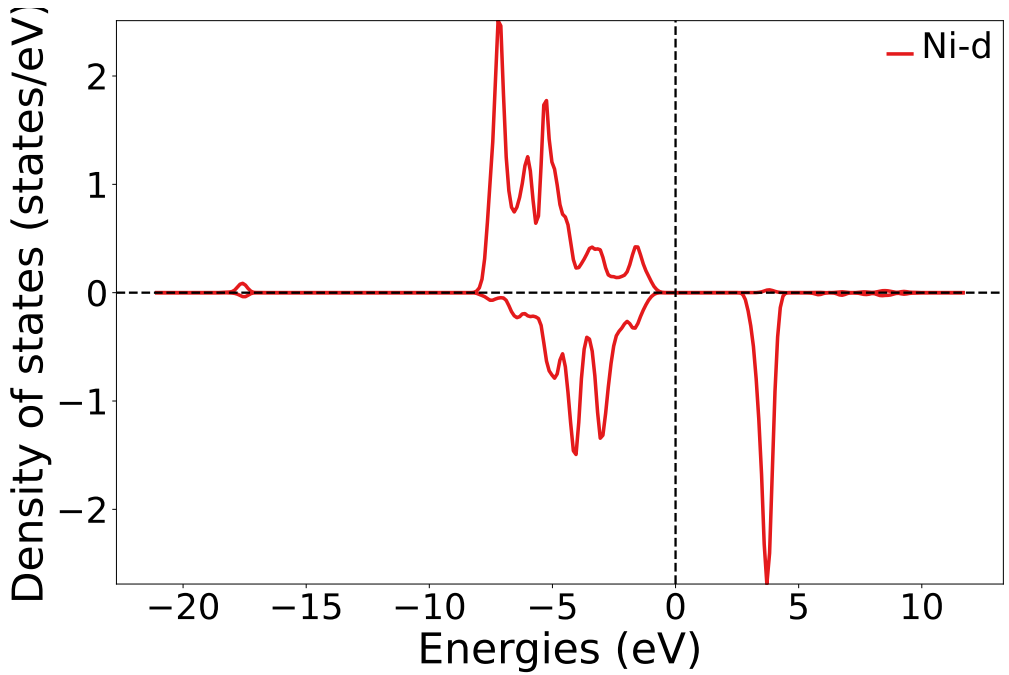
```
 magnetization (x)
# of ion       s       p       d       tot
------------------------------------------------
    1        -0.001  -0.005   1.768   1.761
    2         0.001   0.005  -1.768  -1.761
    3         0.000   0.000   0.000   0.000
    4         0.000   0.000   0.000   0.000
------------------------------------------------
tot           0.000   0.000   0.000   0.000
```

4.Transfer vasprun.xml to XXX/NiO_files/Spin_AFM_U8.0

5.XXX/NiO_files/Spin_AFM_U8.0/python dos_tot.py

6.XXX/NiO_files/Spin_AFM_U8.0/python dos_pdos.py





Tasks

Spin_AFM_U=0, 4.0, and 8.0 eV

Identify a trend for magnetization in Ni-d.

Plot dos together.

Estimate rough band gaps using OUTCARs.

Thank you