

DFT+Hubbard hands-on

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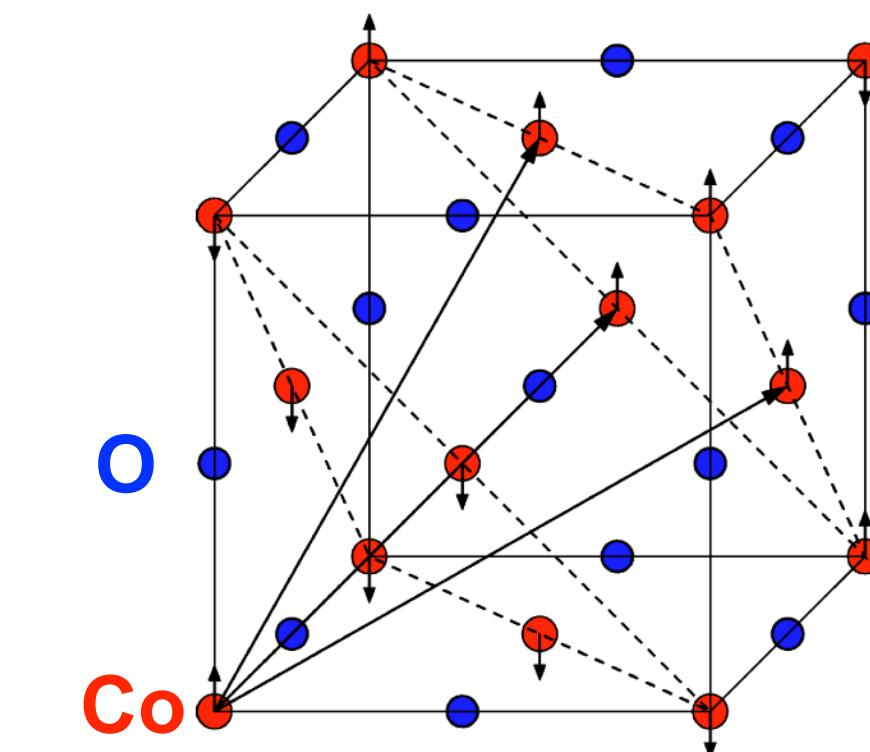


Exercise 1

**Projected density of states of CoO
with and without the Hubbard U correction**

Input file CoO.scf.in

```
&control
  calculation='scf'           ← Self-consistent-field (SCF) calculation
  restart_mode='from_scratch',
  prefix='CoO'
  pseudo_dir = '../files/pseudo'
 outdir='./tmp'
  verbosity='high'
/
&system
  ibrav = 0,
  celldm(1) = 8.00,          ← Specification of the lattice (see CELL_PARAMETERS)
  nat = 4,
  ntyp = 3,
  ecutwfc = 35.0             ← Number of atoms and atomic types
  ecutrho = 280.0             ← Kinetic-energy cutoff for the wavefunctions and density/potential
  nspin = 2
  starting_magnetization(1) = 0.5,
  starting_magnetization(2) = -0.5, ← Spin-polarized collinear calculation (AFM)
  occupations = 'smearing',
  smearing = 'mv',            ← Marzari-Vanderbilt smearing with a broadening parameter of 0.02 Ry
  degauss = 0.02
/
&electrons
  conv_thr = 1.d-10          ← Convergence threshold for self-consistency
/
ATOMIC_SPECIES
  Co1 58.933194  co_pbesol_v1.2.uspp.F.UPF
  Co2 58.933194  co_pbesol_v1.2.uspp.F.UPF
  O   15.999    O.pbesol-n-kjpaw_psl.0.1.UPF
ATOMIC_POSITIONS {crystal}
  Co1    0.0000000  0.0000000  0.0000000
  Co2    0.5000000  0.5000000  0.5000000
  O     0.2500000  0.2500000  0.2500000
  O     0.7500000  0.7500000  0.7500000
CELL_PARAMETERS {alat}
  0.570726115  0.570726115  1.031099100
  0.570726115  1.031099100  0.570726115
  1.031099100  0.570726115  0.570726115
K_POINTS {automatic}
  3 3 3 0 0 0
```



Cell parameters optimized using DFT with the PBEsol functional

Quantum ESPRESSO input generator

Quantum ESPRESSO input generator and structure visualizer

- ▶ About the Quantum ESPRESSO input generator and structure visualizer
- ▶ Instructions
- ▶ Acknowledgements

Upload your structure

Upload a crystal structure: no file selected

Select here the file format: Quantum ESPRESSO input [parser: qetools]

Select here the pseudopotential library: SSSP Efficiency PBEsol (version 1.1)

Select here the magnetism/smearing: non-magnetic metal (fractional occupations)

Select here the k-points distance (1/Å) fine (0.20 1/Å, 0.2 eV)

(and smearing (eV) in case of fractional occupations):

Refine cell (using spglib): No

By continuing, you agree with the [terms of use](#) of this service.

[Generate the PWscf input file](#)

Otherwise, pick an example

Select here a structure: Al

Select here the pseudopotential library: SSSP Efficiency PBEsol (version 1.1)

Select here the magnetism/smearing: non-magnetic metal (fractional occupations)

Select here the k-points distance (1/Å) fine (0.20 1/Å, 0.2 eV)

(and smearing (eV) in case of fractional occupations):

By continuing, you agree with the [terms of use](#) of this service.

[Generate the PWscf input file](#)

<https://www.materialscloud.org/work/tools/qeinputgenerator>

SSSP pseudopotential library

SSSP Efficiency (version 1.1.2)

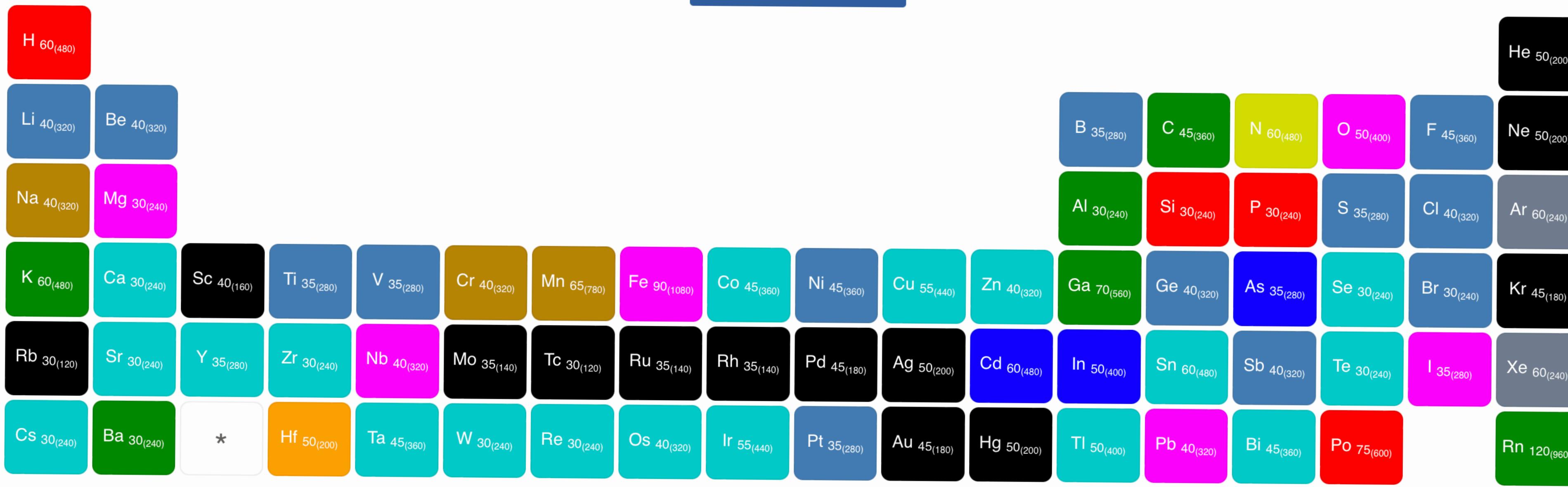
$\Delta_{\text{eff}} = 0.44 \text{ meV}$

 Cutoffs table

 Pseudo

Switch to SSSP Precision

Updates v1.2.0 be



<https://www.materialscloud.org/discover/sssp/table/efficiency>

Input file CoO.scf.in

```
&control
  calculation='scf'
  restart_mode='from_scratch',
  prefix='CoO'
  pseudo_dir = '../files/pseudo'
 outdir='./tmp'
  verbosity='high'
/
&system
  ibrav = 0,
  celldm(1) = 8.00,
  nat = 4,
  ntyp = 3,
  ecutwfc = 35.0
  ecutrho = 280.0
  nspin = 2
  starting_magnetization(1) = 0.5,
  starting_magnetization(2) = -0.5,
  occupations = 'smearing',
  smearing = 'mv',
  degauss = 0.02
/
&electrons
  conv_thr = 1.d-10
/
ATOMIC_SPECIES
Co1 58.933194 co_pbesol_v1.2.uspp.F.UPF
Co2 58.933194 co_pbesol_v1.2.uspp.F.UPF
O   15.999   O.pbesol-n-kjpaw_psl.0.1.UPF
ATOMIC_POSITIONS {crystal}
Co1    0.00000000    0.00000000    0.00000000
Co2    0.50000000    0.50000000    0.50000000
O     0.25000000    0.25000000    0.25000000
O     0.75000000    0.75000000    0.75000000
CELL_PARAMETERS {alat}
  0.570726115    0.570726115    1.031099100
  0.570726115    1.031099100    0.570726115
  1.031099100    0.570726115    0.570726115
K_POINTS {automatic}
  3 3 3 0 0 0
```

Input file CoO.nscf.in

```
&control
  calculation='nscf'
  restart_mode='from_scratch',
  prefix='CoO'
  pseudo_dir = '../files/pseudo'
 outdir='./tmp'
  verbosity='high'
/
&system
  ibrav = 0,
  celldm(1) = 8.00,
  nat = 4,
  ntyp = 3,
  ecutwfc = 35.0
  ecutrho = 280.0
  nspin = 2
  starting_magnetization(1) = 0.5,
  starting_magnetization(2) = -0.5,
  occupations = 'smearing',
  smearing = 'mv',
  degauss = 0.02
  nbnd = 40
/
&electrons
  conv_thr = 1.d-10
/
ATOMIC_SPECIES
Co1 58.933194 co_pbesol_v1.2.uspp.F.UPF
Co2 58.933194 co_pbesol_v1.2.uspp.F.UPF
O   15.999   O.pbesol-n-kjpaw_psl.0.1.UPF
ATOMIC_POSITIONS {crystal}
Co1    0.00000000    0.00000000    0.00000000
Co2    0.50000000    0.50000000    0.50000000
O     0.25000000    0.25000000    0.25000000
O     0.75000000    0.75000000    0.75000000
CELL_PARAMETERS {alat}
  0.500380664    0.500380664    1.004818266
  0.500380664    1.004818266    0.500380664
  1.004818266    0.500380664    0.500380664
K_POINTS {automatic}
  6 6 6 0 0 0
```

Input file CoO.projwfc.in

```
&projwfc
    prefix='CoO'
    outdir='./tmp'
    ngauss = 0, ← Gaussian broadening for PDOS
    degauss = 0.005, ← Value of the Gaussian broadening (in Ry)
    Emin = -15.0, ← Minimum and maximum energy for the plot (in eV)
    Emax = 30.0, ←
    DeltaE = 0.01 ← Energy grid step
/

```

Gnuplot script: plot_pdos.gp

Inspect the script. It aims at plotting Co-3d states (majority spin and minority spin) and O-2p states.

PDOS is shifted such that the Fermi energy corresponds to zero of energy.

After running the script, visualize the file CoO_PDOS.eps.

Run the calculations

```
pw.x < Co0.scf.in |tee Co0.scf.out
```

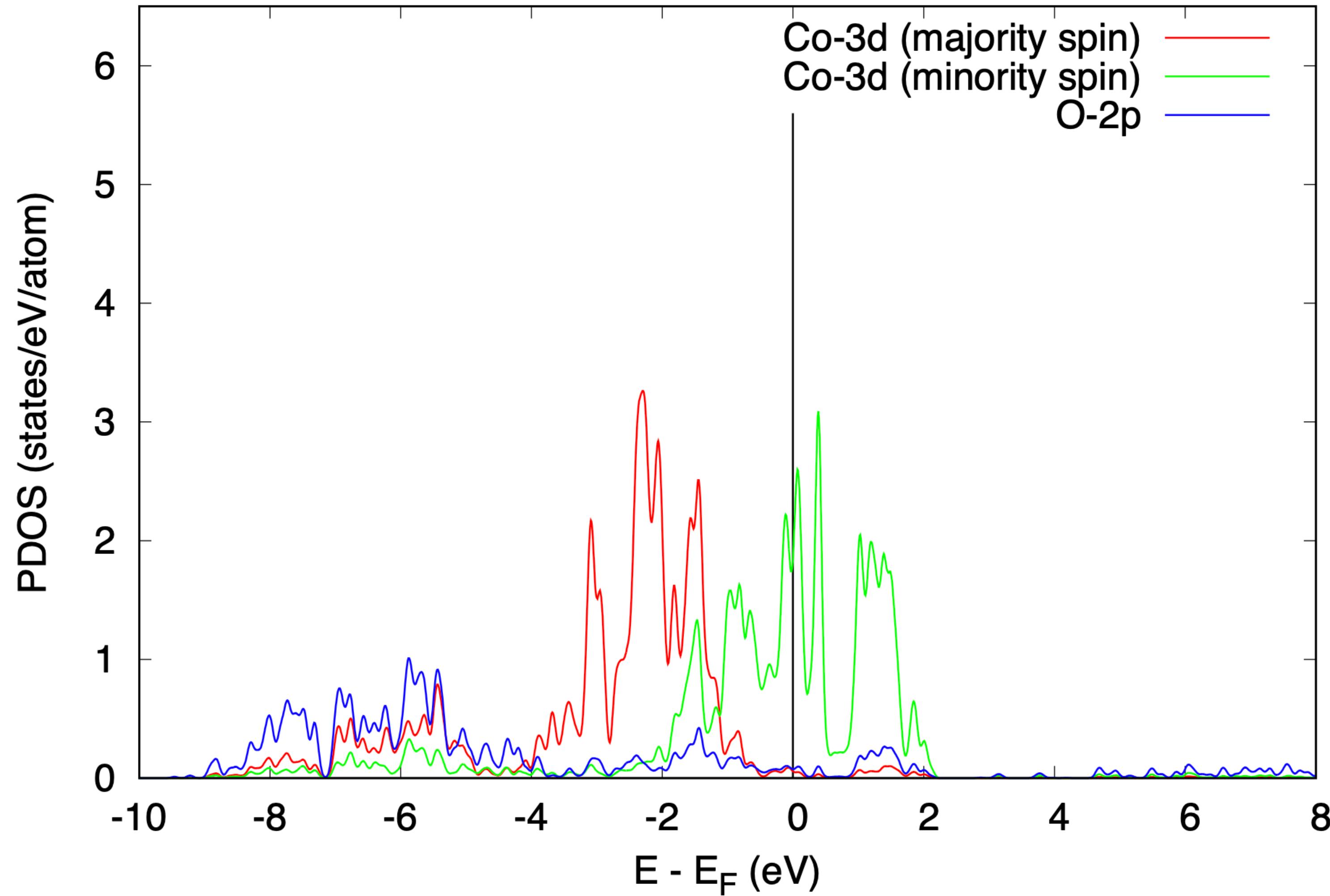
```
pw.x < Co0.nscf.in |tee Co0.nscf.out
```

```
projwfc.x < Co0.projwfc.in |tee Co0.projwfc.out
```

```
gnuplot plot_pdos.gp
```

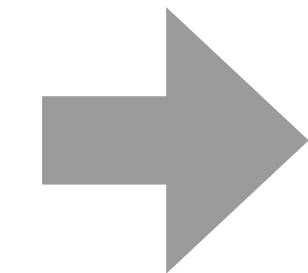
```
evince Co0_PDOS.eps
```

PDOS using DFT (PBEsol)



DFT predicts CoO to be metallic (**this is wrong**)

Experimentally CoO is insulating



Let's try DFT+*U*

Input file CoO.scf.in

```
&control
  calculation='scf'
  restart_mode='from_scratch',
  prefix='CoO'
  pseudo_dir = '../..../files/pseudo'
 outdir='./tmp'
  verbosity='high'
/
&system
  ibrav = 0,
  celldm(1) = 8.00,
  nat = 4,
  ntyp = 3,
  ecutwfc = 35.0
  ecutrho = 280.0
  nspin = 2
  starting_magnetization(1) = 0.5,
  starting_magnetization(2) = -0.5,
  occupations = 'smearing',
  smearing = 'mv',
  degauss = 0.02
/
&electrons
  conv_thr = 1.d-10
/
ATOMIC_SPECIES
Co1 58.933194 co_pbesol_v1.2.uspp.F.UPF
Co2 58.933194 co_pbesol_v1.2.uspp.F.UPF
O 15.999 O.pbesol-n-kjpaw_psl.0.1.UPF
ATOMIC_POSITIONS {crystal}
Co1    0.0000000    0.0000000    0.0000000
Co2    0.5000000    0.5000000    0.5000000
O     0.2500000    0.2500000    0.2500000
O     0.7500000    0.7500000    0.7500000
CELL_PARAMETERS {alat}
  0.570726115  0.570726115  1.031099100
  0.570726115  1.031099100  0.570726115
  1.031099100  0.570726115  0.570726115
K_POINTS {automatic}
  3 3 3 0 0 0
HUBBARD {ortho-atomic}
U Co1-3d 6.3
U Co2-3d 6.3
```



HUBBARD card

Input file CoO.scf.in

```
&control
  calculation='scf'
  restart_mode='from_scratch',
  prefix='CoO'
  pseudo_dir = '../files/pseudo'
  outdir='./tmp'
  verbosity='high'
/
&system
  ibrav = 0,
  celldm(1) = 8.00,
  nat = 4,
  ntyp = 3,
  ecutwfc = 35.0
  ecutrho = 280.0
  nspin = 2
  starting_magnetization(1) = 0.5,
  starting_magnetization(2) = -0.5,
  occupations = 'smearing',
  smearing = 'mv',
  degauss = 0.02
/
&electrons
  conv_thr = 1.d-10
/
ATOMIC_SPECIES
  Co1 58.933194 co_pbesol_v1.2.uspp.F.UPF
  Co2 58.933194 co_pbesol_v1.2.uspp.F.UPF
  O 15.999 O.pbesol-n-kjpaw_psl.0.1.UPF
ATOMIC_POSITIONS {crystal}
  Co1 0.0000000 0.0000000 0.0000000
  Co2 0.5000000 0.5000000 0.5000000
  O 0.2500000 0.2500000 0.2500000
  O 0.7500000 0.7500000 0.7500000
CELL_PARAMETERS {alat}
  0.570726115 0.570726115 1.031099100
  0.570726115 1.031099100 0.570726115
  1.031099100 0.570726115 0.570726115
K_POINTS {automatic}
  3 3 3 0 0 0
HUBBARD {ortho-atomic}
  U Co1-3d 6.3
  U Co2-3d 6.3
```

Name of the card

Type of the Hubbard projectors

HUBBARD {ortho-atomic}		
U	Co1-3d	6.3
U	Co2-3d	6.3

Value of the Hubbard parameter (in eV)

Name of the Hubbard parameter

Hubbard manifold to which we want to apply the Hubbard correction

Atomic type of the chemical element to which we want to apply the Hubbard correction

Detailed description of the new Hubbard input syntax (since v7.1):
Quantum ESPRESSO folder -> Doc/Hubbard_input.pdf

HUBBARD card

Input file CoO.scf.in

```
&control
  calculation='scf'
  restart_mode='from_scratch',
  prefix='CoO'
  pseudo_dir = '../files/pseudo'
 outdir='./tmp'
  verbosity='high'
/
&system
  ibrav = 0,
  celldm(1) = 8.00,
  nat = 4,
  ntyp = 3,
  ecutwfc = 35.0
  ecutrho = 280.0
  nspin = 2
  starting_magnetization(1) = 0.5,
  starting_magnetization(2) = -0.5,
  occupations = 'smearing',
  smearing = 'mv',
  degauss = 0.02
/
&electrons
  conv_thr = 1.d-10
/
ATOMIC_SPECIES
  Co1 58.933194 co_pbesol_v1.2.uspp.F.UPF
  Co2 58.933194 co_pbesol_v1.2.uspp.F.UPF
  O 15.999 0.pbesol-n-kjpaw_psl.0.1.UPF
ATOMIC_POSITIONS {crystal}
  Co1    0.0000000    0.0000000    0.0000000
  Co2    0.5000000    0.5000000    0.5000000
  O     0.2500000    0.2500000    0.2500000
  O     0.7500000    0.7500000    0.7500000
CELL_PARAMETERS {alat}
  0.570726115  0.570726115  1.031099100
  0.570726115  1.031099100  0.570726115
  1.031099100  0.570726115  0.570726115
K_POINTS {automatic}
  3 3 3 0 0 0
HUBBARD {ortho-atomic}
U Co1-3d 6.3
U Co2-3d 6.3
```

Input file CoO.nscf.in

```
&control
  calculation='nscf'
  restart_mode='from_scratch',
  prefix='CoO'
  pseudo_dir = '../files/pseudo'
 outdir='./tmp'
  verbosity='high'
/
&system
  ibrav = 0,
  celldm(1) = 8.00,
  nat = 4,
  ntyp = 3,
  ecutwfc = 35.0
  ecutrho = 280.0
  nspin = 2
  starting_magnetization(1) = 0.5,
  starting_magnetization(2) = -0.5,
  occupations = 'smearing',
  smearing = 'mv',
  degauss = 0.02
  nbnd = 40
/
&electrons
  conv_thr = 1.d-10
/
ATOMIC_SPECIES
  Co1 58.933194 co_pbesol_v1.2.uspp.F.UPF
  Co2 58.933194 co_pbesol_v1.2.uspp.F.UPF
  O 15.999 0.pbesol-n-kjpaw_psl.0.1.UPF
ATOMIC_POSITIONS {crystal}
  Co1    0.0000000    0.0000000    0.0000000
  Co2    0.5000000    0.5000000    0.5000000
  O     0.2500000    0.2500000    0.2500000
  O     0.7500000    0.7500000    0.7500000
CELL_PARAMETERS {alat}
  0.500380664  0.500380664  1.004818266
  0.500380664  1.004818266  0.500380664
  1.004818266  0.500380664  0.500380664
K_POINTS {automatic}
  6 6 6 0 0 0
HUBBARD {ortho-atomic}
U Co1-3d 6.3
U Co2-3d 6.3
```

Input file CoO.projwfc.in

```
&projwfc
  prefix='CoO'
  outdir='./tmp'
  ngauss = 0, ← Gaussian broadening for PDOS
  degauss = 0.005, ← Value of the Gaussian broadening (in Ry)
  Emin = -15.0, ← Minimum and maximum energy for the plot (in eV)
  Emax = 30.0, ←
  DeltaE = 0.01 ← Energy grid step
/

```

This is exactly the same as before (i.e. DFT-PBEsol case)

Gnuplot script: plot_pdos.gp

Inspect the script. It aims at plotting Co-3d states (majority spin and minority spin) and O-2p states.

PDOS is shifted such that the Fermi energy corresponds to zero of energy.

After running the script, visualize the file CoO_PDOS.eps.

Run the calculations

```
pw.x < Co0.scf.in |tee Co0.scf.out
```

```
pw.x < Co0.nscf.in |tee Co0.nscf.out
```

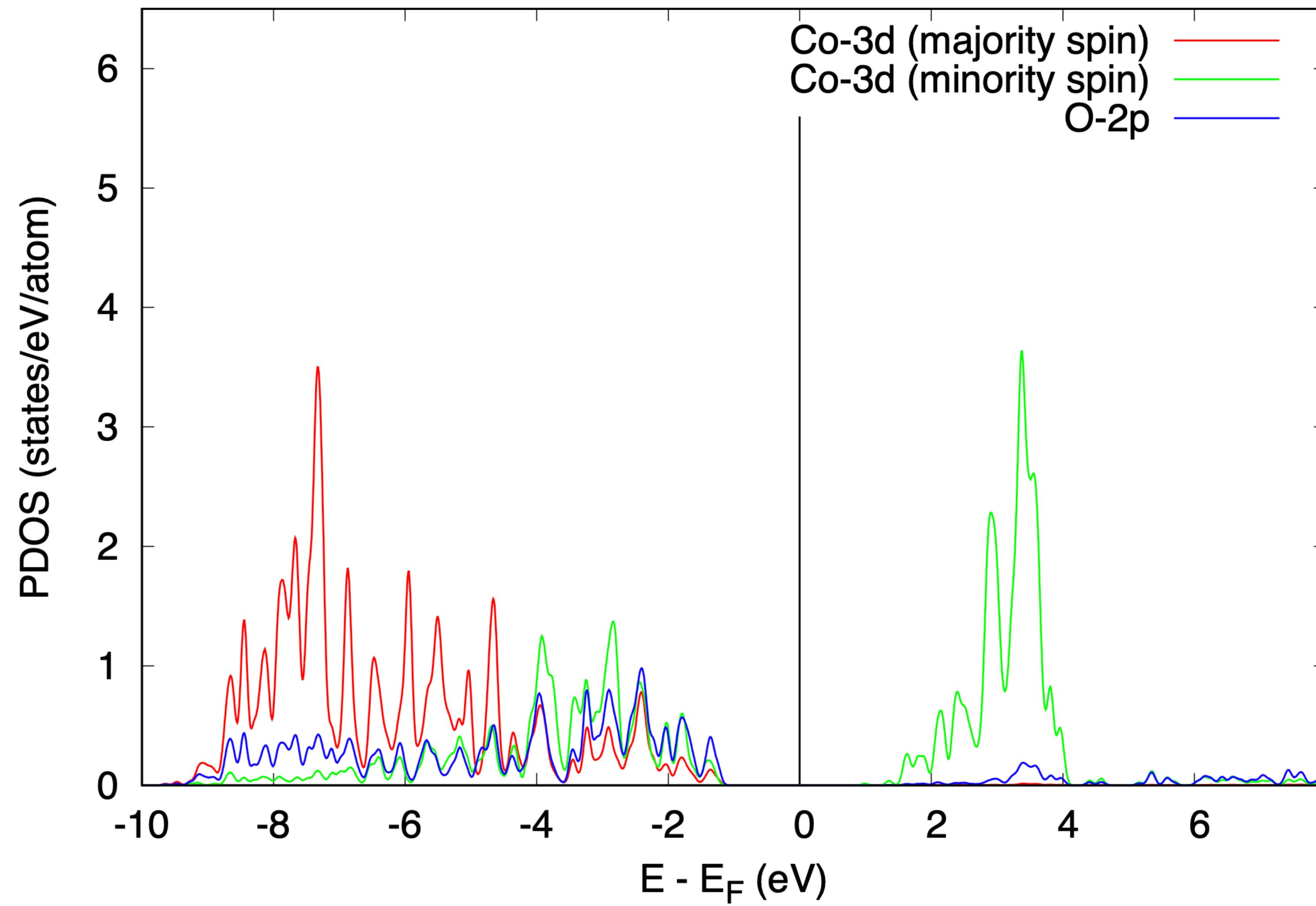
```
projwfc.x < Co0.projwfc.in |tee Co0.projwfc.out
```

```
gnuplot plot_pdos.gp
```

```
evince Co0_PDOS.eps
```

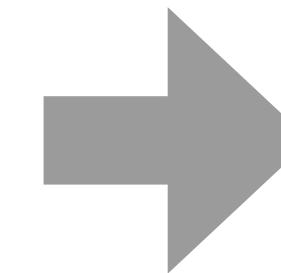
This is exactly the same as before (i.e. DFT-PBEsol case)

PDOS using DFT+ U (more precisely, PBEsol+ U)



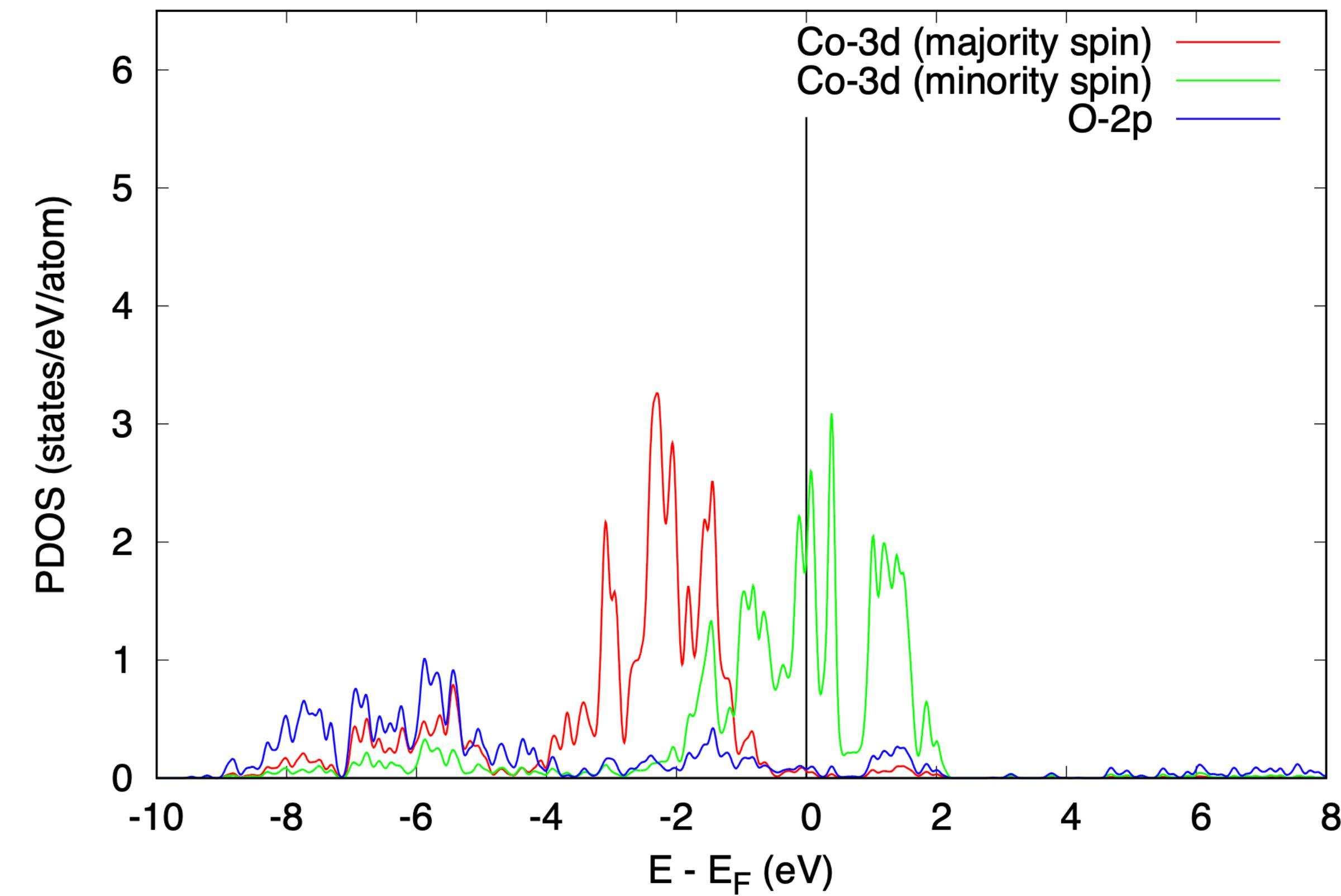
DFT+ U predicts CoO to be insulating ([this is correct](#))

Experimentally CoO is insulating

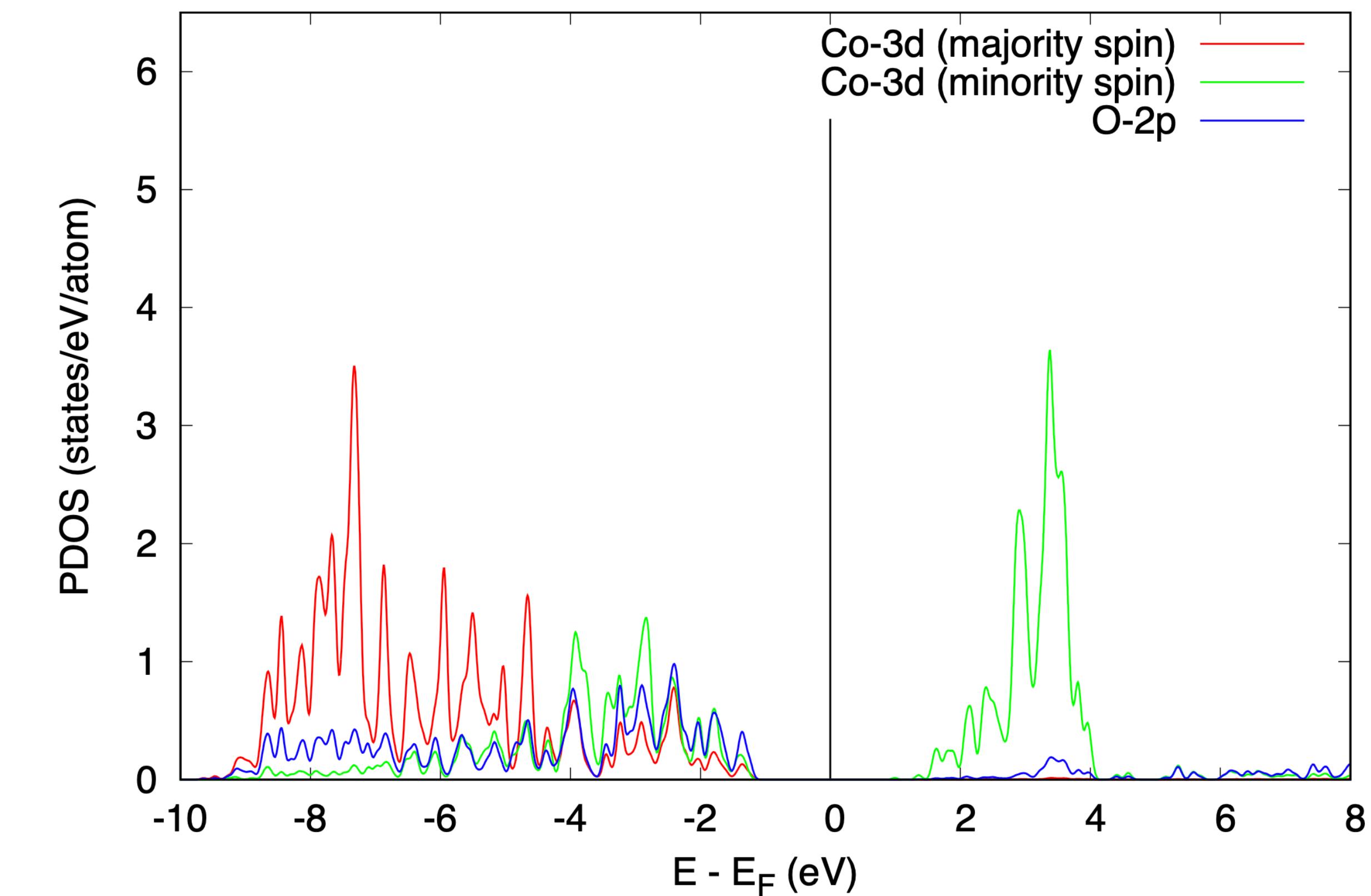


Agreement with experiment

PDOS using DFT



PDOS using DFT+ U



Co-3d (minority spin) states are split

Co-3d (majority spin) states are shifted to lower energies

DFT+ U band gap: 2.6 eV

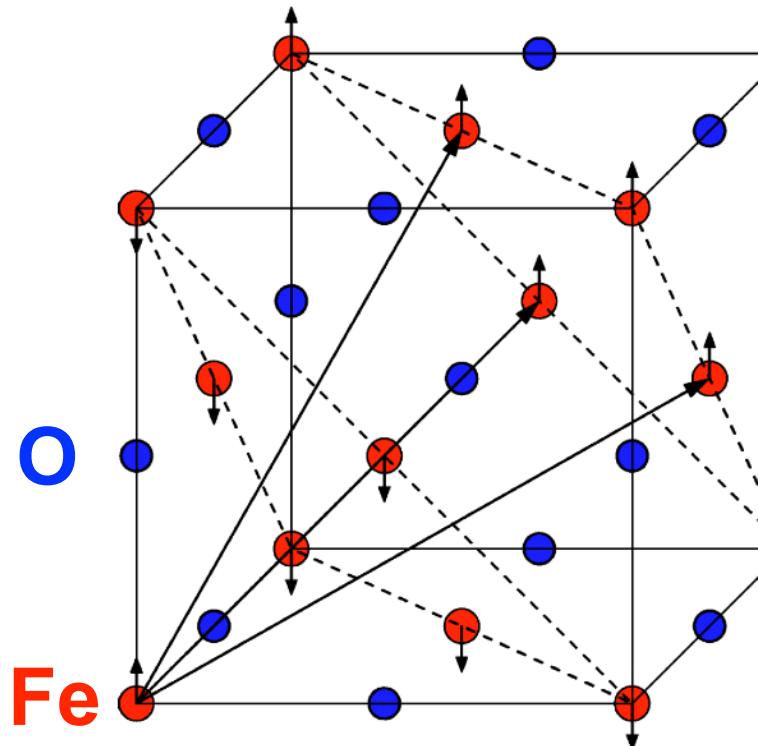
Experimental gap: 2.5 ± 0.3 eV

Exercise 2

**Projected density of states of FeO
with and without the Hubbard U correction**

Input file FeO.scf.in

```
&control
  calculation='scf'
  restart_mode='from_scratch',
  prefix='FeO'
  pseudo_dir = '../files/pseudo'
 outdir='./tmp'
  verbosity='high'
/
&system
  ibrav = 0,
  celldm(1) = 8.00,
  nat = 4,
  ntyp = 3,
  ecutwfc = 35.0
  ecutrho = 280.0
  nspin = 2
  starting_magnetization(1) = 0.5,
  starting_magnetization(2) = -0.5,
  occupations = 'smearing',
  smearing = 'mv',
  degauss = 0.02
/
&electrons
  conv_thr = 1.d-10
/
ATOMIC_SPECIES
  Fe1 55.845 Fe.pbesol-spn-kjpaw_psl.0.2.1.UPF
  Fe2 55.845 Fe.pbesol-spn-kjpaw_psl.0.2.1.UPF
  O 15.999 O.pbesol-n-kjpaw_psl.0.1.UPF
ATOMIC_POSITIONS {crystal}
  Fe1    0.0000000    0.0000000    0.0000000
  Fe2    0.5000000    0.5000000    0.5000000
  O     0.2500000    0.2500000    0.2500000
  O     0.7500000    0.7500000    0.7500000
CELL_PARAMETERS {alat}
  0.582729109  0.582729109  1.045799900
  0.582729109  1.045799900  0.582729109
  1.045799900  0.582729109  0.582729109
K_POINTS {automatic}
  3 3 3 0 0 0
HUBBARD {ortho-atomic}
U Fe1-3d 0.0001
U Fe2-3d 0.0001
```



Input file FeO.nscf.in

```
&control
  calculation='nscf'
  restart_mode='from_scratch',
  prefix='FeO'
  pseudo_dir = '../files/pseudo'
 outdir='./tmp'
  verbosity='high'
/
&system
  ibrav = 0,
  celldm(1) = 8.00,
  nat = 4,
  ntyp = 3,
  ecutwfc = 35.0
  ecutrho = 280.0
  nspin = 2
  starting_magnetization(1) = 0.5,
  starting_magnetization(2) = -0.5,
  occupations = 'smearing',
  smearing = 'mv',
  degauss = 0.02
  nbnd = 40
/
&electrons
  conv_thr = 1.d-9
/
ATOMIC_SPECIES
  Fe1 55.845 Fe.pbesol-spn-kjpaw_psl.0.2.1.UPF
  Fe2 55.845 Fe.pbesol-spn-kjpaw_psl.0.2.1.UPF
  O 15.999 O.pbesol-n-kjpaw_psl.0.1.UPF
ATOMIC_POSITIONS {crystal}
  Fe1    0.0000000    0.0000000    0.0000000
  Fe2    0.5000000    0.5000000    0.5000000
  O     0.2500000    0.2500000    0.2500000
  O     0.7500000    0.7500000    0.7500000
CELL_PARAMETERS {alat}
  0.582729109  0.582729109  1.045799900
  0.582729109  1.045799900  0.582729109
  1.045799900  0.582729109  0.582729109
K_POINTS {automatic}
  6 6 6 0 0 0
HUBBARD {ortho-atomic}
U Fe1-3d 0.0001
U Fe2-3d 0.0001
```

Input file FeO.projwfc.in

```
&projwfc
    prefix='FeO'
    outdir='./tmp'
    ngauss = 0, ← Gaussian broadening for PDOS
    degauss = 0.005, ← Value of the Gaussian broadening (in Ry)
    Emin = -15.0, ← Minimum and maximum energy for the plot (in eV)
    Emax = 30.0, ←
    DeltaE = 0.01 ← Energy grid step
/

```

Gnuplot script: plot_pdos.gp

Inspect the script. It aims at plotting Fe-3d states (majority spin and minority spin) and O-2p states.

PDOS is shifted such that the Fermi energy corresponds to zero of energy.

After running the script, visualize the file FeO_PDOS.eps.

Run the calculations

```
pw.x < Fe0.scf.in |tee Fe0.scf.out
```

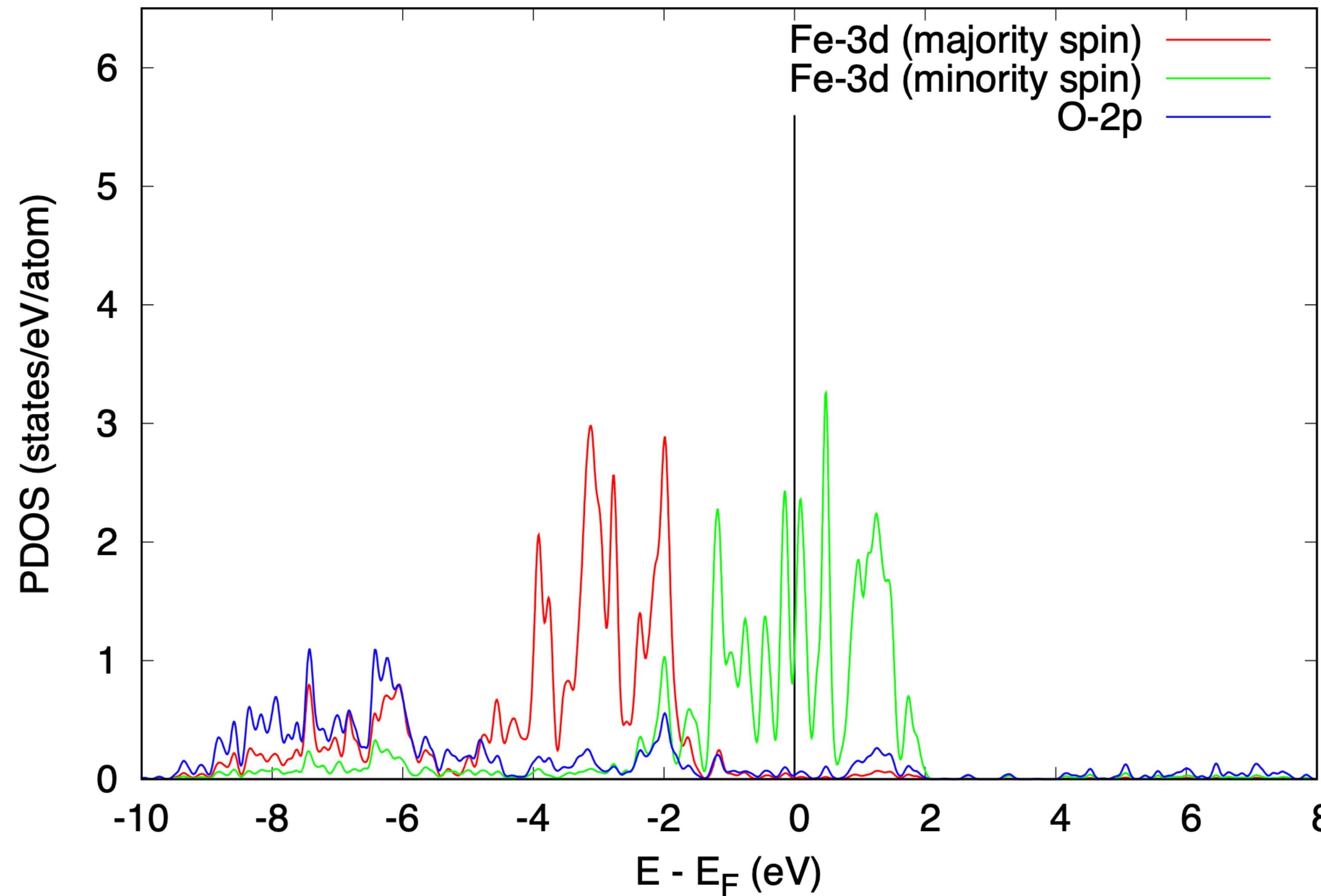
```
pw.x < Fe0.nscf.in |tee Fe0.nscf.out
```

```
projwfc.x < Fe0.projwfc.in |tee Fe0.projwfc.out
```

```
gnuplot plot_pdos.gp
```

```
evince Fe0_PDOS.eps
```

PDOS using DFT (PBEsol)



DFT predicts FeO to be metallic (**this is wrong**)

Experimentally FeO is insulating

Let's try DFT+*U*

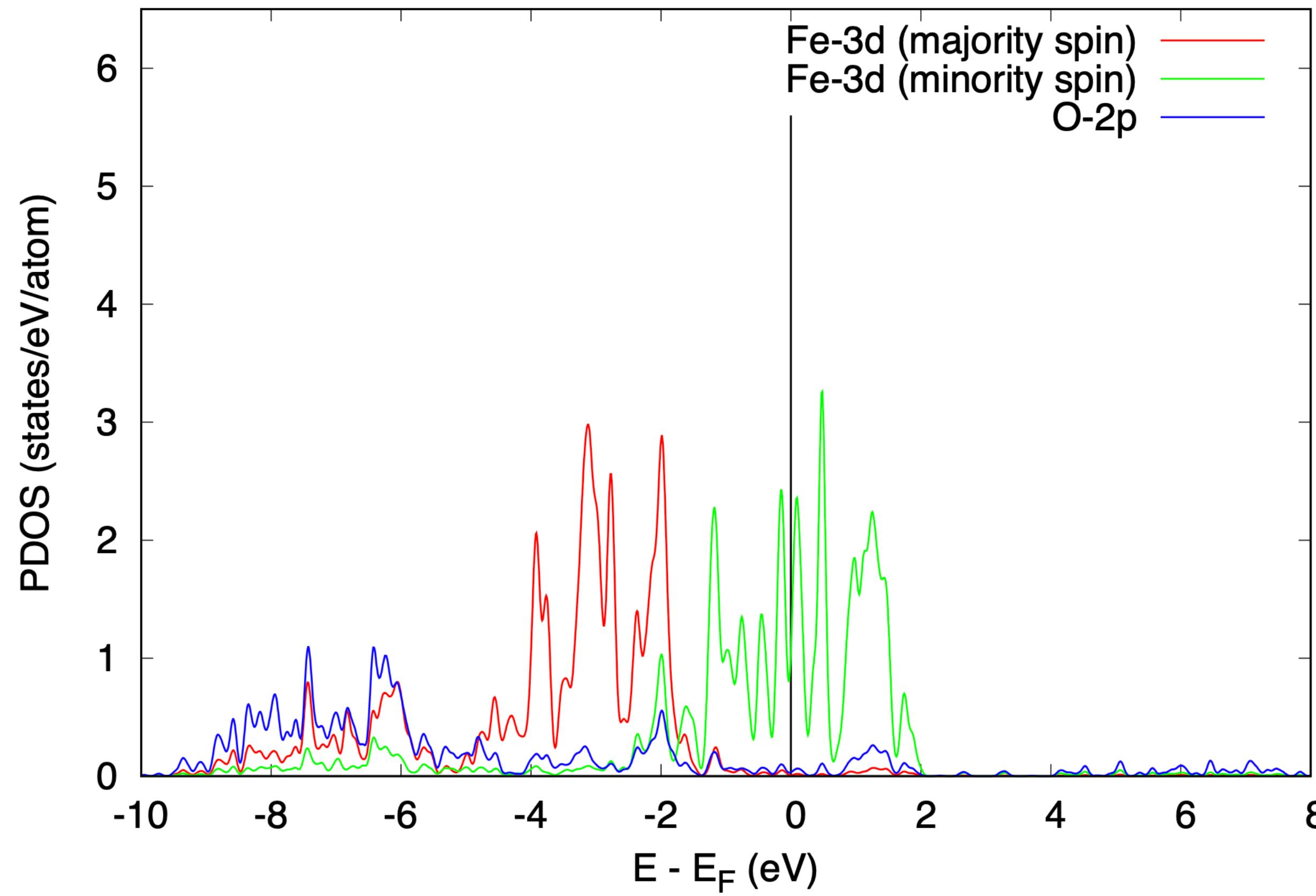
Input file FeO.scf.in

```
&control
  calculation='scf'
  restart_mode='from_scratch',
  prefix='FeO'
  pseudo_dir = '../files/pseudo'
 outdir='./tmp'
  verbosity='high'
/
&system
  ibrav = 0,
  celldm(1) = 8.00,
  nat = 4,
  ntyp = 3,
  ecutwfc = 35.0
  ecutrho = 280.0
  nspin = 2
  starting_magnetization(1) = 0.5,
  starting_magnetization(2) = -0.5,
  occupations = 'smearing',
  smearing = 'mv',
  degauss = 0.02
/
&electrons
  conv_thr = 1.d-10
/
ATOMIC_SPECIES
  Fe1 55.845 Fe.pbesol-spn-kjpaw_psl.0.2.1.UPF
  Fe2 55.845 Fe.pbesol-spn-kjpaw_psl.0.2.1.UPF
  O 15.999 O.pbesol-n-kjpaw_psl.0.1.UPF
ATOMIC_POSITIONS {crystal}
  Fe1    0.0000000    0.0000000    0.0000000
  Fe2    0.5000000    0.5000000    0.5000000
  O     0.2500000    0.2500000    0.2500000
  O     0.7500000    0.7500000    0.7500000
CELL_PARAMETERS {alat}
  0.582729109  0.582729109  1.045799900
  0.582729109  1.045799900  0.582729109
  1.045799900  0.582729109  0.582729109
K_POINTS {automatic}
  3 3 3 0 0 0
HUBBARD {ortho-atomic}
U Fe1-3d 5.36
U Fe2-3d 5.36
```

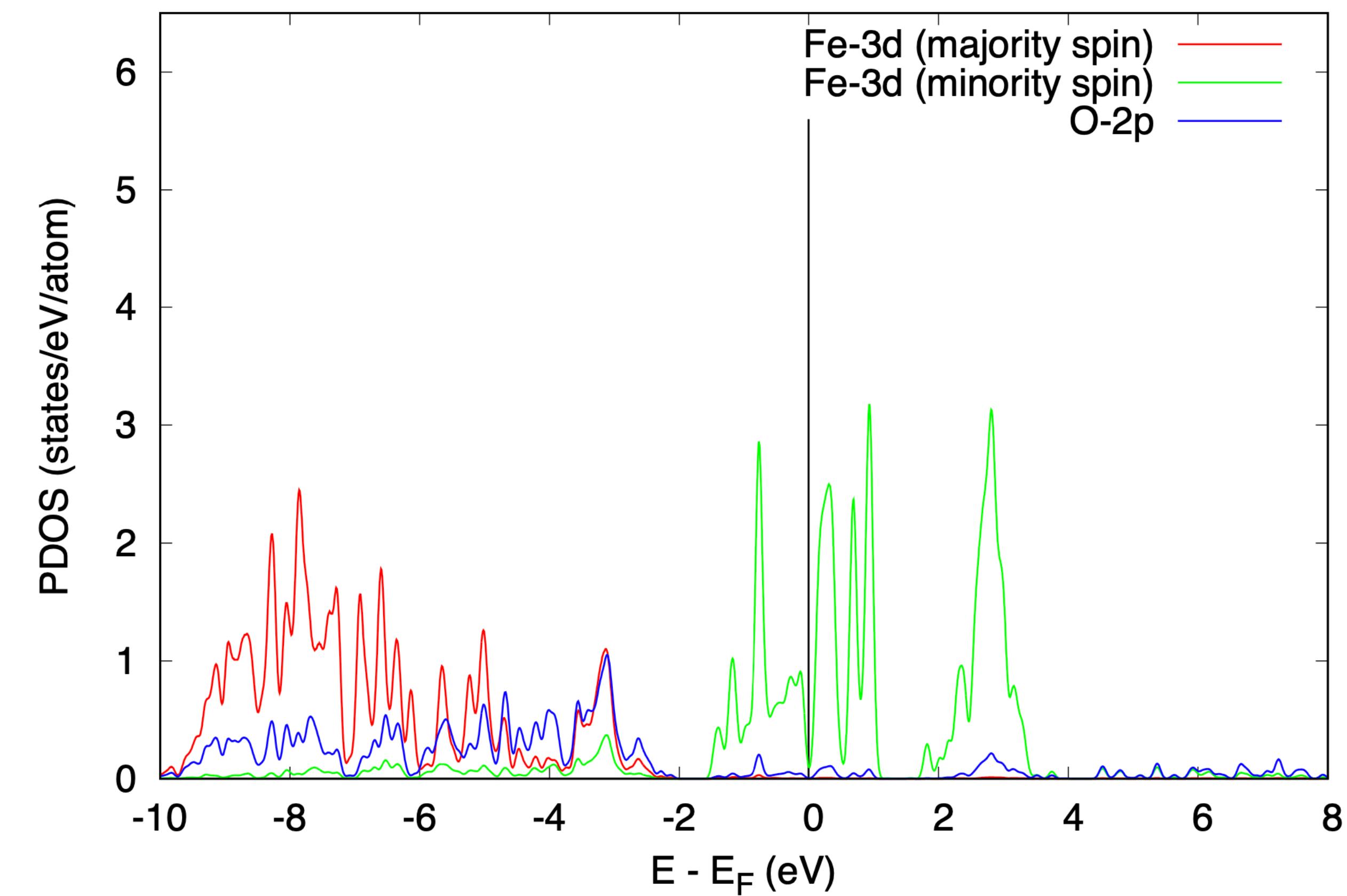
Input file FeO.nscf.in

```
&control
  calculation='nscf'
  restart_mode='from_scratch',
  prefix='FeO'
  pseudo_dir = '../files/pseudo'
 outdir='./tmp'
  verbosity='high'
/
&system
  ibrav = 0,
  celldm(1) = 8.00,
  nat = 4,
  ntyp = 3,
  ecutwfc = 35.0
  ecutrho = 280.0
  nspin = 2
  starting_magnetization(1) = 0.5,
  starting_magnetization(2) = -0.5,
  occupations = 'smearing',
  smearing = 'mv',
  degauss = 0.02
  nbnd = 40
/
&electrons
  conv_thr = 1.d-9
/
ATOMIC_SPECIES
  Fe1 55.845 Fe.pbesol-spn-kjpaw_psl.0.2.1.UPF
  Fe2 55.845 Fe.pbesol-spn-kjpaw_psl.0.2.1.UPF
  O 15.999 O.pbesol-n-kjpaw_psl.0.1.UPF
ATOMIC_POSITIONS {crystal}
  Fe1    0.0000000    0.0000000    0.0000000
  Fe2    0.5000000    0.5000000    0.5000000
  O     0.2500000    0.2500000    0.2500000
  O     0.7500000    0.7500000    0.7500000
CELL_PARAMETERS {alat}
  0.582729109  0.582729109  1.045799900
  0.582729109  1.045799900  0.582729109
  1.045799900  0.582729109  0.582729109
K_POINTS {automatic}
  6 6 6 0 0 0
HUBBARD {ortho-atomic}
U Fe1-3d 5.36
U Fe2-3d 5.36
```

PDOS using DFT



PDOS using DFT+ U



Even a standard DFT+ U calculation does not manage to open a gap in FeO

Output file FeO.scf.out from the DFT+U calculation

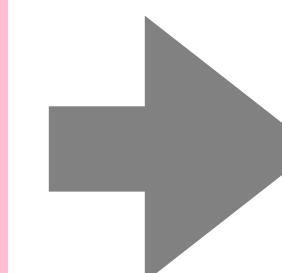
After the 1st SCF iteration:

```
===== HUBBARD OCCUPATIONS =====
----- ATOM    1 -----
Tr[ns( 1)] (up, down, total) =   4.98138   0.94209   5.92348
Atomic magnetic moment for atom 1 =   4.03929
SPIN 1
eigenvalues:
  0.996  0.996  0.996  0.997  0.997
SPIN 2
eigenvalues:
  0.075  0.075  0.253  0.253  0.285
----- ATOM    2 -----
Tr[ns( 2)] (up, down, total) =   0.94168   4.98133   5.92301
Atomic magnetic moment for atom 2 = -4.03965
SPIN 1
eigenvalues:
  0.075  0.075  0.253  0.253  0.285
SPIN 2
eigenvalues:
  0.996  0.996  0.996  0.997  0.997
```

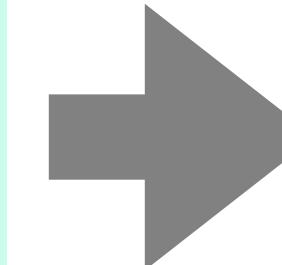
Output file FeO.scf.out from the DFT+*U* calculation

After the 1st SCF iteration:

```
===== HUBBARD OCCUPATIONS =====
----- ATOM 1 -----
Tr[ns( 1)] (up, down, total) = 4.98138 0.94209 5.92348
Atomic magnetic moment for atom 1 = 4.03929
SPIN 1
eigenvalues:
 0.996 0.996 0.996 0.997 0.997
SPIN 2
eigenvalues:
 0.075 0.075 0.253 0.253 0.285
----- ATOM 2 -----
Tr[ns( 2)] (up, down, total) = 0.94168 4.98133 5.92301
Atomic magnetic moment for atom 2 = -4.03965
SPIN 1
eigenvalues:
 0.075 0.075 0.253 0.253 0.285
SPIN 2
eigenvalues:
 0.996 0.996 0.996 0.997 0.997
```



starting_ns_eigenvalue(5,2,1) = 1.0

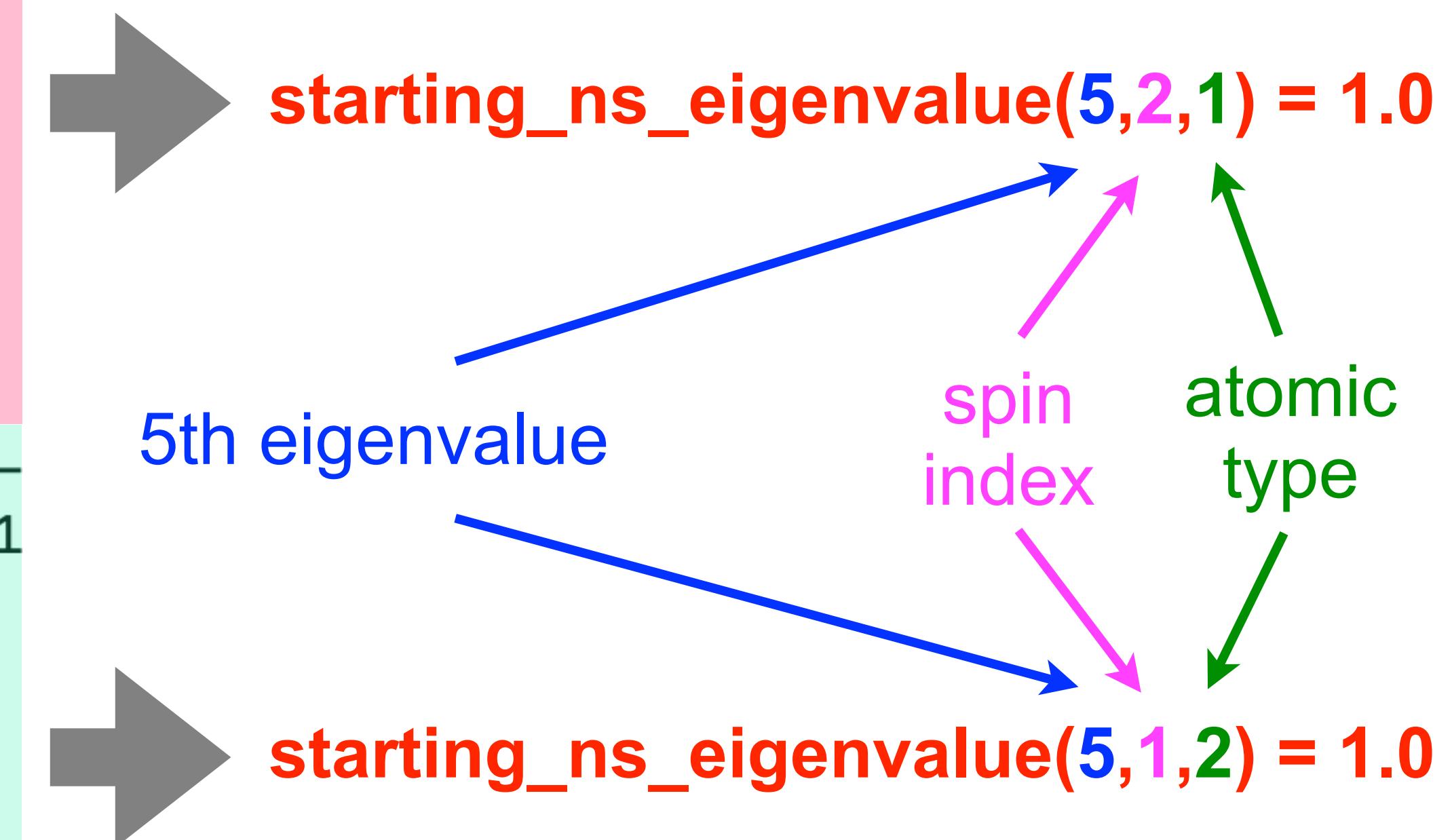


starting_ns_eigenvalue(5,1,2) = 1.0

Output file FeO.scf.out from the DFT+U calculation

After the 1st SCF iteration:

```
===== HUBBARD OCCUPATIONS =====
----- ATOM 1 -----
Tr[ns( 1)] (up, down, total) = 4.98138 0.94209 5.92348
Atomic magnetic moment for atom 1 = 4.03929
SPIN 1
eigenvalues:
 0.996 0.996 0.996 0.997 0.997
SPIN 2
eigenvalues:
 0.075 0.075 0.253 0.253 0.285
----- ATOM 2 -----
Tr[ns( 2)] (up, down, total) = 0.94168 4.98133 5.92301
Atomic magnetic moment for atom 2 = -4.03965
SPIN 1
eigenvalues:
 0.075 0.075 0.253 0.253 0.285
SPIN 2
eigenvalues:
 0.996 0.996 0.996 0.997 0.997
```



Input file FeO.scf.in

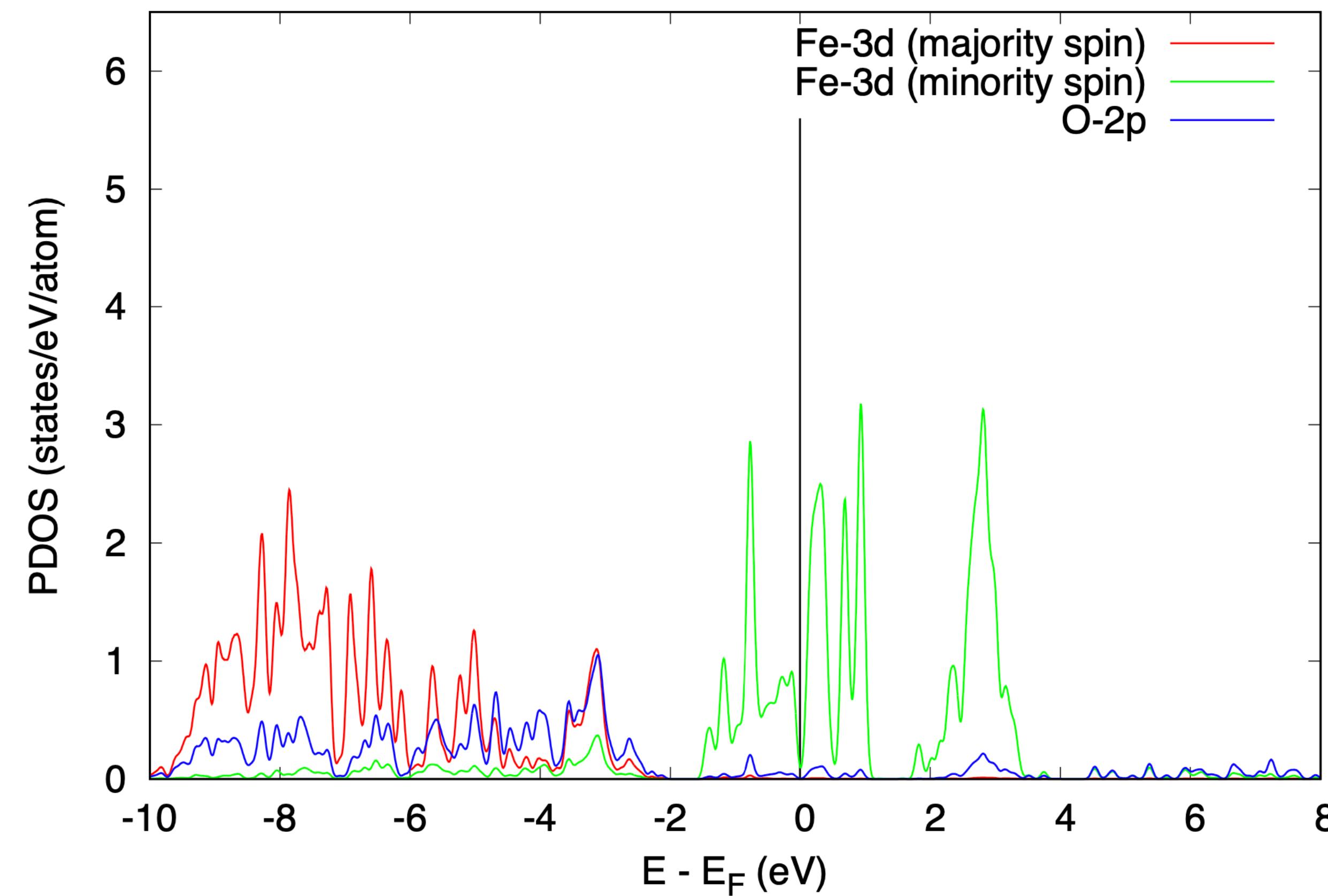
```
&control
  calculation='scf'
  restart_mode='from_scratch',
  prefix='FeO'
  pseudo_dir = '../files/pseudo'
 outdir='./tmp'
  verbosity='high'
/
&system
  ibrav = 0,
  celldm(1) = 8.00,
  nat = 4,
  ntyp = 3,
  ecutwfc = 35.0
  ecutrho = 280.0
  nspin = 2
  starting_magnetization(1) = 0.5,
  starting_magnetization(2) = -0.5,
  occupations = 'smearing',
  smearing = 'mv',
  degauss = 0.02
  starting_ns_eigenvalue(5,2,1) = 1.0
  starting_ns_eigenvalue(5,1,2) = 1.0
/
&electrons
  conv_thr = 1.d-10
/
ATOMIC_SPECIES
  Fe1 55.845 Fe.pbesol-spn-kjpaw_psl.0.2.1.UPF
  Fe2 55.845 Fe.pbesol-spn-kjpaw_psl.0.2.1.UPF
  O 15.999 O.pbesol-n-kjpaw_psl.0.1.UPF
ATOMIC_POSITIONS {crystal}
  Fe1    0.0000000    0.0000000    0.0000000
  Fe2    0.5000000    0.5000000    0.5000000
  O     0.2500000    0.2500000    0.2500000
  O     0.7500000    0.7500000    0.7500000
CELL_PARAMETERS {alat}
  0.582729109  0.582729109  1.045799900
  0.582729109  1.045799900  0.582729109
  1.045799900  0.582729109  0.582729109
K_POINTS {automatic}
  3 3 3 0 0 0
HUBBARD {ortho-atomic}
U Fe1-3d 5.36
U Fe2-3d 5.36
```

Input file FeO.nscf.in

```
&control
  calculation='nscf'
  restart_mode='from_scratch',
  prefix='FeO'
  pseudo_dir = '../files/pseudo'
  outdir='./tmp'
  verbosity='high'
/
&system
  ibrav = 0,
  celldm(1) = 8.00,
  nat = 4,
  ntyp = 3,
  ecutwfc = 35.0
  ecutrho = 280.0
  nspin = 2
  starting_magnetization(1) = 0.5,
  starting_magnetization(2) = -0.5,
  occupations = 'smearing',
  smearing = 'mv',
  degauss = 0.02
  starting_ns_eigenvalue(5,2,1) = 1.0
  starting_ns_eigenvalue(5,1,2) = 1.0
  nbnd = 40
/
&electrons
  conv_thr = 1.d-9
/
ATOMIC_SPECIES
  Fe1 55.845 Fe.pbesol-spn-kjpaw_psl.0.2.1.UPF
  Fe2 55.845 Fe.pbesol-spn-kjpaw_psl.0.2.1.UPF
  O 15.999 O.pbesol-n-kjpaw_psl.0.1.UPF
ATOMIC_POSITIONS {crystal}
  Fe1    0.0000000    0.0000000    0.0000000
  Fe2    0.5000000    0.5000000    0.5000000
  O     0.2500000    0.2500000    0.2500000
  O     0.7500000    0.7500000    0.7500000
CELL_PARAMETERS {alat}
  0.582729109  0.582729109  1.045799900
  0.582729109  1.045799900  0.582729109
  1.045799900  0.582729109  0.582729109
K_POINTS {automatic}
  6 6 6 0 0 0
HUBBARD {ortho-atomic}
U Fe1-3d 5.36
U Fe2-3d 5.36
```

PDOS using DFT+U

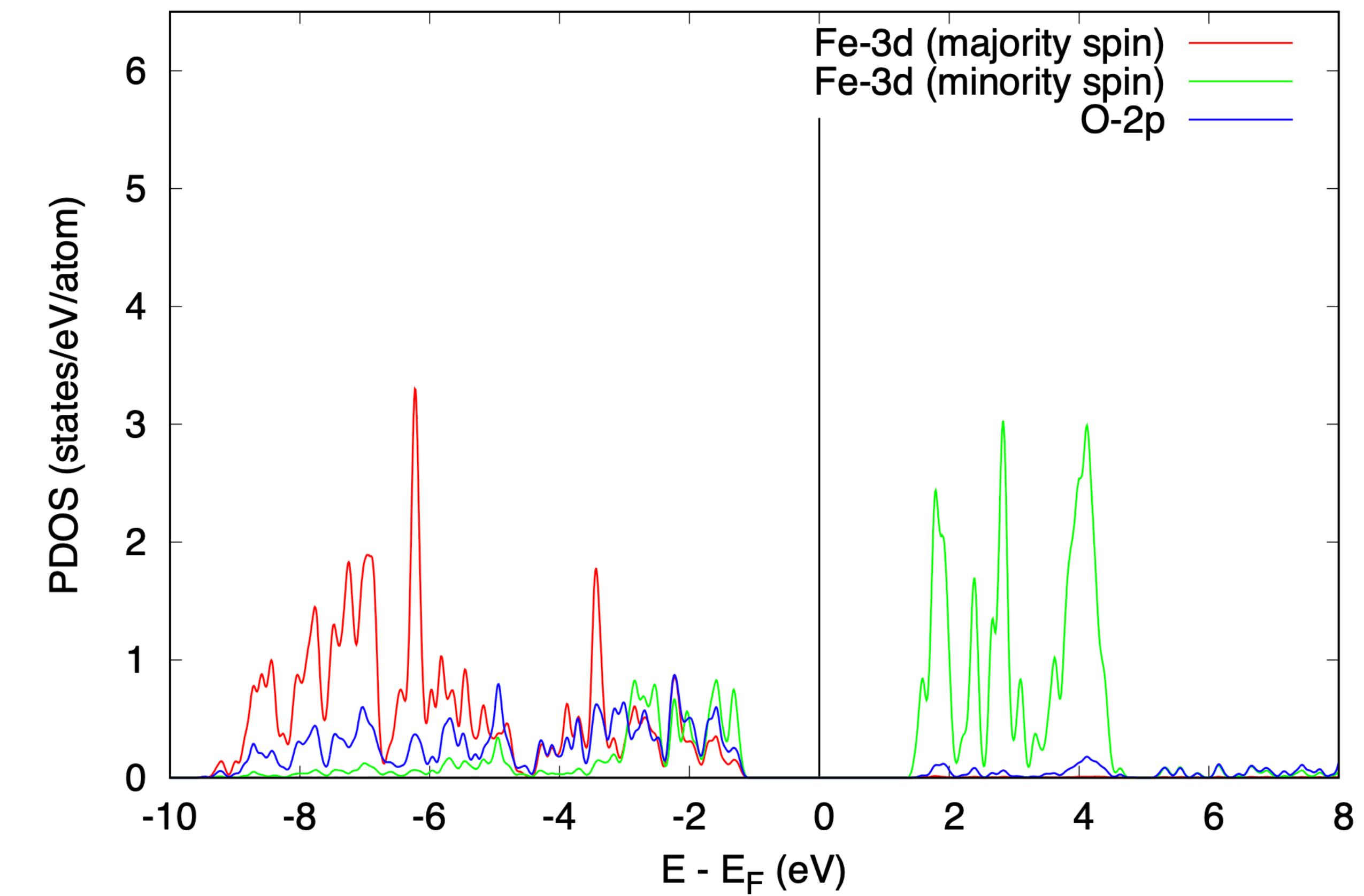
PDOS using DFT+U (with starting_ns_eigenvalue)



$$E_{\text{TOT}} = -735.372 \text{ Ry}$$

DFT+U with starting_ns_eigenvalue opens the band gap in FeO

DFT+U band gap: 2.76 eV



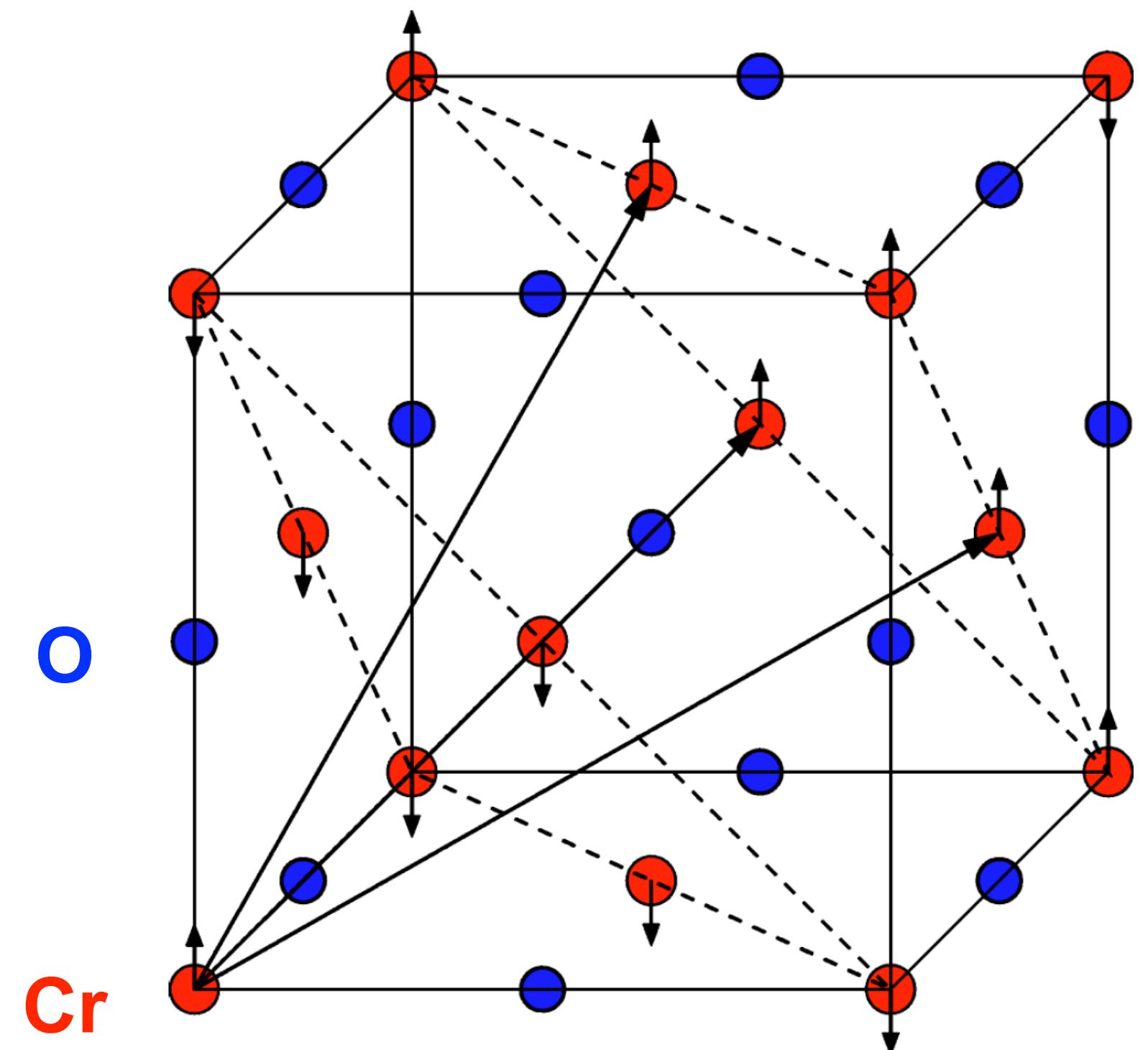
$$E_{\text{TOT}} = -735.480 \text{ Ry}$$

Experimental gap: 2.4 eV

Exercise 3

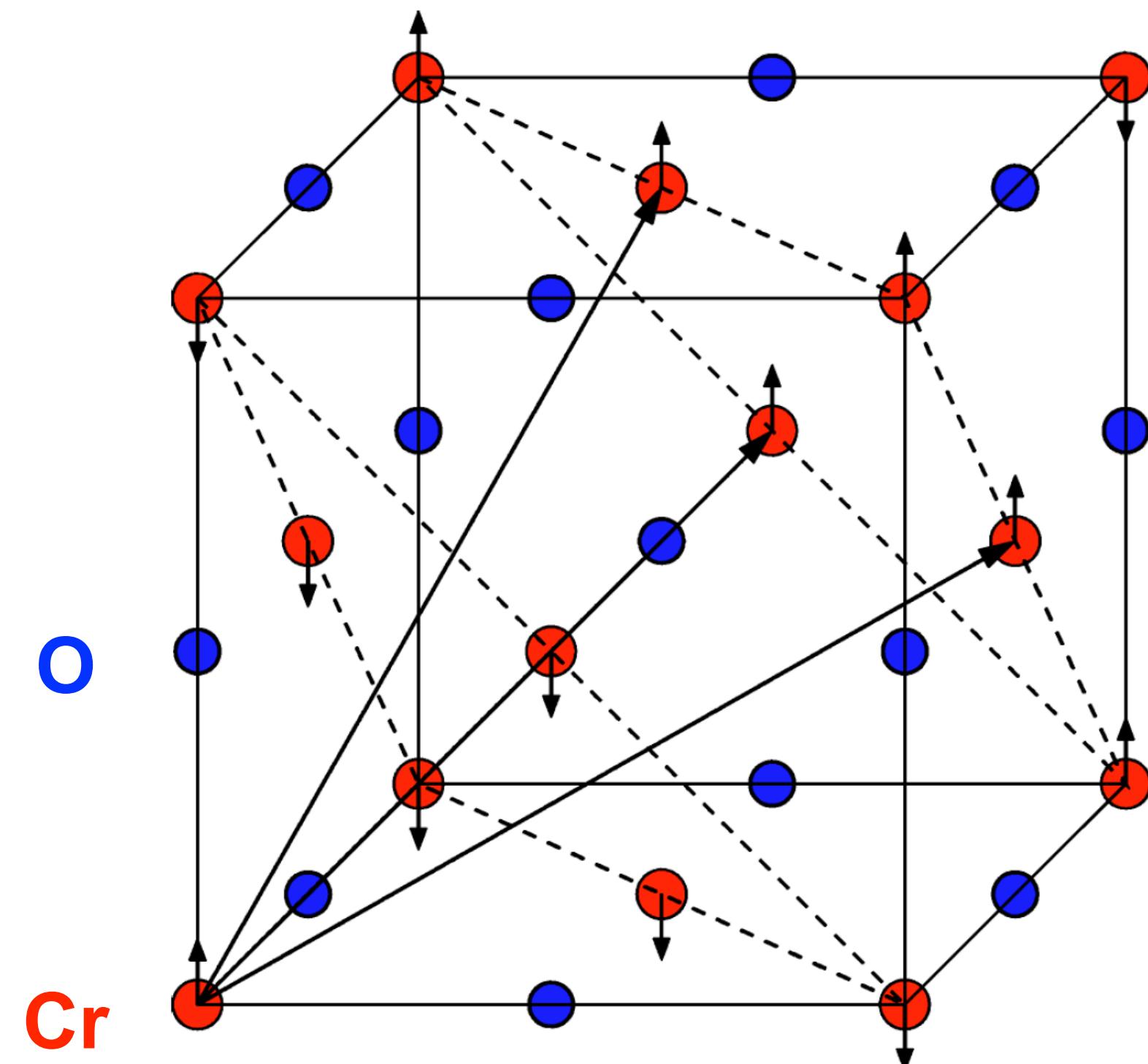
**Band structure of CrO
with and without the Hubbard U correction**

Another transition-metal monoxide: cubic CrO



Same crystal structure
as FeO and CoO

Another transition-metal monoxide: cubic CrO

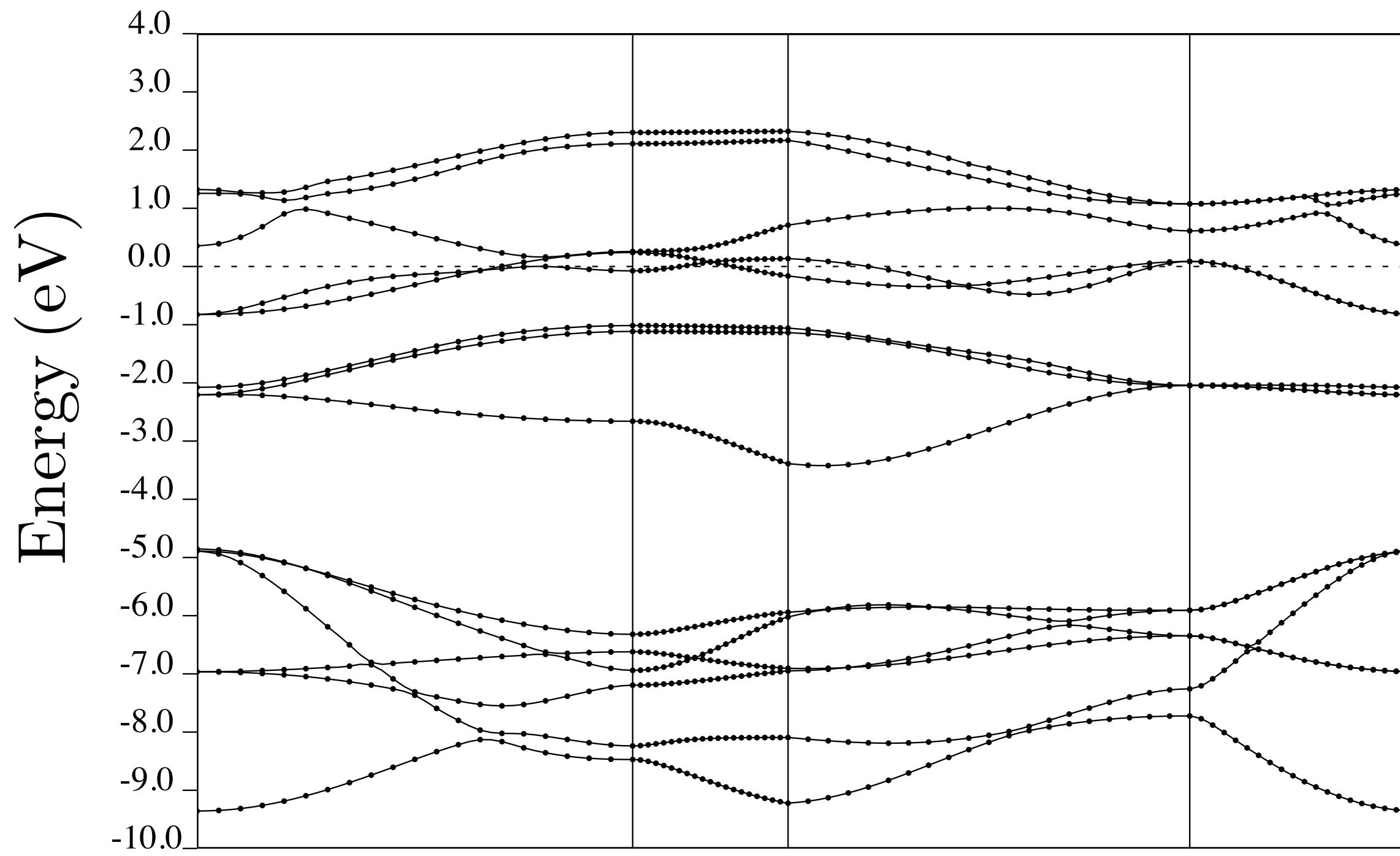


Same crystal structure
as FeO and CoO

However, Cr^{2+} has 4 d electrons all in the same (majority) spin channel

CrO band structure from DFT and DFT+ U

PBEsol

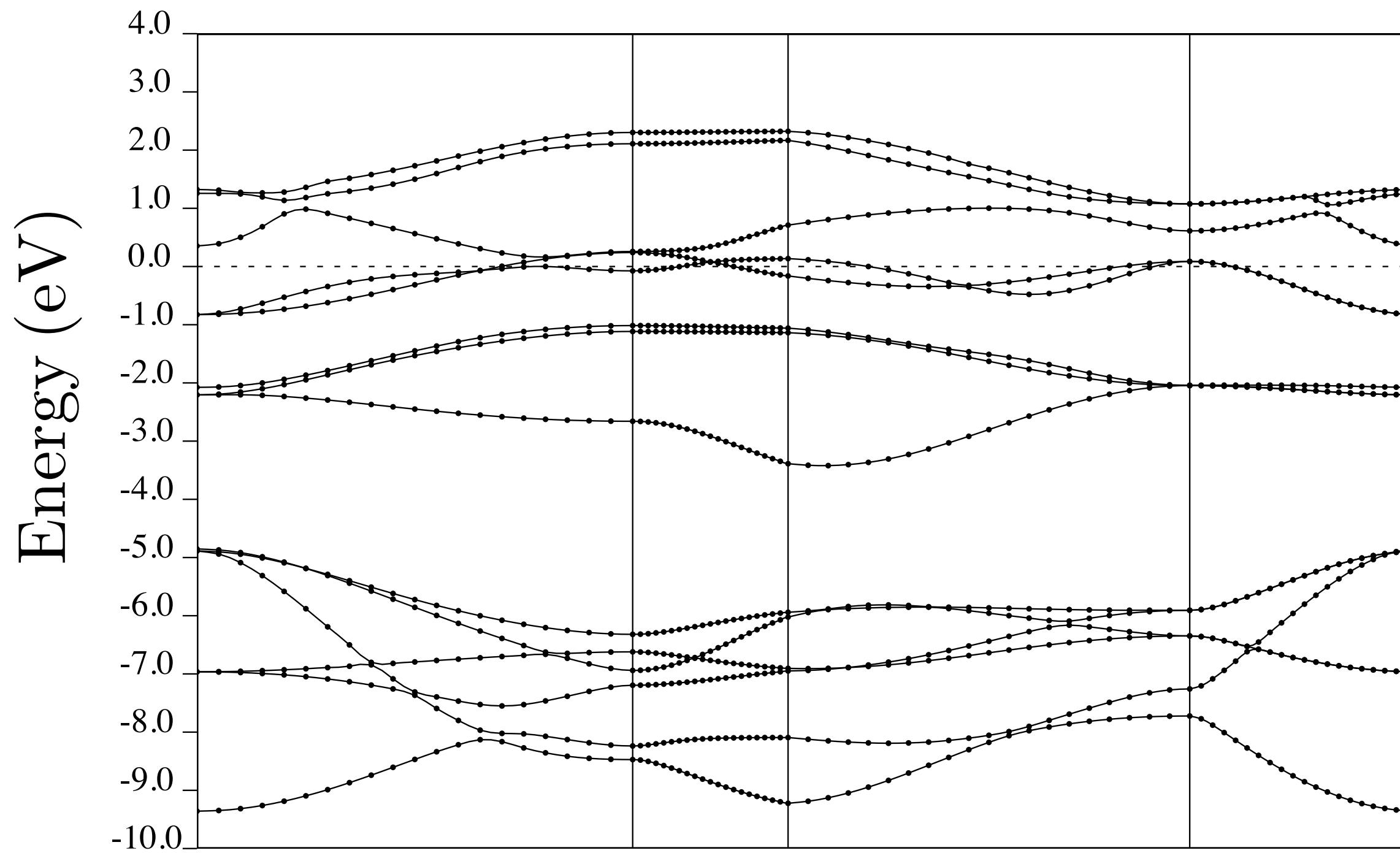


Energy (eV)

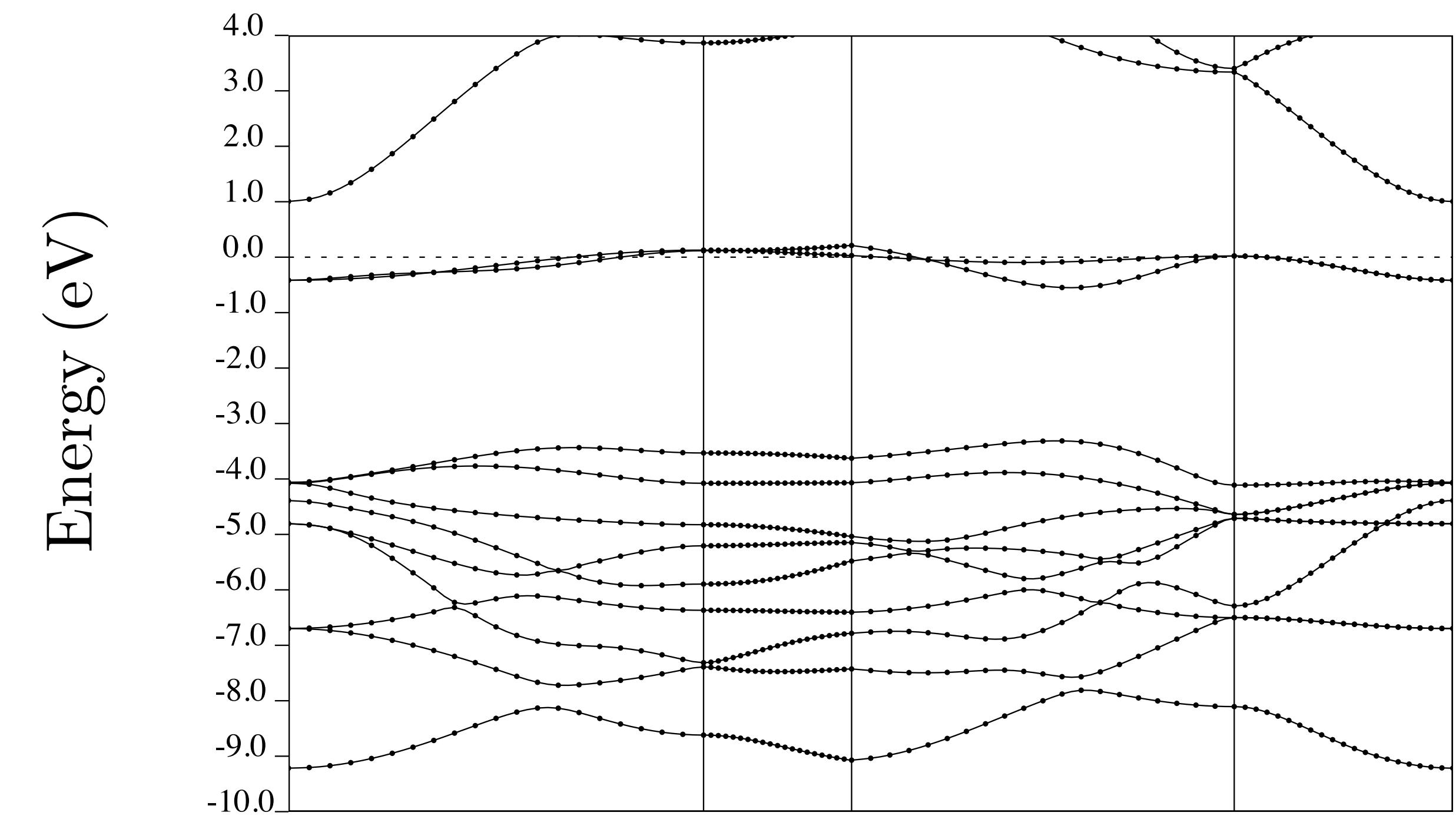
No gap opens in the band structure; is this right?

CrO band structure from DFT and DFT+ U

PBEsol



PBEsol+ U ($U=7.86$ eV, ortho-atomic)



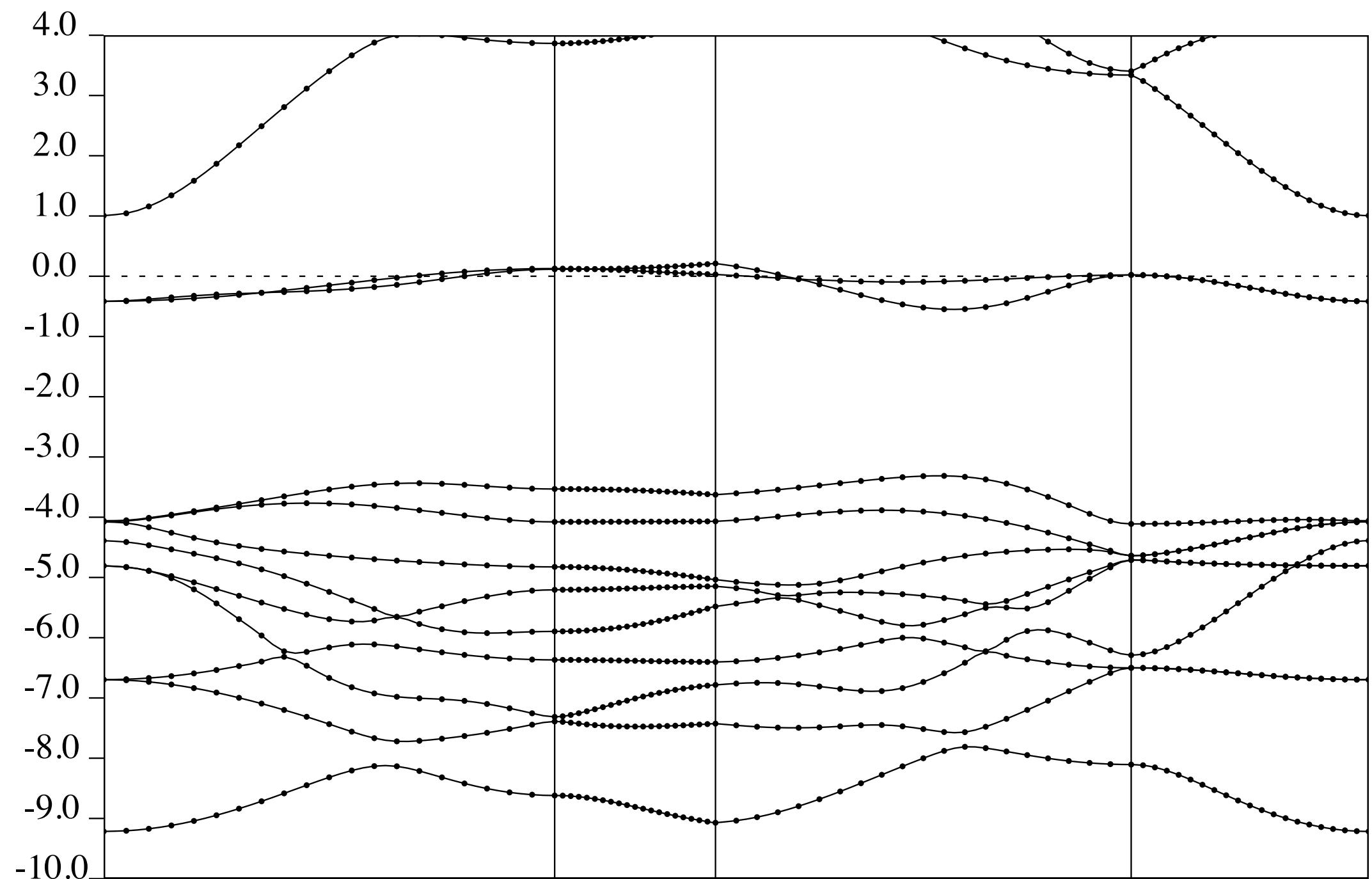
No gap opens in the band structure; is this right?

Cr *d* states occupation

```
----- ATOM 1 -----
Tr[ns( 1)] (up, down, total) = 4.21157 0.20845 4.42002
Atomic magnetic moment for atom 1 = 4.00312
SPIN 1
eigenvalues:
  0.629  0.629  0.984  0.985  0.985
eigenvectors (columns):
  0.665  0.747  0.000 -0.030  0.003
  0.008 -0.024 -0.577 -0.471 -0.667
 -0.024  0.005 -0.577 -0.342  0.741
 -0.747  0.665 -0.000 -0.003 -0.030
 -0.017 -0.019  0.577 -0.813  0.075
occupation matrix ns (before diag.):
  0.629  0.004  0.004  0.000  0.009
  0.004  0.985 -0.000  0.008  0.000
  0.004 -0.000  0.985 -0.008  0.000
  0.000  0.008 -0.008  0.629 -0.000
  0.009  0.000  0.000 -0.000  0.985
SPIN 2
eigenvalues:
  0.022  0.023  0.023  0.070  0.070
eigenvectors (columns):
 -0.000  0.038 -0.001  0.658  0.752
 -0.577 -0.424 -0.697 -0.010  0.029
 -0.577 -0.391  0.716  0.030 -0.006
  0.000  0.001  0.038 -0.752  0.658
  0.577 -0.816  0.019  0.020  0.023
occupation matrix ns (before diag.):
  0.070  0.001  0.001  0.000  0.001
  0.001  0.023 -0.000  0.001  0.000
  0.001 -0.000  0.023 -0.001  0.000
  0.000  0.001 -0.001  0.070 -0.000
  0.001  0.000  0.000 -0.000  0.023
```

Cr²⁺ has 4 d electrons, all in the majority spin channel

PBE+U

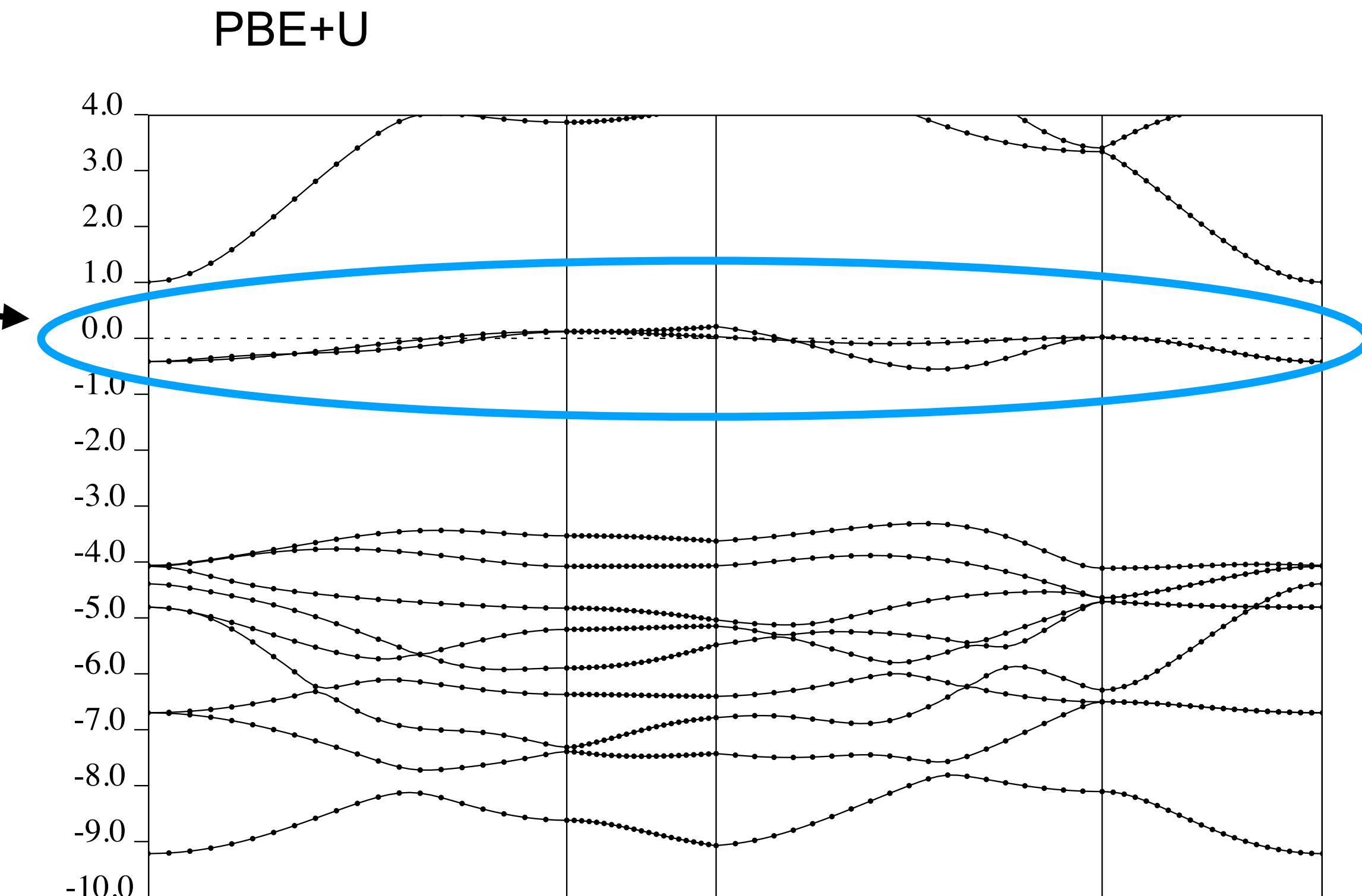


Cr *d* states occupation

```
----- ATOM      1 -----  
Tr[ns( 1)] (up, down, total) =   4.21157  0.20845  4.42002  
Atomic magnetic moment for atom 1 =    4.00312  
SPIN 1  
eigenvalues:  
0.629 0.629 0.984 0.985 0.985  
eigenvectors (columns):  
  0.665  0.747  0.000 -0.030  0.003  
  0.008 -0.024 -0.577 -0.471 -0.667  
 -0.024  0.005 -0.577 -0.342  0.741  
 -0.747  0.665 -0.000 -0.003 -0.030  
 -0.017 -0.019  0.577 -0.813  0.075  
occupation matrix ns (before diag.):  
  0.629  0.004  0.004  0.000  0.009  
  0.004  0.985 -0.000  0.008  0.000  
  0.004 -0.000  0.985 -0.008  0.000  
  0.000  0.008 -0.008  0.629 -0.000  
  0.009  0.000  0.000 -0.000  0.985  
SPIN 2  
eigenvalues:  
  0.022  0.023  0.023  0.070  0.070  
eigenvectors (columns):  
 -0.000  0.038 -0.001  0.658  0.752  
 -0.577 -0.424 -0.697 -0.010  0.029  
 -0.577 -0.391  0.716  0.030 -0.006  
  0.000  0.001  0.038 -0.752  0.658  
  0.577 -0.816  0.019  0.020  0.023  
occupation matrix ns (before diag.):  
  0.070  0.001  0.001  0.000  0.001  
  0.001  0.023 -0.000  0.001  0.000  
  0.001 -0.000  0.023 -0.001  0.000  
  0.000  0.001 -0.001  0.070 -0.000  
  0.001  0.000  0.000 -0.000  0.023
```

Cr²⁺ has 4 d electrons, all in the majority spin channel

Degenerate,
half-filled states



Cr d states occupation

```

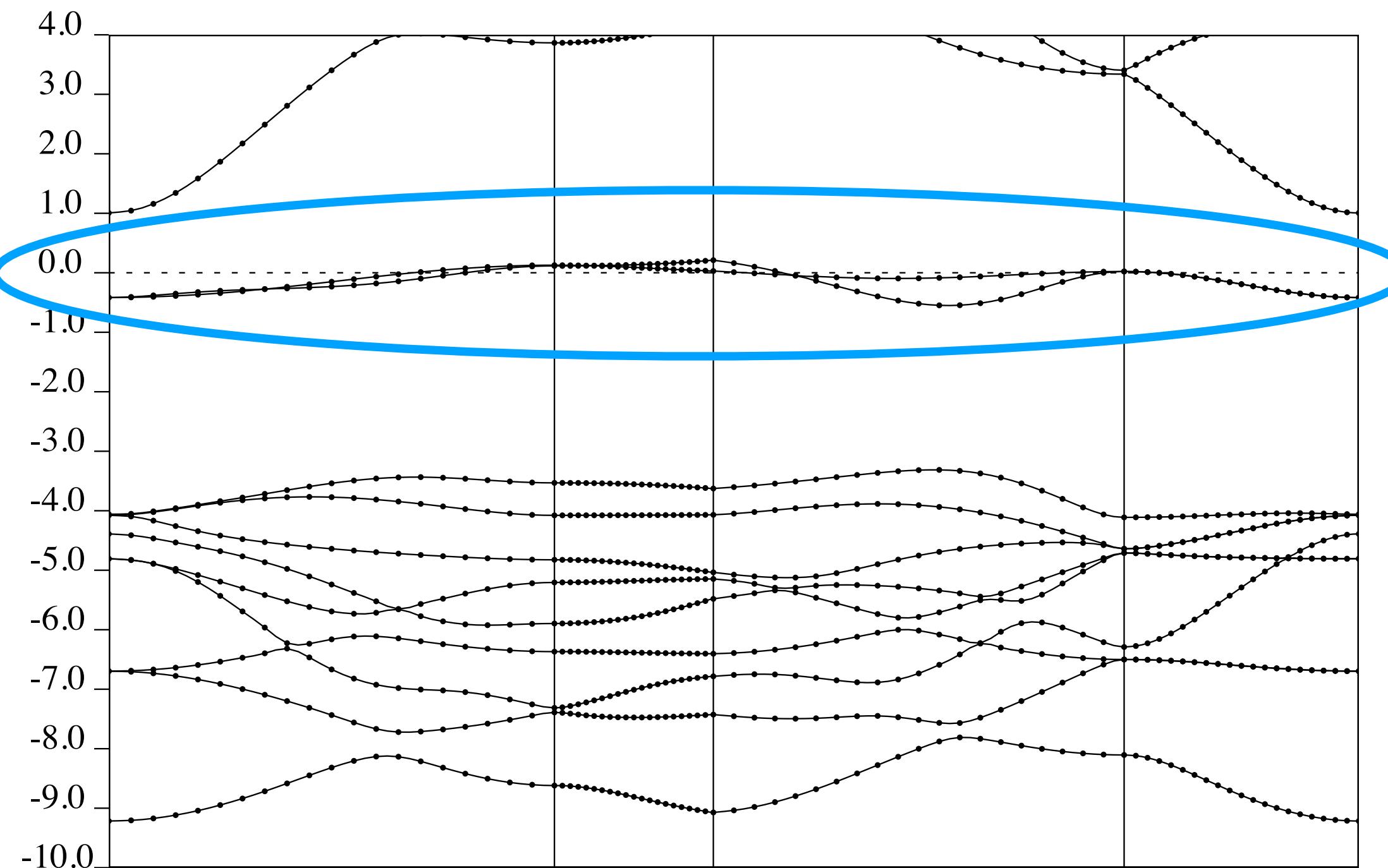
----- ATOM      1 -----
Tr[ns( 1)] (up, down, total) =   4.21157  0.20845  4.42002
Atomic magnetic moment for atom 1 =    4.00312
SPIN 1
eigenvalues:
 0.629  0.629  0.984  0.985  0.985
eigenvectors (columns):
 0.665  0.747  0.000 -0.030  0.003
 0.008 -0.024 -0.577 -0.471 -0.667
-0.024  0.005 -0.577 -0.342  0.741
-0.747  0.665 -0.000 -0.003 -0.030
-0.017 -0.019  0.577 -0.813  0.075
occupation matrix ns (before diag.):
 0.629  0.004  0.004  0.000  0.009
 0.004  0.985 -0.000  0.008  0.000
 0.004 -0.000  0.985 -0.008  0.000
 0.000  0.008 -0.008  0.629 -0.000
 0.009  0.000  0.000 -0.000  0.985
SPIN 2
eigenvalues:
 0.022  0.023  0.023  0.070  0.070
eigenvectors (columns):
-0.000  0.038 -0.001  0.658  0.752
-0.577 -0.424 -0.697 -0.010  0.029
-0.577 -0.391  0.716  0.030 -0.006
 0.000  0.001  0.038 -0.752  0.658
 0.577 -0.816  0.019  0.020  0.023
occupation matrix ns (before diag.):
 0.070  0.001  0.001  0.000  0.001
 0.001  0.023 -0.000  0.001  0.000
 0.001 -0.000  0.023 -0.001  0.000
 0.000  0.001 -0.001  0.070 -0.000
 0.001  0.000  0.000 -0.000  0.023

```

Degenerate,
half-filled states

Cr²⁺ has 4 d electrons, all in the majority spin channel

PBE+U



Maybe an insulating state can be achieved fully occupying the
degenerate states and forcing the third state to be empty?

The new ground state

Input

```
.  
. &system  
  ibrav= 0, celldm(1)=8.0, nat= 4, ntyp= 3,  
  nspin = 2,  
  starting_magnetization(1) = 0.4,  
  starting_magnetization(2) = -0.4,  
  ecutwfc = $ecut,  
  ecutrho = $ecutrho,  
  occupations='smearing',  
  smearing='mv',  
  degauss=0.01  
  starting_ns_eigenvalue(3,1,1) = 0.0  
  starting_ns_eigenvalue(1,1,1) = 1.0  
  starting_ns_eigenvalue(2,1,1) = 1.0  
  starting_ns_eigenvalue(3,2,2) = 0.0  
  starting_ns_eigenvalue(1,2,2) = 1.0  
  starting_ns_eigenvalue(2,2,2) = 1.0  
 /  
. .
```

The new ground state

Input

```
&system
    ibrav= 0, celldm(1)=8.0, nat= 4, ntyp= 3,
    nspin = 2,
    starting_magnetization(1) = 0.4,
    starting_magnetization(2) = -0.4,
    ecutwfc = $ecut,
    ecutrho = $ecutrho,
    occupations='smearing',
    smearing='mv',
    degauss=0.01
    starting_ns_eigenvalue(3,1,1) = 0.0
    starting_ns_eigenvalue(1,1,1) = 1.0
    starting_ns_eigenvalue(2,1,1) = 1.0
    starting_ns_eigenvalue(3,2,2) = 0.0
    starting_ns_eigenvalue(1,2,2) = 1.0
    starting_ns_eigenvalue(2,2,2) = 1.0
/
.
```

Run scf
calculation



Output

```
===== HUBBARD OCCUPATIONS =====
----- ATOM 1 -----
Tr[ns( 1)] (up, down, total) = 3.99608 0.24396 4.24004
Atomic magnetic moment for atom 1 = 3.75212
SPIN 1
eigenvalues:
  0.046  0.983  0.983  0.992  0.992
eigenvectors (columns):
  0.000  0.075  0.011  0.643  0.762
  0.577  0.507 -0.637  0.021 -0.058
  0.577  0.298  0.758 -0.061  0.011
 -0.000  0.011 -0.075 -0.762  0.643
 -0.577  0.805  0.120 -0.040 -0.047
occupation matrix ns (before diag.):
  0.992 -0.000 -0.000  0.000 -0.001
 -0.000  0.671 -0.312 -0.000  0.312
 -0.000 -0.312  0.671  0.000  0.312
  0.000 -0.000  0.000  0.992 -0.000
 -0.001  0.312  0.312 -0.000  0.671
```

The new ground state

Input

```
&system
  ibrav= 0, celldm(1)=8.0, nat= 4, ntyp= 3,
  nspin = 2,
  starting_magnetization(1) = 0.4,
  starting_magnetization(2) = -0.4,
  ecutwfc = $ecut,
  ecutrho = $ecutrho,
  occupations='smearing',
  smearing='mv',
  degauss=0.01
  starting_ns_eigenvalue(3,1,1) = 0.0
  starting_ns_eigenvalue(1,1,1) = 1.0
  starting_ns_eigenvalue(2,1,1) = 1.0
  starting_ns_eigenvalue(3,2,2) = 0.0
  starting_ns_eigenvalue(1,2,2) = 1.0
  starting_ns_eigenvalue(2,2,2) = 1.0
/
.
```

Run scf
calculation

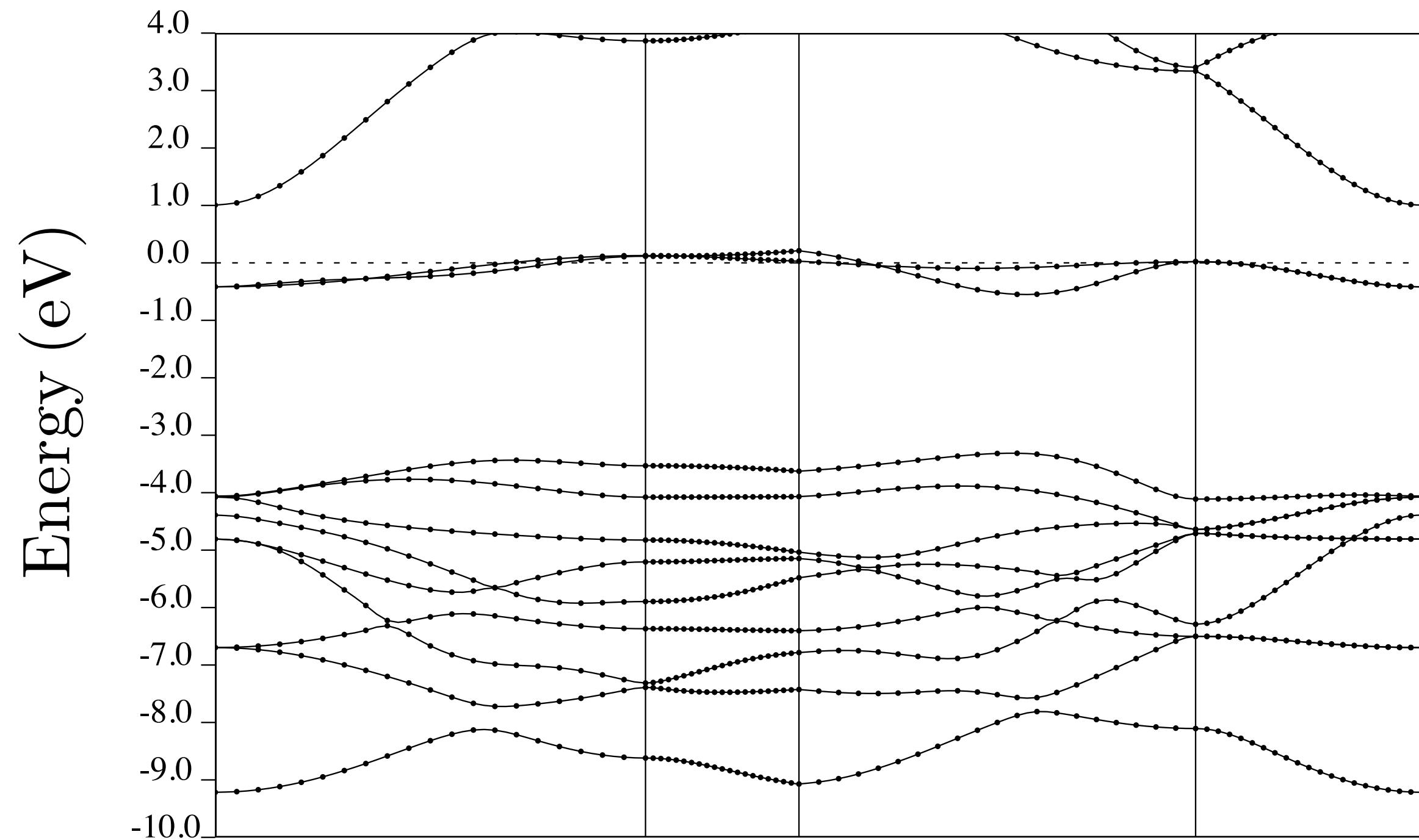
Output

```
===== HUBBARD OCCUPATIONS =====
----- ATOM 1 -----
Tr[ns( 1)] (up, down, total) = 3.99608 0.24396 4.24004
Atomic magnetic moment for atom 1 = 3.75212
SPIN 1
eigenvalues:
  0.046  0.983  0.983  0.992  0.992
eigenvectors (columns):
  0.000  0.075  0.011  0.643  0.762
  0.577  0.507 -0.637  0.021 -0.058
  0.577  0.298  0.758 -0.061  0.011
 -0.000  0.011 -0.075 -0.762  0.643
 -0.577  0.805  0.120 -0.040 -0.047
occupation matrix ns (before diag.):
  0.992 -0.000 -0.000  0.000 -0.001
 -0.000  0.671 -0.312 -0.000  0.312
 -0.000 -0.312  0.671  0.000  0.312
  0.000 -0.000  0.000  0.992 -0.000
 -0.001  0.312  0.312 -0.000  0.671
```

The occupation scheme suggested in input has been retained by the system.
Each Cr ion fully occupies 4 d states of its majority spin manifold.

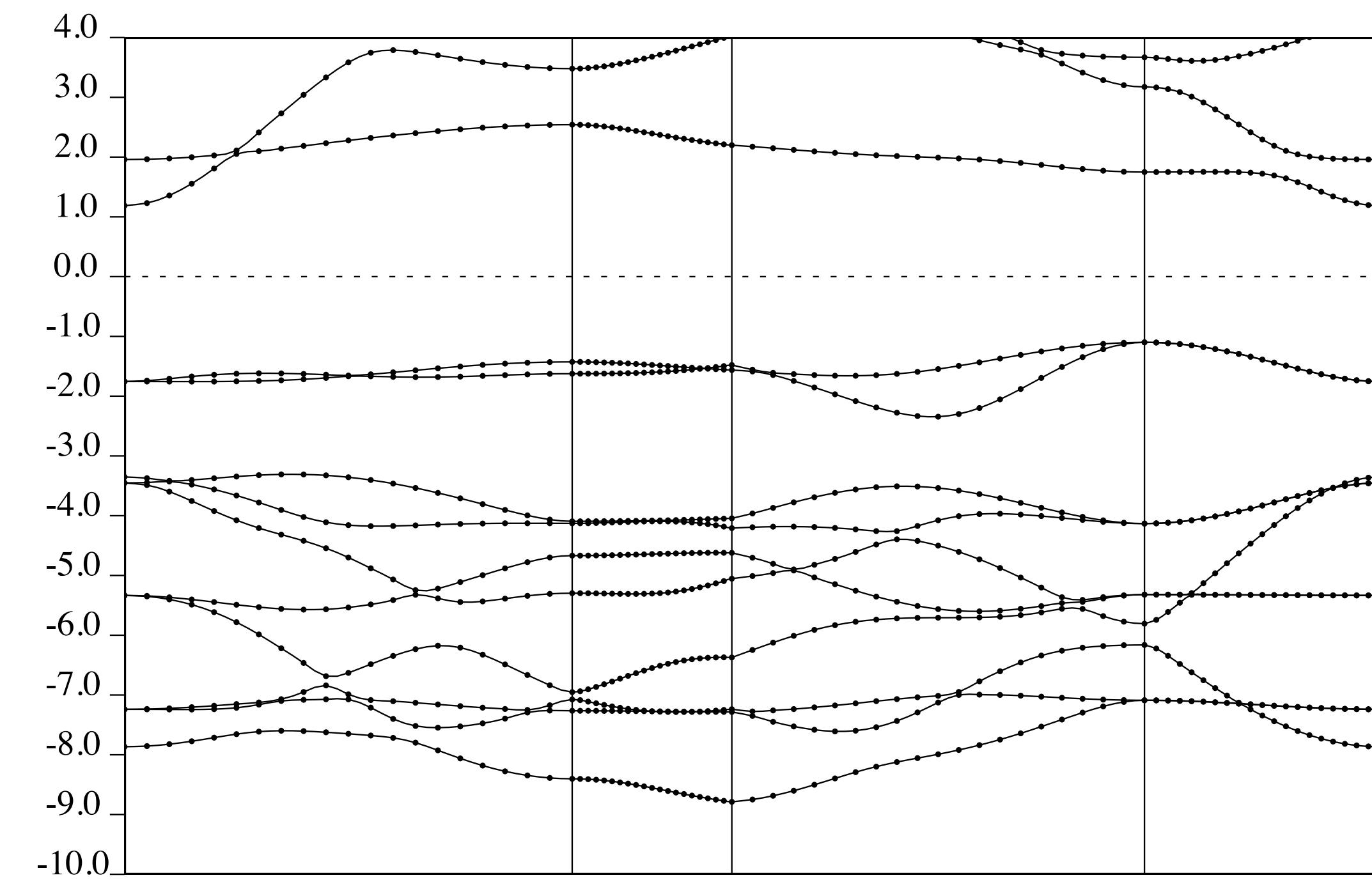
An insulating ground state

No adjustment



$$E_{TOT} = -432.63 \text{ Ry}$$

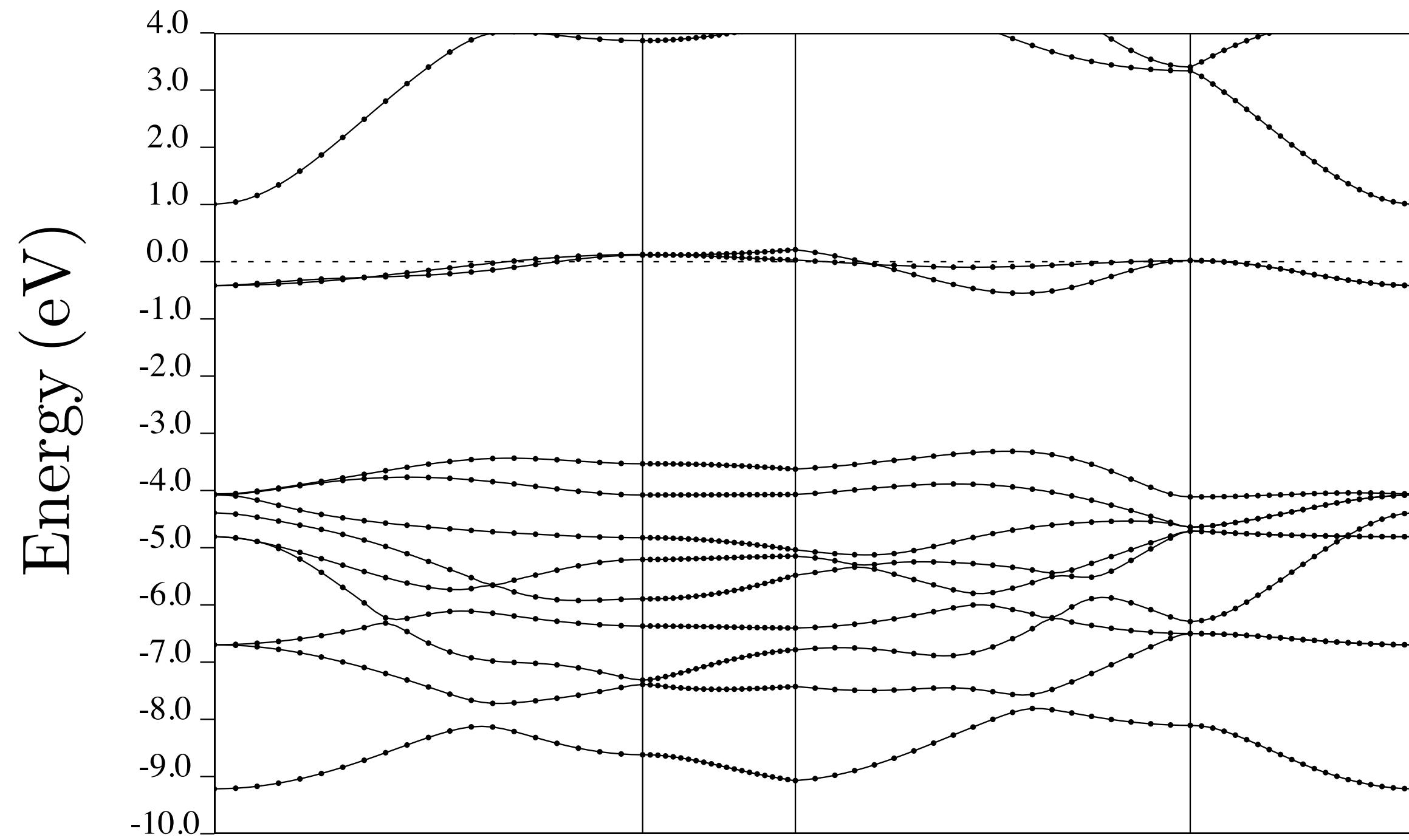
Adjusted occupations



$$E_{TOT} = -432.59 \text{ Ry}$$

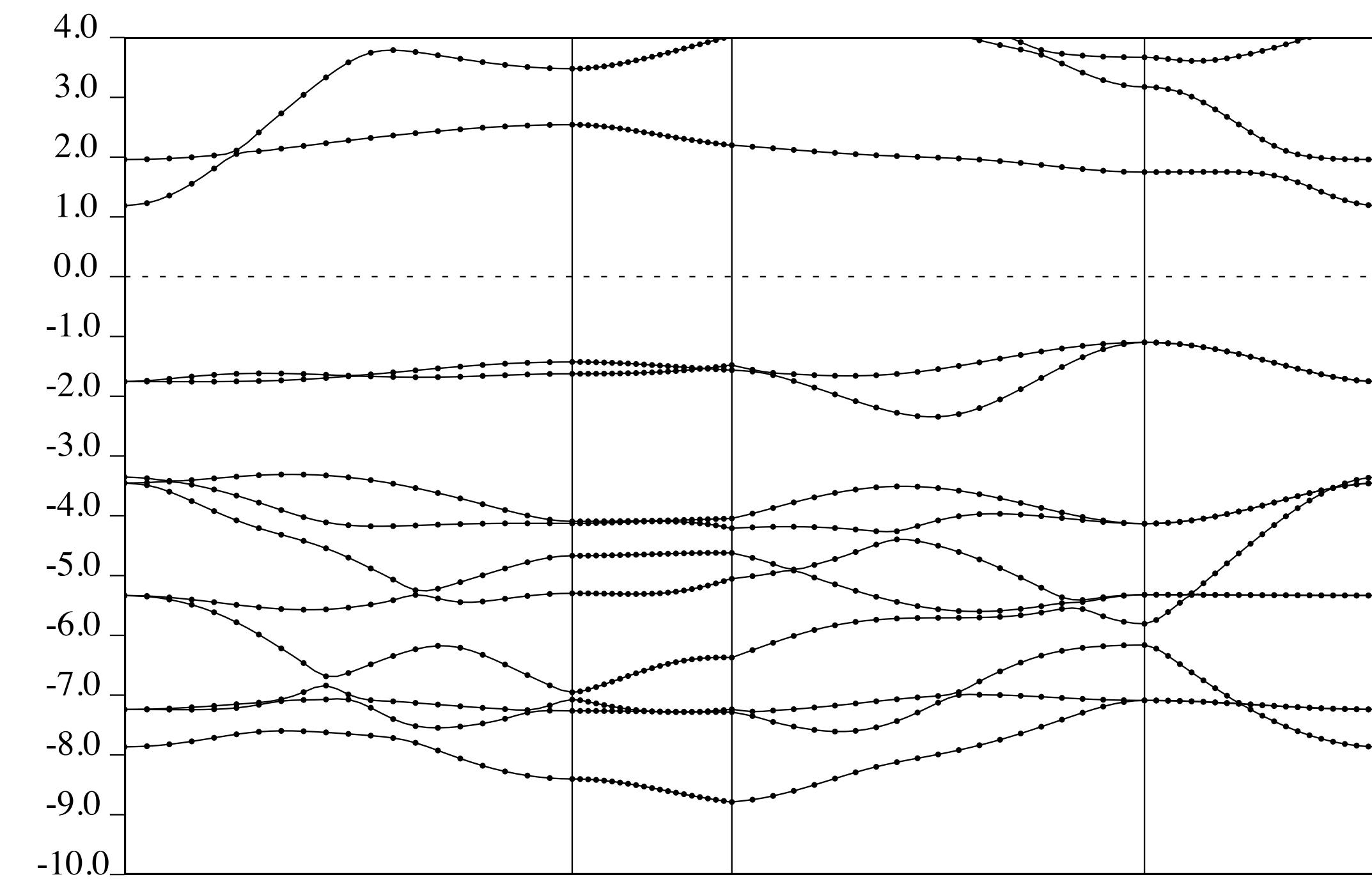
An insulating ground state

No adjustment



$$E_{\text{TOT}} = -432.63 \text{ Ry}$$

Adjusted occupations



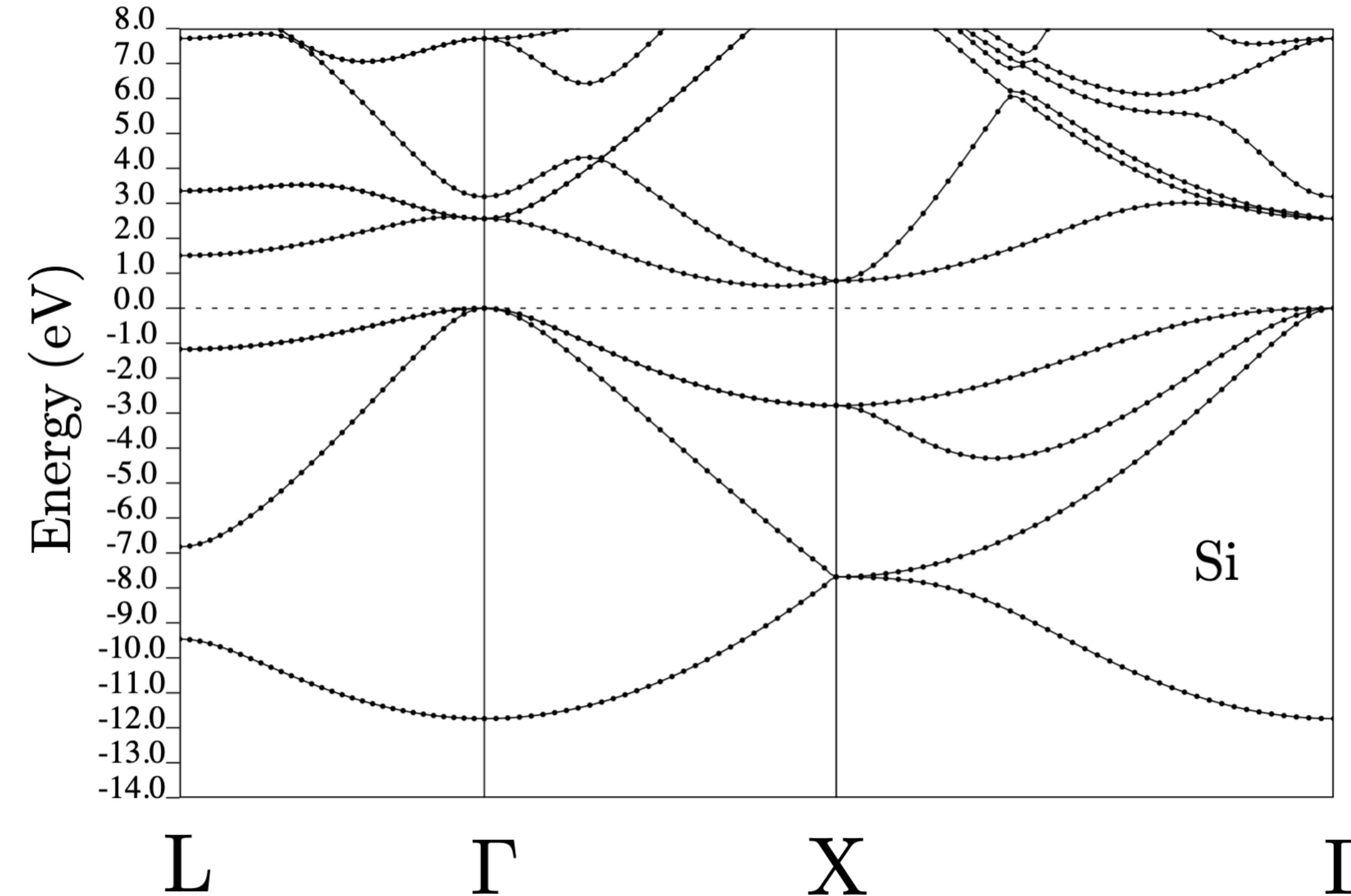
$$E_{\text{TOT}} = -432.59 \text{ Ry}$$

The insulating state is **metastable**. Perhaps a more stable insulating state can be found by using a supercell of lower symmetry.

Exercise 4

DFT+ U + V calculation of a band gap of Si

Band structure of Si (PBE)



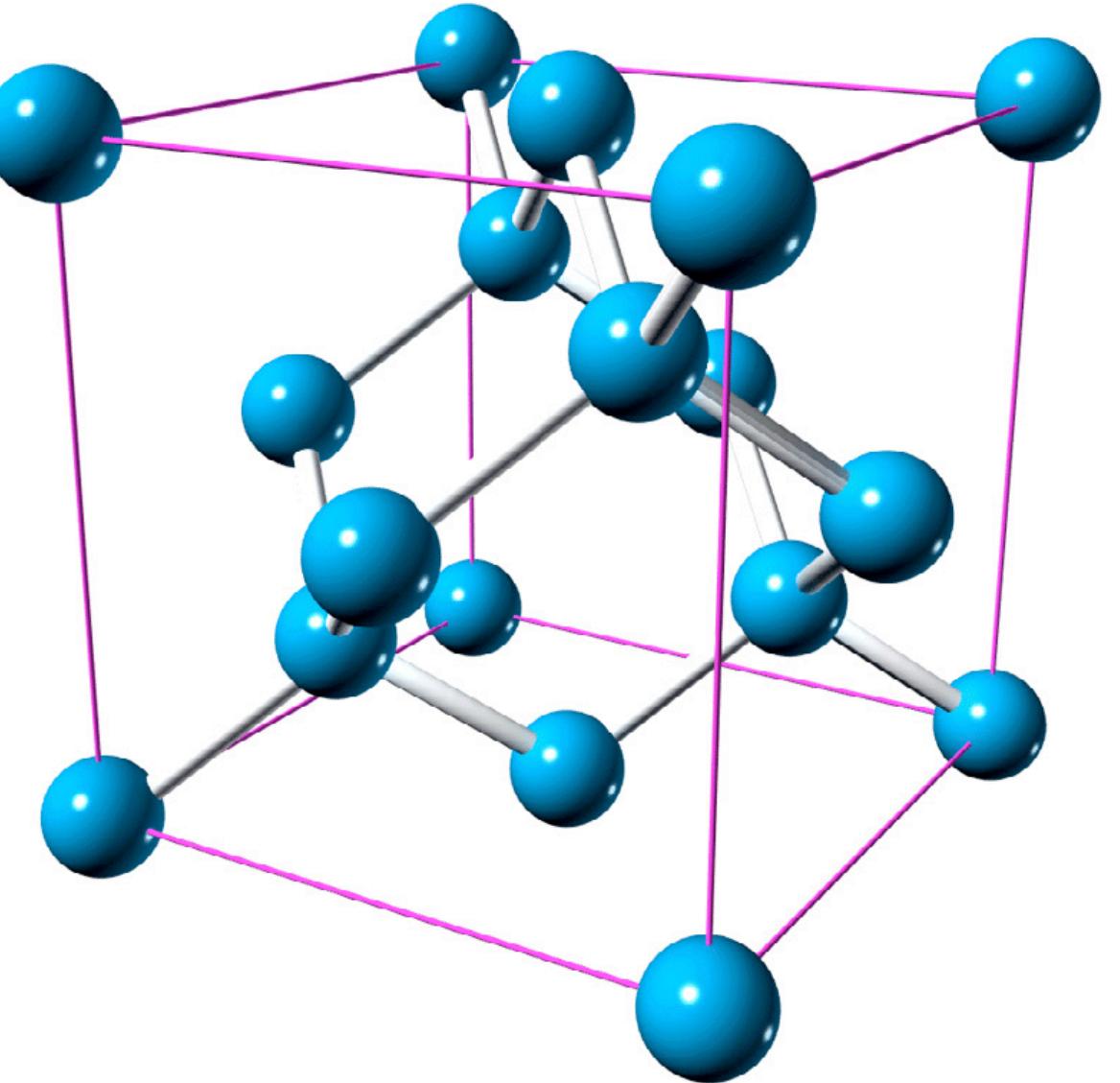
Approximate functionals correctly predict an insulating ground state but the energy band gap is underestimated.

This problem is typically tackled with hybrid functionals, meta-GGA, or self-interaction corrected approaches. Can we use DFT+U?

A simple DFT+U+V calculation: bulk Si

PBE+U

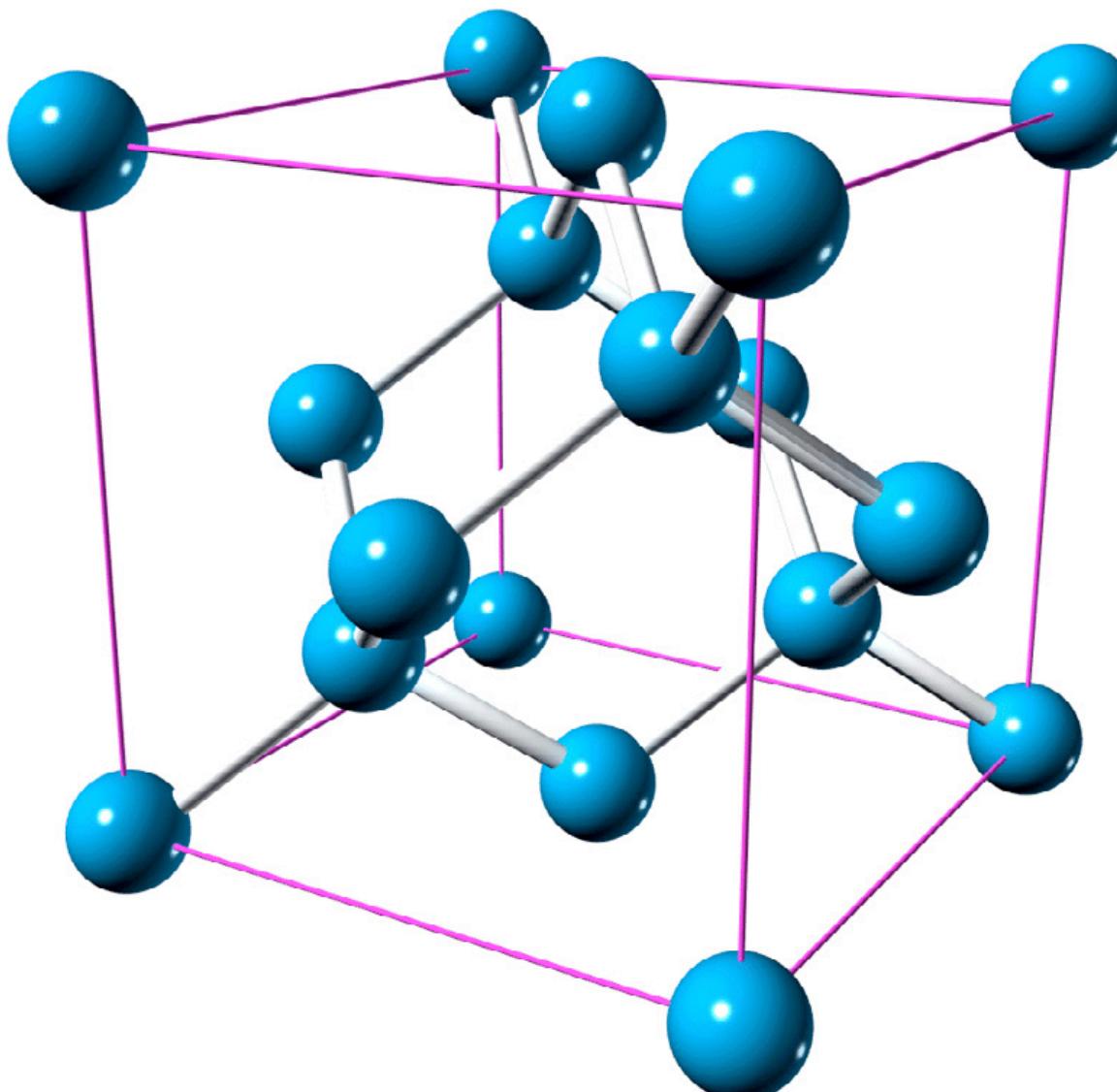
```
&control
  calculation = 'scf',
  verbosity = 'high',
  pseudo_dir = '.../.../files/pseudo'
 outdir='./tmp'
  restart_mode='from_scratch'
  verbosity = 'high',
  prefix='si',
/
&system
  ibrav= 2, celldm(1)=10.346, nat= 2, ntyp= 1,
  ecutwfc = 30,
  occupations='fixed',
  nbnd = 10,
/
&electrons
  mixing_beta = 0.3
  conv_thr = 1.0d-8,
/
ATOMIC_SPECIES
Si 1. Si.pbe-rrkj.UPF
ATOMIC_POSITIONS crystal
Si 0.0 0.0 0.0
Si 0.25 0.25 0.25
K_POINTS automatic
8 8 8 0 0 0
HUBBARD ortho-atomic
U Si-3p 1.42
```



A simple DFT+U+V calculation: bulk Si

PBE+U

```
&control
  calculation = 'scf',
  verbosity = 'high',
  pseudo_dir = '../files/pseudo'
  outdir='./tmp'
  restart_mode='from_scratch'
  verbosity = 'high',
  prefix='si',
/
&system
  ibrav= 2, celldm(1)=10.346, nat= 2, ntyp= 1,
  ecutwfc = 30,
  occupations='fixed',
  nbnd = 10,
/
&electrons
  mixing_beta = 0.3
  conv_thr = 1.0d-8,
/
ATOMIC_SPECIES
Si 1. Si.pbe-rrkj.UPF
ATOMIC_POSITIONS crystal
Si 0.0 0.0 0.0
Si 0.25 0.25 0.25
K_POINTS automatic
8 8 8 0 0 0
HUBBARD ortho-atomic
U Si-3p 1.42
```



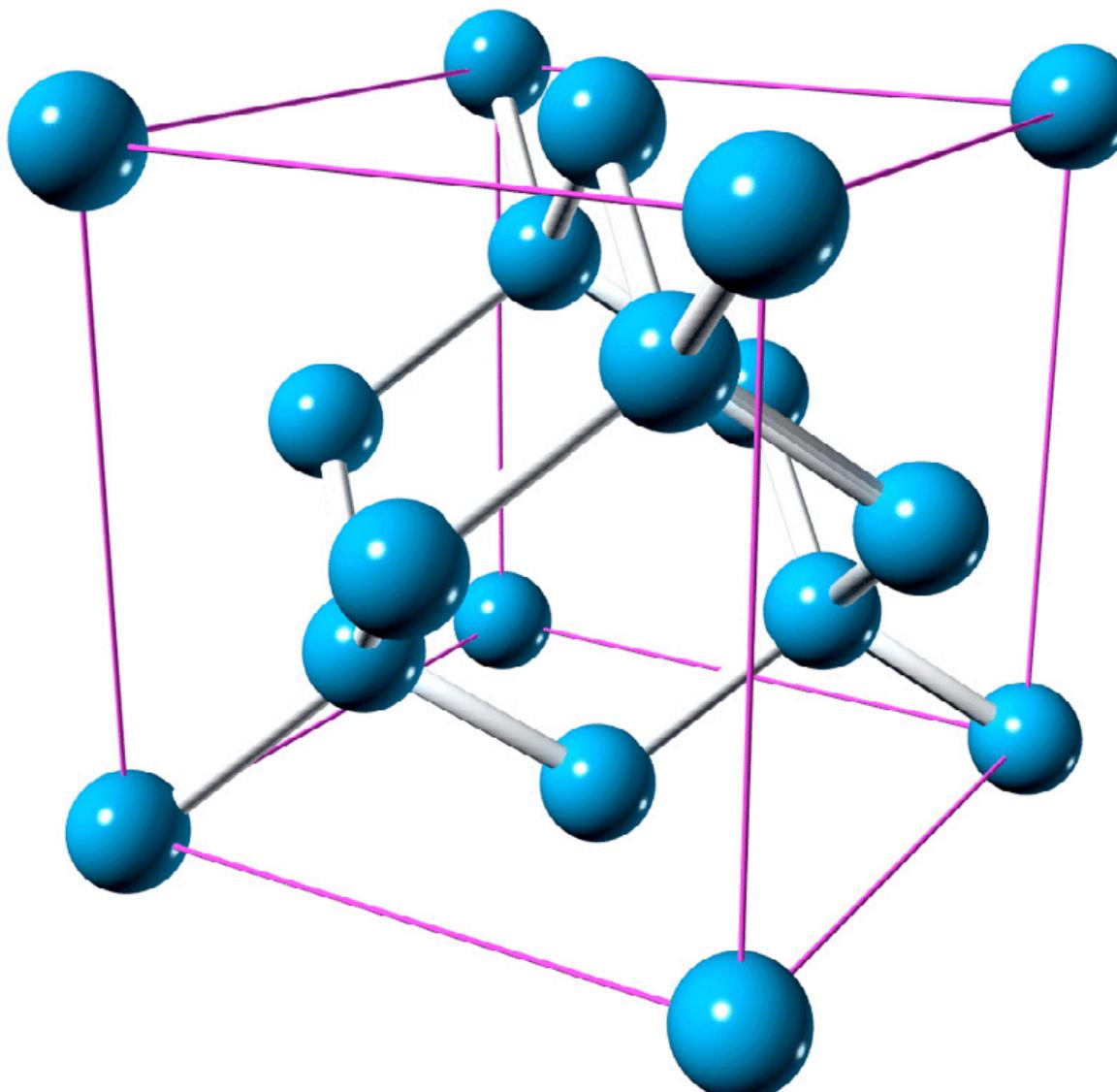
PBE+U+V

```
&control
  calculation = 'scf',
  verbosity = 'high',
  pseudo_dir = '../files/pseudo'
  outdir='./tmp'
  restart_mode='from_scratch'
  verbosity = 'high',
  prefix='si',
/
&system
  ibrav= 2, celldm(1)=10.346, nat= 2, ntyp= 2,
  ecutwfc = 30,
  occupations='fixed',
  nbnd = 10,
/
&electrons
  mixing_beta = 0.3
  conv_thr = 1.0d-8,
/
ATOMIC_SPECIES
Si 1. Si.pbe-rrkj.UPF
ATOMIC_POSITIONS crystal
Si 0.0 0.0 0.0
Si 0.25 0.25 0.25
K_POINTS automatic
8 8 8 0 0 0
HUBBARD ortho-atomic
V Si-3p Si-3p 1 1 1.42
V Si-3p Si-3p 1 2 0.25
```

A simple DFT+U+V calculation: bulk Si

PBE+U

```
&control
  calculation = 'scf',
  verbosity = 'high',
  pseudo_dir = '../files/pseudo'
  outdir='./tmp'
  restart_mode='from_scratch'
  verbosity = 'high',
  prefix='si',
/
&system
  ibrav= 2, celldm(1)=10.346, nat= 2, ntyp= 1,
  ecutwfc = 30,
  occupations='fixed',
  nbnd = 10,
/
&electrons
  mixing_beta = 0.3
  conv_thr = 1.0d-8,
/
ATOMIC_SPECIES
Si 1. Si.pbe-rrkj.UPF
ATOMIC_POSITIONS crystal
Si 0.0 0.0 0.0
Si 0.25 0.25 0.25
K_POINTS automatic
8 8 8 0 0 0
HUBBARD ortho-atomic
V Si-3p Si-3p 1 1 1.42
V Si-3p Si-3p 1 2 0.25
on-site: Si 3p states
inter-site: Si 3p - Si 3p states
U Si-3p 1.42
```



PBE+U+V

```
&control
  calculation = 'scf',
  verbosity = 'high',
  pseudo_dir = '../files/pseudo'
  outdir='./tmp'
  restart_mode='from_scratch'
  verbosity = 'high',
  prefix='si',
/
&system
  ibrav= 2, celldm(1)=10.346, nat= 2, ntyp= 1,
  ecutwfc = 30,
  occupations='fixed',
  nbnd = 10,
/
&electrons
  mixing_beta = 0.3
  conv_thr = 1.0d-8,
/
ATOMIC_SPECIES
Si 1. Si.pbe-rrkj.UPF
ATOMIC_POSITIONS crystal
Si 0.0 0.0 0.0
Si 0.25 0.25 0.25
K_POINTS automatic
8 8 8 0 0 0
HUBBARD ortho-atomic
V Si-3p Si-3p 1 1 1.42
V Si-3p Si-3p 1 2 0.25
```

Input file Si.scf.in

```
&control
  calculation = 'scf',
  verbosity = 'high',
  pseudo_dir = '../..../files/pseudo'
  outdir='./tmp'
  restart_mode='from_scratch'
  verbosity = 'high',
  prefix='Si',
/
&system
  ibrav = 2,
  celldm(1) = 10.346,
  nat = 2,
  ntyp = 1,
  ecutwfc = 30,
  occupations = 'fixed',
  nbnd = 10,
/
&electrons
  mixing_beta = 0.3
  conv_thr = 1.0d-8,
/
ATOMIC_SPECIES
  Si 1. Si.pbe-rrkj.UPF
ATOMIC_POSITIONS crystal
  Si 0.0 0.0 0.0
  Si 0.25 0.25 0.25
K_POINTS automatic
  8 8 8 0 0 0
HUBBARD ortho-atomic
  V Si-3p Si-3p 1 1 1.42
  V Si-3p Si-3p 1 2 0.25
```

Input file Si.bands.in

```
&control
  calculation = 'bands',
  verbosity = 'high',
  pseudo_dir = '../..../files/pseudo'
  outdir='./tmp'
  restart_mode='from_scratch'
  verbosity = 'high',
  prefix='Si',
/
&system
  ibrav = 2,
  celldm(1) = 10.346,
  nat = 2,
  ntyp = 1,
  ecutwfc = 30,
  occupations = 'fixed',
  nbnd = 10,
/
&electrons
  mixing_beta = 0.3
  diagonalization = 'cg'
  conv_thr = 1.0d-8,
/
ATOMIC_SPECIES
  Si 1. Si.pbe-rrkj.UPF
ATOMIC_POSITIONS crystal
  Si 0.0 0.0 0.0
  Si 0.25 0.25 0.25
K_POINTS crystal_b
  6
  0.5 0.5 0.5 30
  0.0 0.0 0.0 30
  0.5 0.5 0.0 0
  0.5 0.5 1.0 10
  0.375 0.375 0.75 30
  0.0 0.0 0.0 1
HUBBARD ortho-atomic
  V Si-3p Si-3p 1 1 1.42
  V Si-3p Si-3p 1 2 0.25
```

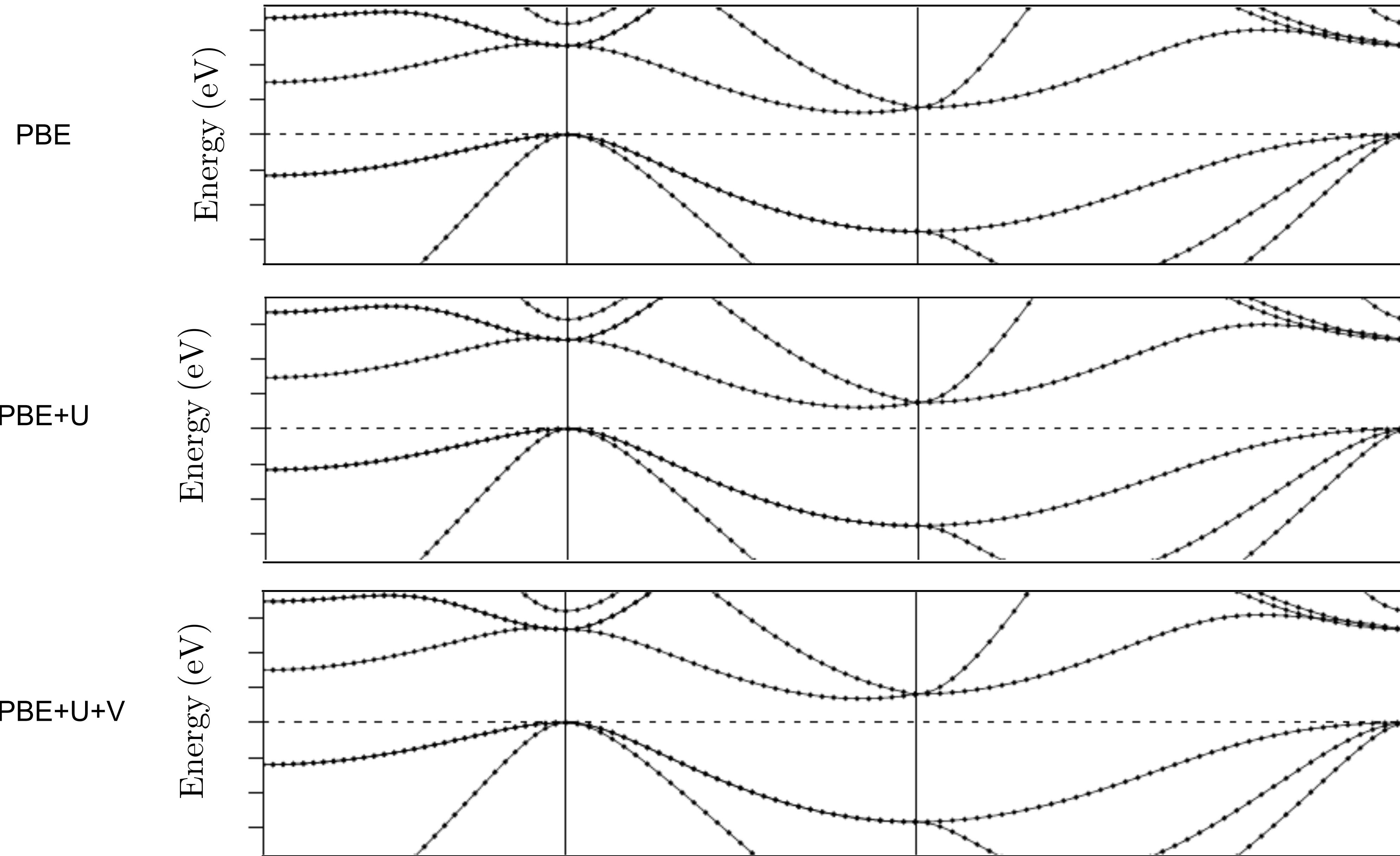
Input file Si.bands.pp.in

```
&bands
  prefix = 'Si',
  outdir = './tmp'
  filband = 'Si_bands.dat'
/
```

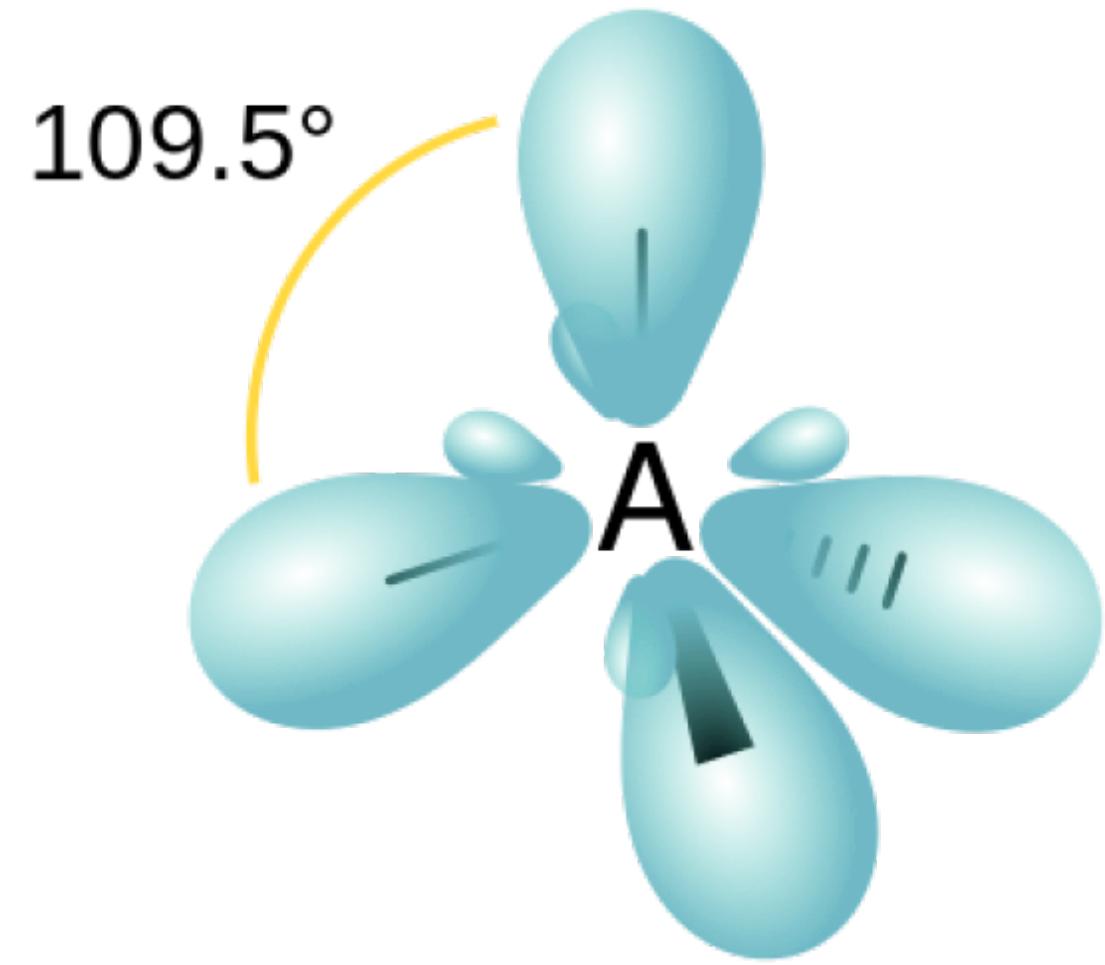
Run the calculations

```
pw.x < Si.scf.in |tee Si.scf.out  
pw.x < Si.bands.in |tee Si.bands.out  
bands.x < Si.bands.pp.in |tee Si.bands.pp.out  
plotband.x < Si.plotband.in |tee Si.plotband.out  
evince Si_bands.ps
```

The band gap of Si

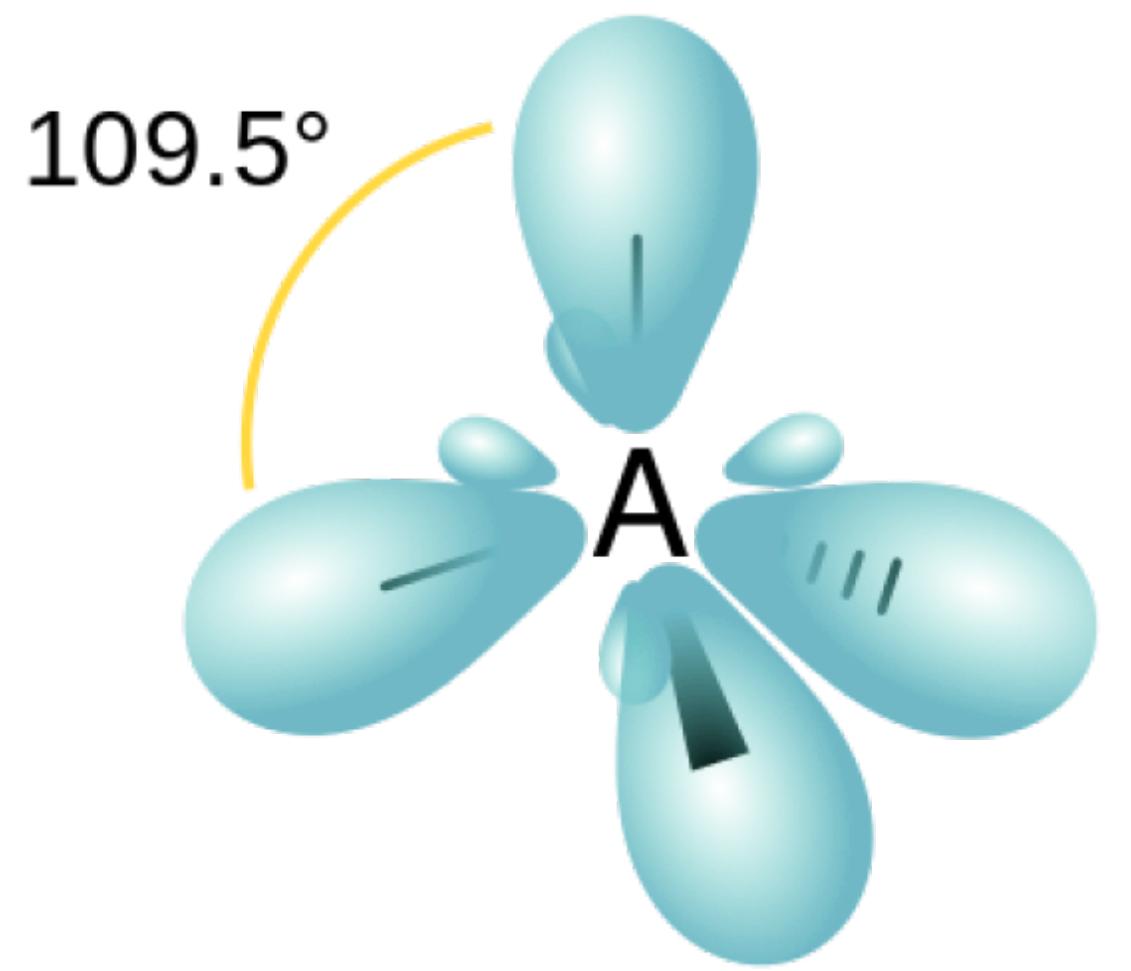


On-site V: sp³ hybridisation



s and p states should be treated similarly

On-site V: sp^3 hybridisation

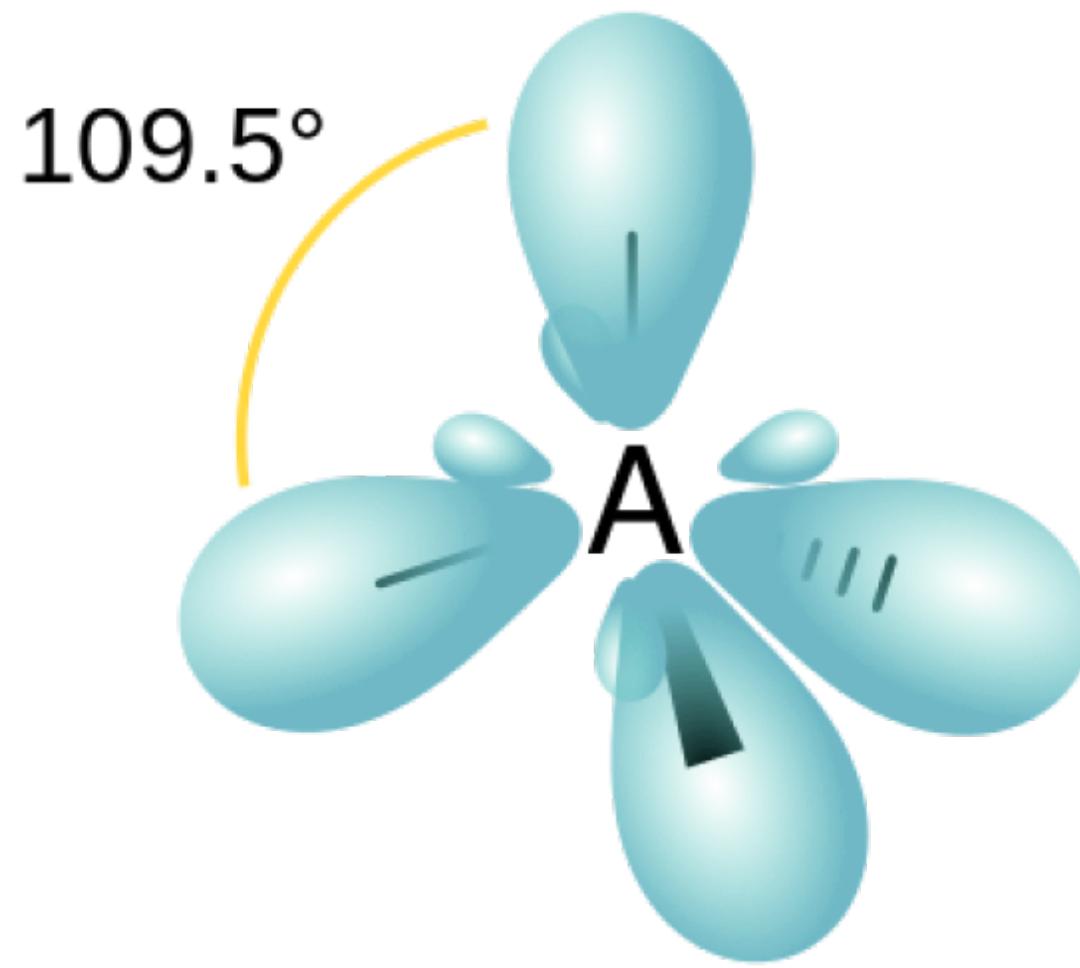


s and p states should be treated similarly

HUBBARD ortho-atomic

V Si-3p	Si-3p	1	1	1.42	on-site: Si 3p states
V Si-3p	Si-3s	1	1	1.42	
V Si-3s	Si-3s	1	1	1.42	
V Si-3s	Si-3p	1	1	1.42	
V Si-3p	Si-3p	1	2	0.25	inter-site: Si 3p - Si 3p states
V Si-3p	Si-3s	1	2	0.25	
V Si-3s	Si-3s	1	2	0.25	
V Si-3s	Si-3p	1	2	0.25	

On-site V: sp^3 hybridisation



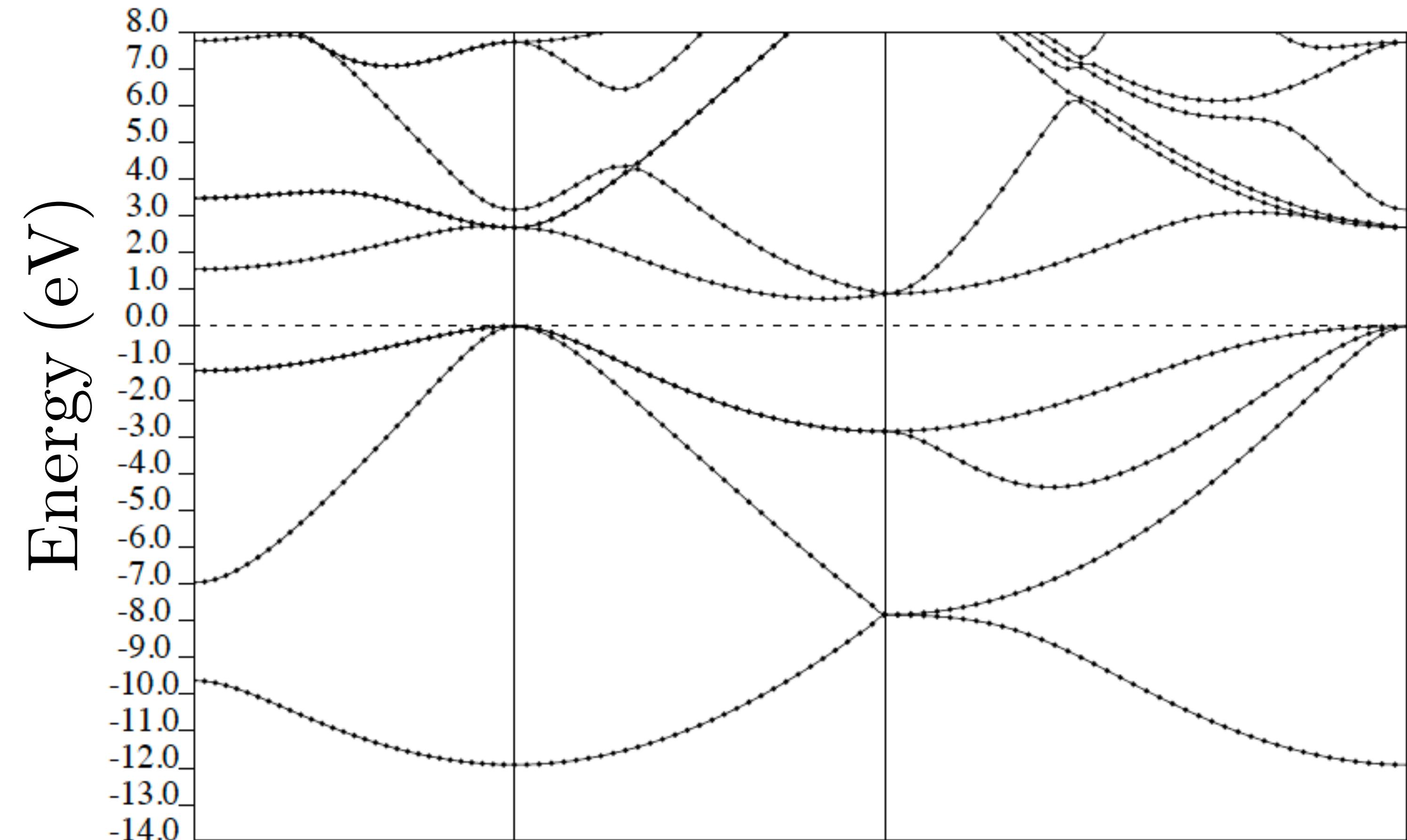
s and p states should be treated similarly

HUBBARD ortho-atomic

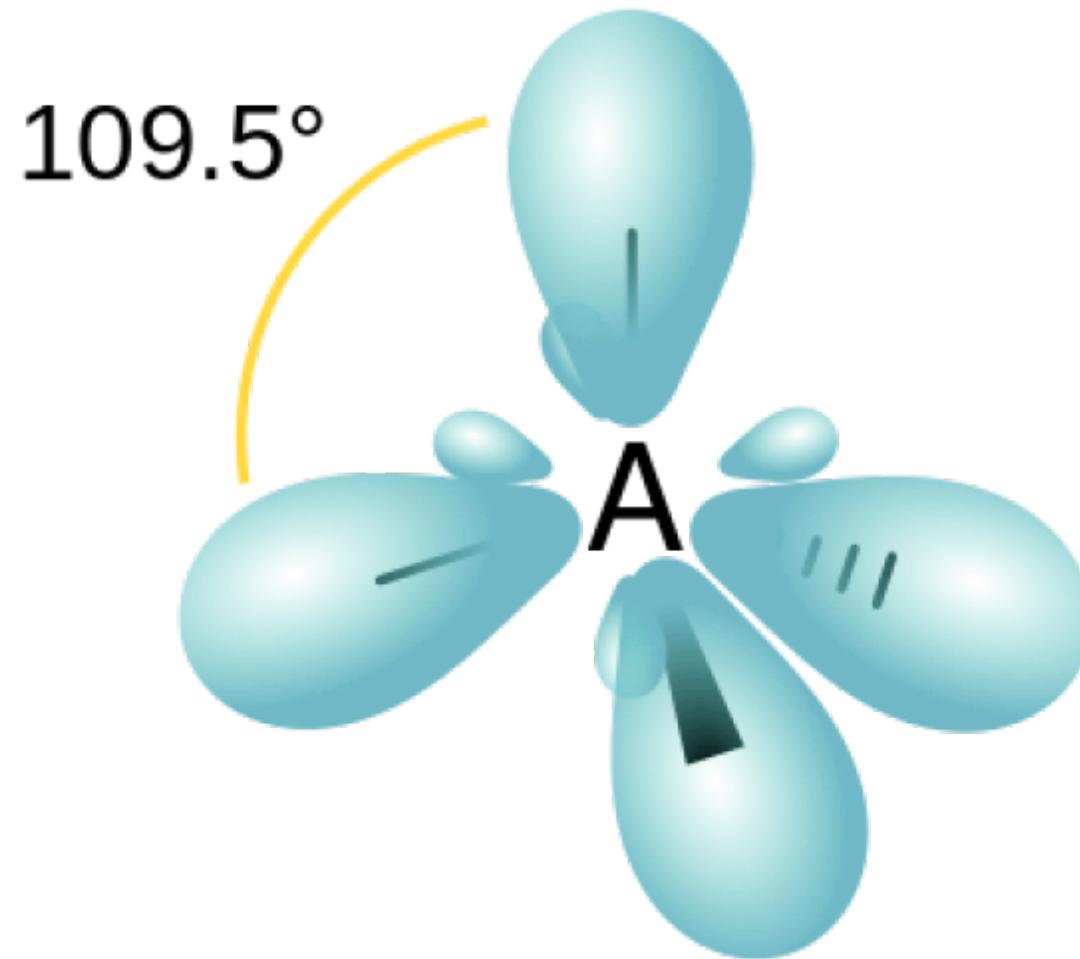
V Si-3p	Si-3p	1	1	1.42
V Si-3p	Si-3s	1	1	1.42
V Si-3s	Si-3s	1	1	1.42
V Si-3s	Si-3p	1	1	1.42
V Si-3p	Si-3p	1	2	0.25
V Si-3p	Si-3s	1	2	0.25
V Si-3s	Si-3s	1	2	0.25
V Si-3s	Si-3p	1	2	0.25

on-site: Si 3p states

inter-site: Si 3p - Si 3p states



On-site V: sp^3 hybridisation



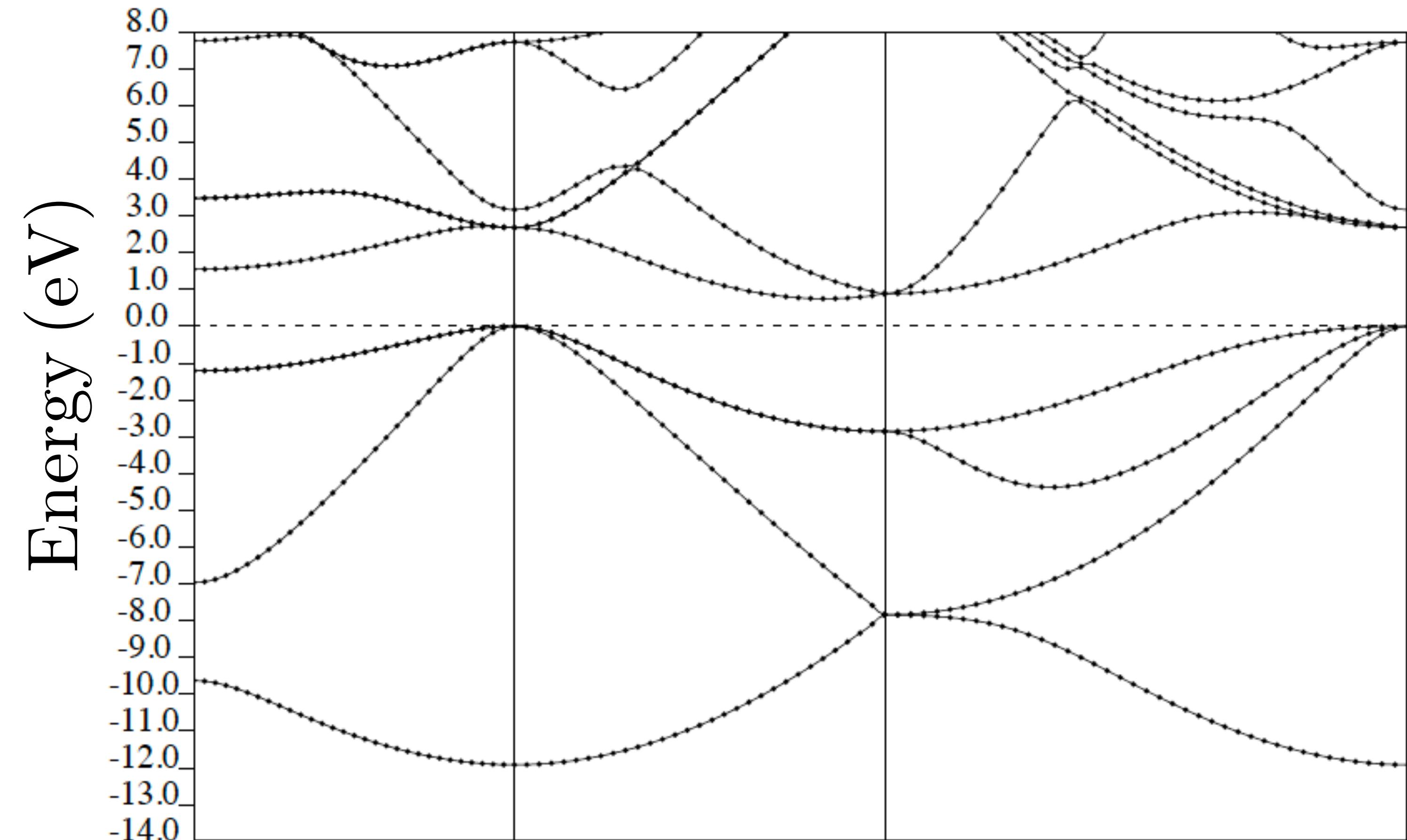
s and p states should be treated similarly

HUBBARD ortho-atomic

V Si-3p	Si-3p	1	1	1.42
V Si-3p	Si-3s	1	1	1.42
V Si-3s	Si-3s	1	1	1.42
V Si-3s	Si-3p	1	1	1.42
V Si-3p	Si-3p	1	2	0.25
V Si-3p	Si-3s	1	2	0.25
V Si-3s	Si-3s	1	2	0.25
V Si-3s	Si-3p	1	2	0.25

on-site: Si 3p states

inter-site: Si 3p - Si 3p states



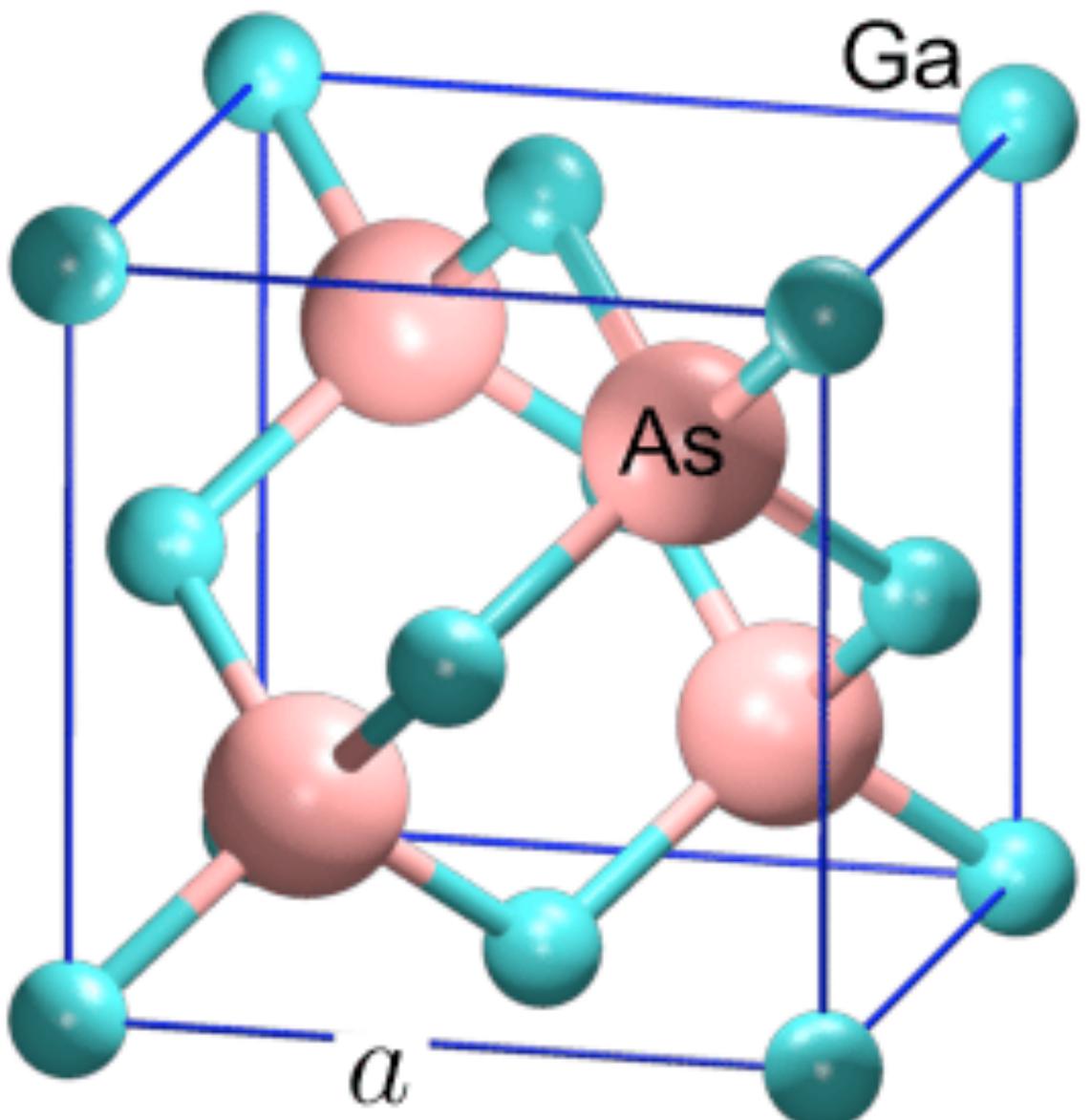
Differences are hardly visible (although with on-site V the gap opens a bit more). In order to get more accurate results U and V should be determined consistently with the crystal structure

GaAs

```

&control
  calculation = 'scf',
  verbosity = 'high',
  pseudo_dir = '$PSEUDODIR'
  outdir='$tmpdir'
  restart_mode='from_scratch'
  verbosity = 'high',
  wf_collect = .true.
  prefix='gaas',
/
&system
  ibrav= 2, celldm(1)=10.68, nat= 2, ntyp= 2,
  ecutwfc = $ecut,
  ecutrho = $ecutrho,
  occupations='smearing',
  smearing='gauss',
  degauss=0.01
  nbnd = 14,
/
&electrons
  mixing_beta = 0.2
  conv_thr = 1.0d-10,
/
ATOMIC_SPECIES
Ga 69.723 Ga.pbesol-dn-rrkjus_psl.1.0.0.UPF
As 74.9216 As.pbesol-n-rrkjus_psl.0.2.UPF
ATOMIC_POSITIONS crystal
  Ga      0.00      0.00      0.00
  As      0.25      0.25      0.25
K_POINTS automatic
6 6 6 0 0 0
HUBBARD ortho-atomic
U Ga-4p 2.0
U As-4p 2.5

```



HUBBARD ortho-atomic

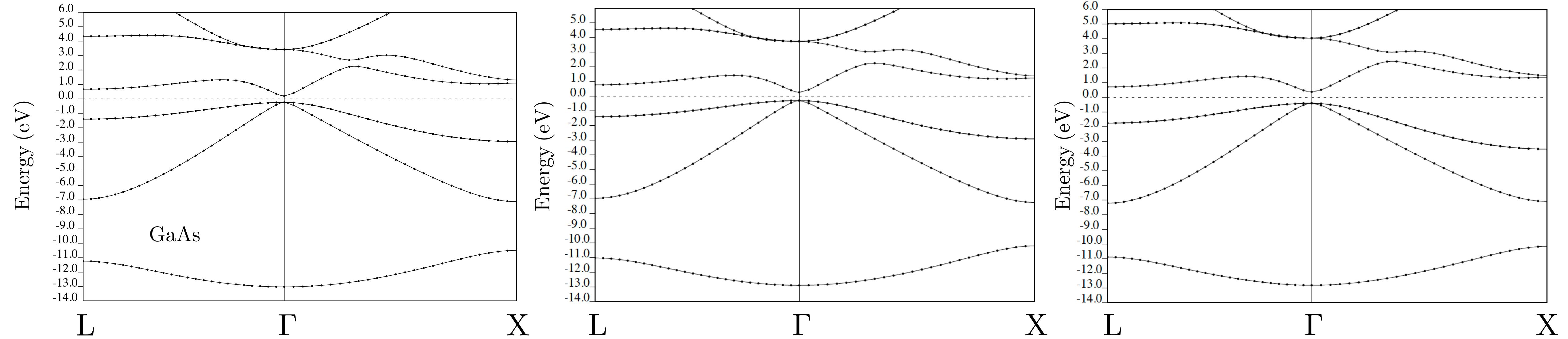
V Ga-4p	Ga-4p	1	1	2.00	on-site: Ga 4p states
V As-4p	As-4p	2	2	2.50	on-site: As 4p states
V Ga-4p	As-4p	1	2	1.5	inter-site: Ga 4p - As 4p states

```

&control
  calculation = 'scf',
  verbosity = 'high',
  pseudo_dir = '$PSEUDODIR'
  outdir='$tmpdir'
  restart_mode='from_scratch'
  verbosity = 'high',
  wf_collect = .true.
  prefix='gaas',
/
&system
  ibrav= 2, celldm(1)=10.68, nat= 2, ntyp= 2,
  ecutwfc = $ecut,
  ecutrho = $ecutrho,
  occupations='smearing',
  smearing='gauss',
  degauss=0.01
  nbnd = 14,
/
&electrons
  mixing_beta = 0.2
  conv_thr = 1.0d-10,
/
ATOMIC_SPECIES
Ga 69.723 Ga.pbesol-dn-rrkjus_psl.1.0.0.UPF
As 74.9216 As.pbesol-n-rrkjus_psl.0.2.UPF
ATOMIC_POSITIONS crystal
  Ga      0.00      0.00      0.00
  As      0.25      0.25      0.25
K_POINTS automatic
6 6 6 0 0 0
HUBBARD ortho-atomic
V Ga-4p Ga-4p 1 1 2.00
V As-4p As-4p 2 2 2.50
V Ga-4p As-4p 1 2 1.5

```

GaAs: DFT vs DFT+U vs DFT+U+V

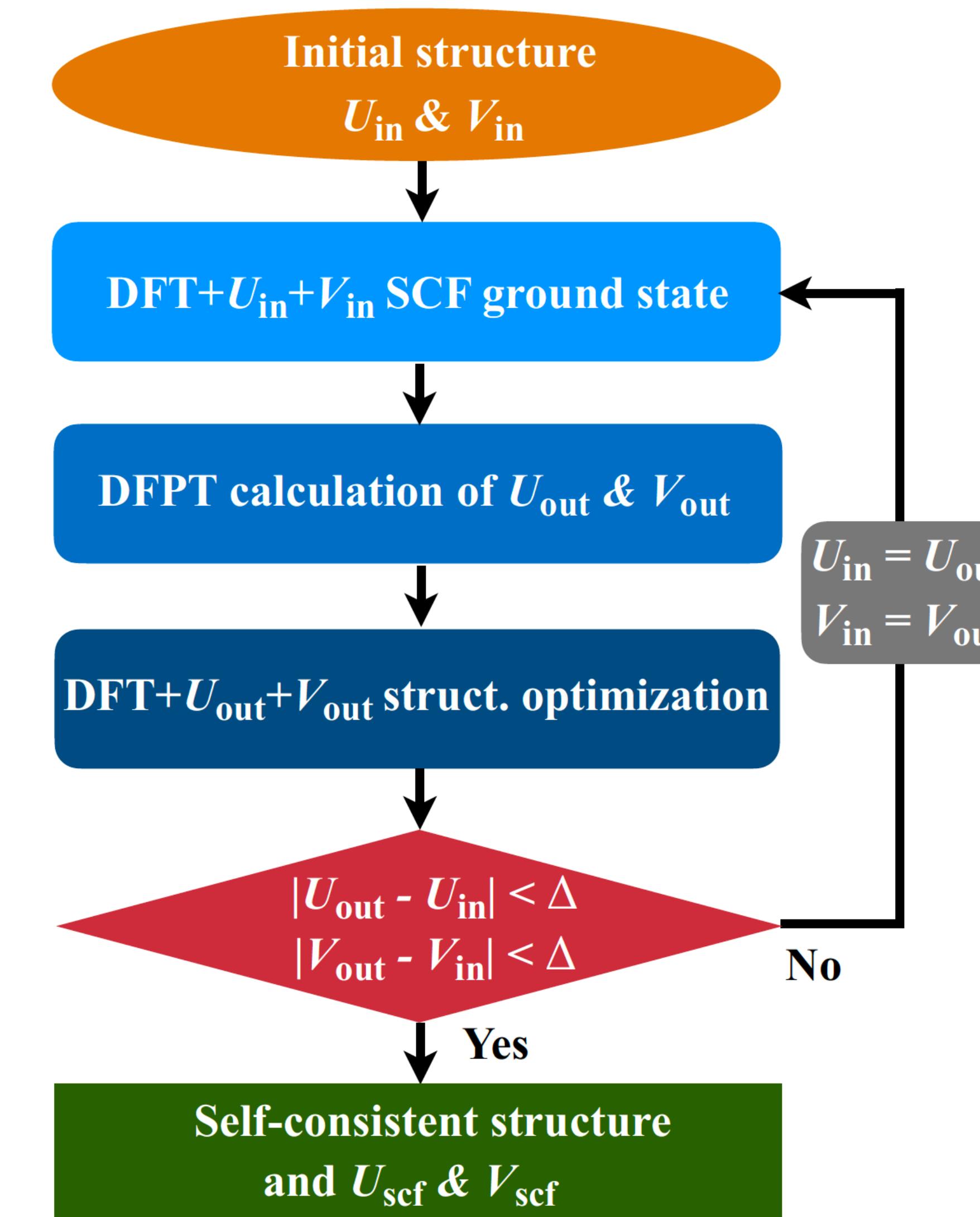


PBE+U+V achieves a slightly wider gap. On site V and self-consistency are also important for GaAs.

Exercise 5

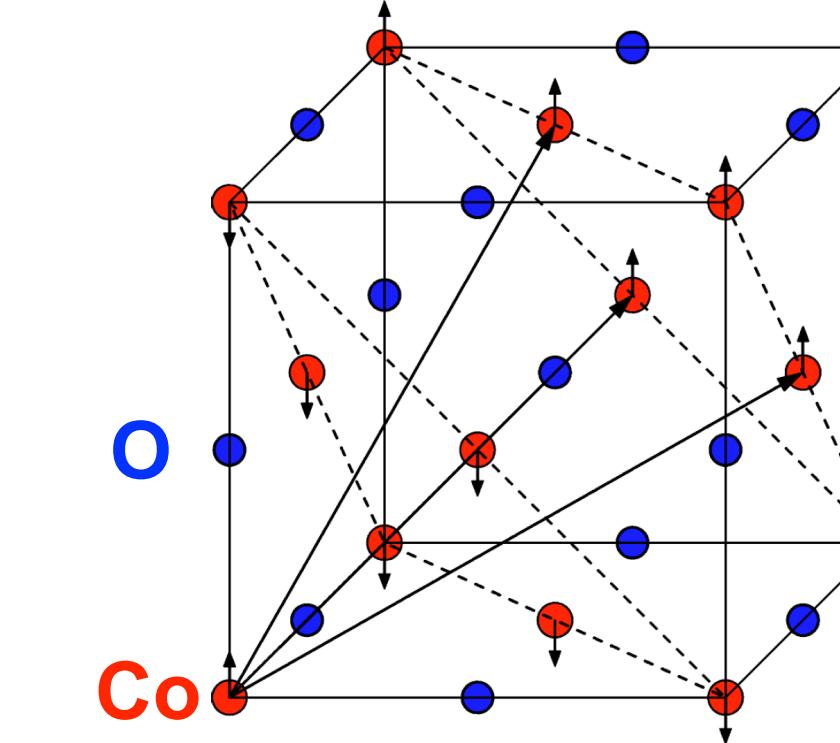
**Self-consistent calculation of the Hubbard U
parameter for Co-3d states in CoO**

Self-consistent calculation of Hubbard parameters



Input file CoO.scf.in

```
&control
  calculation='scf'
  restart_mode='from_scratch',
  prefix='CoO'
  pseudo_dir = '../files/pseudo'
 outdir='./tmp'
  verbosity='high'
/
&system
  ibrav = 0,
  celldm(1) = 8.00,
  nat = 4,
  ntyp = 3,
  ecutwfc = 35.0
  ecutrho = 280.0
  nspin = 2
  starting_magnetization(1) =  0.5,
  starting_magnetization(2) = -0.5,
  occupations = 'smearing',
  smearing = 'mv',
  degauss = 0.02
/
&electrons
  conv_thr = 1.d-10
/
ATOMIC_SPECIES
  Co1 58.933194 co_pbesol_v1.2.uspp.F.UPF
  Co2 58.933194 co_pbesol_v1.2.uspp.F.UPF
  O 15.999 O.pbesol-n-kjpaw_psl.0.1.UPF
ATOMIC_POSITIONS {crystal}
  Co1    0.0000000    0.0000000    0.0000000
  Co2    0.5000000    0.5000000    0.5000000
  O     0.2500000    0.2500000    0.2500000
  O     0.7500000    0.7500000    0.7500000
CELL_PARAMETERS {alat}
  0.570726115  0.570726115  1.031099100
  0.570726115  1.031099100  0.570726115
  1.031099100  0.570726115  0.570726115
K_POINTS {automatic}
  3 3 3 0 0 0
HUBBARD {ortho-atomic}
  U Co1-3d 0.0001
  U Co2-3d 0.0001
```



We treat the system as a metal (i.e. with smearing) because we perform a spin-polarized calculation (fractional occupations) and because the system is indeed a metal at the DFT level

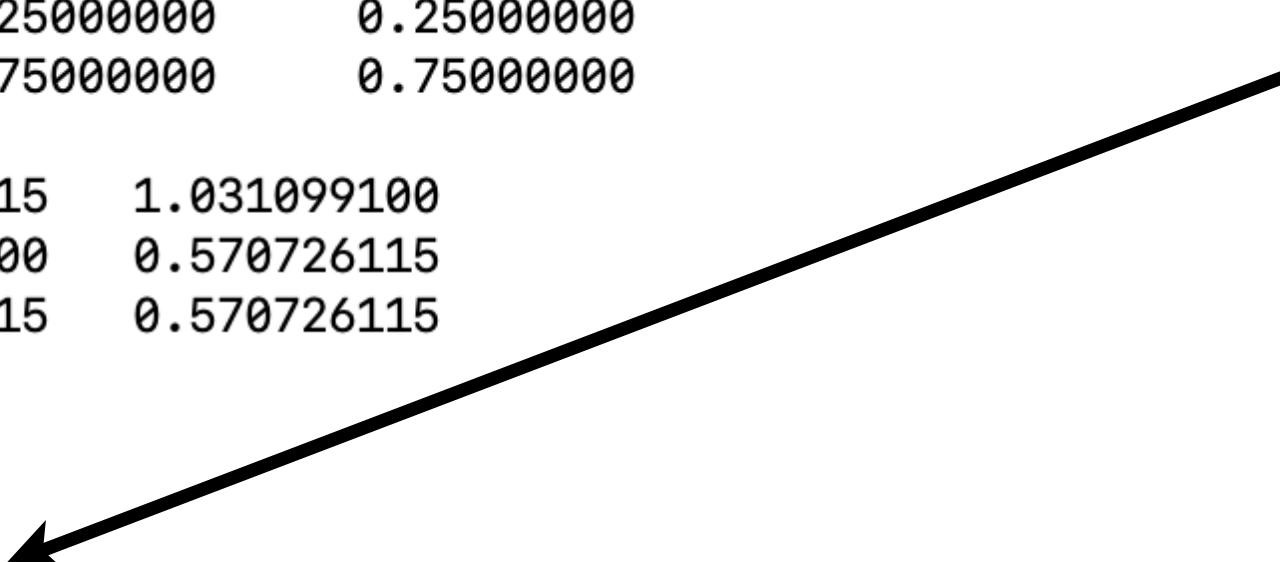
HUBBARD {ortho-atomic}

U Co1-3d 0.0001

U Co2-3d 0.0001



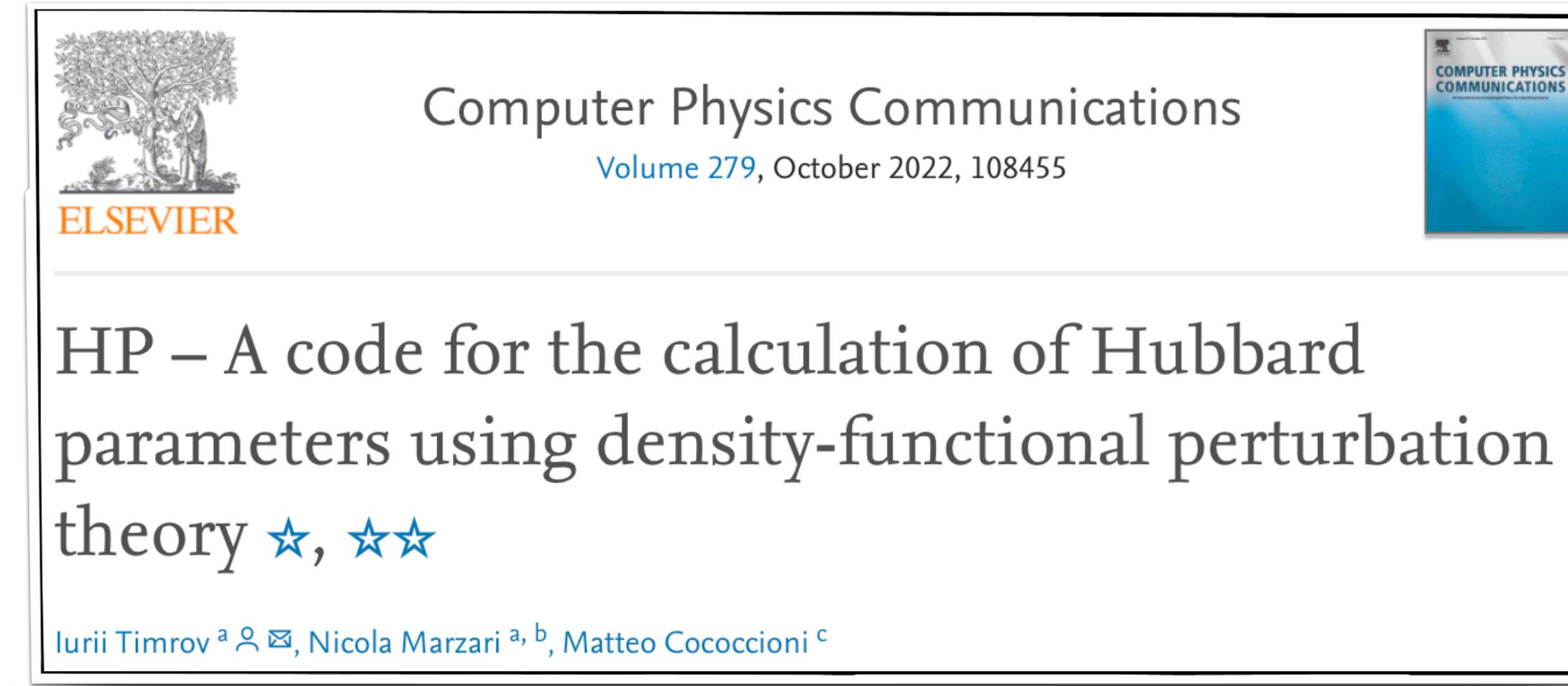
We set some small initial value just to activate the Hubbard machinery in the code



Input file CoO.hp.in

```
&inputhp
```

```
prefix = 'CoO'  
outdir = './tmp' ← The same as in the CoO.scf.in input  
nq1 = 2, nq2 = 2, nq3 = 2 ← Size of the q points mesh  
conv_thr_chi = 1.d-6 ← Convergence threshold for computing the self-consistent  
/ response matrix  $\chi$  (in eV-1)
```

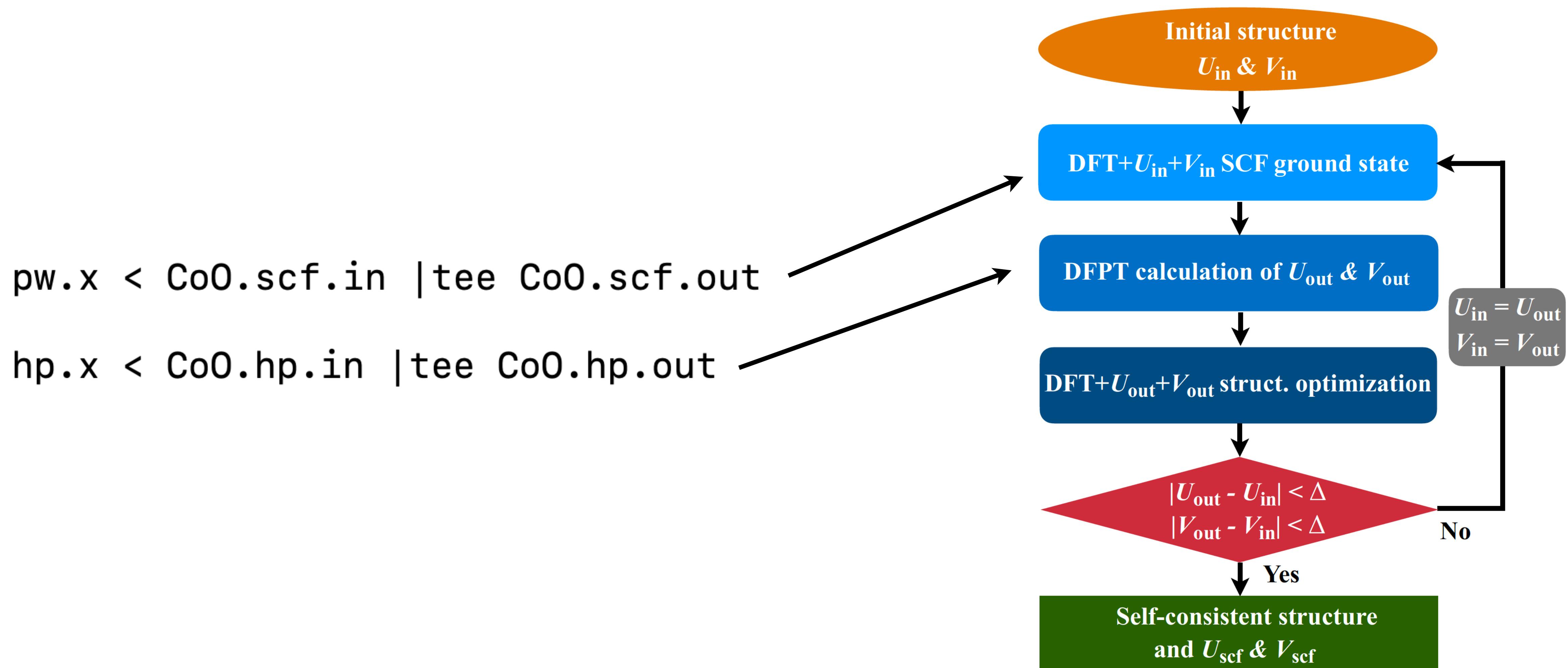


Important notice: The calculation of the Hubbard U parameter must be converged (as any other quantity of interest)!

Hubbard U must be converged with respect to the kinetic-energy cutoff (ecutwfc and ecutrho), **k** points mesh, and **q** points mesh.

For more details see: *I. Timrov, N. Marzari, M. Cococcioni, Phys. Rev. B 98, 085127 (2018)*.

Run the calculations



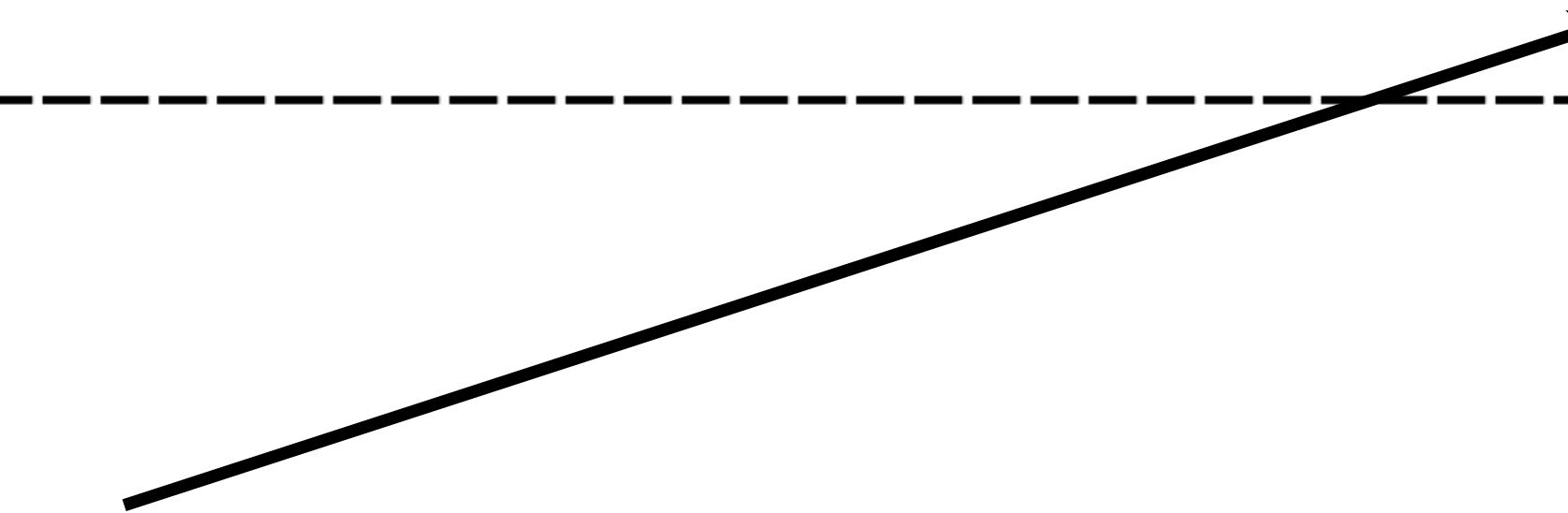
Output file CoO.Hubbard_parameters.dat

=====

Hubbard U parameters:

site	n.	type	label	spin	new_type	new_label	Hubbard U (eV)
1		1	Co1	1	1	Co1	6.7553
2		2	Co2	-1	1	Co1	6.7553

=====



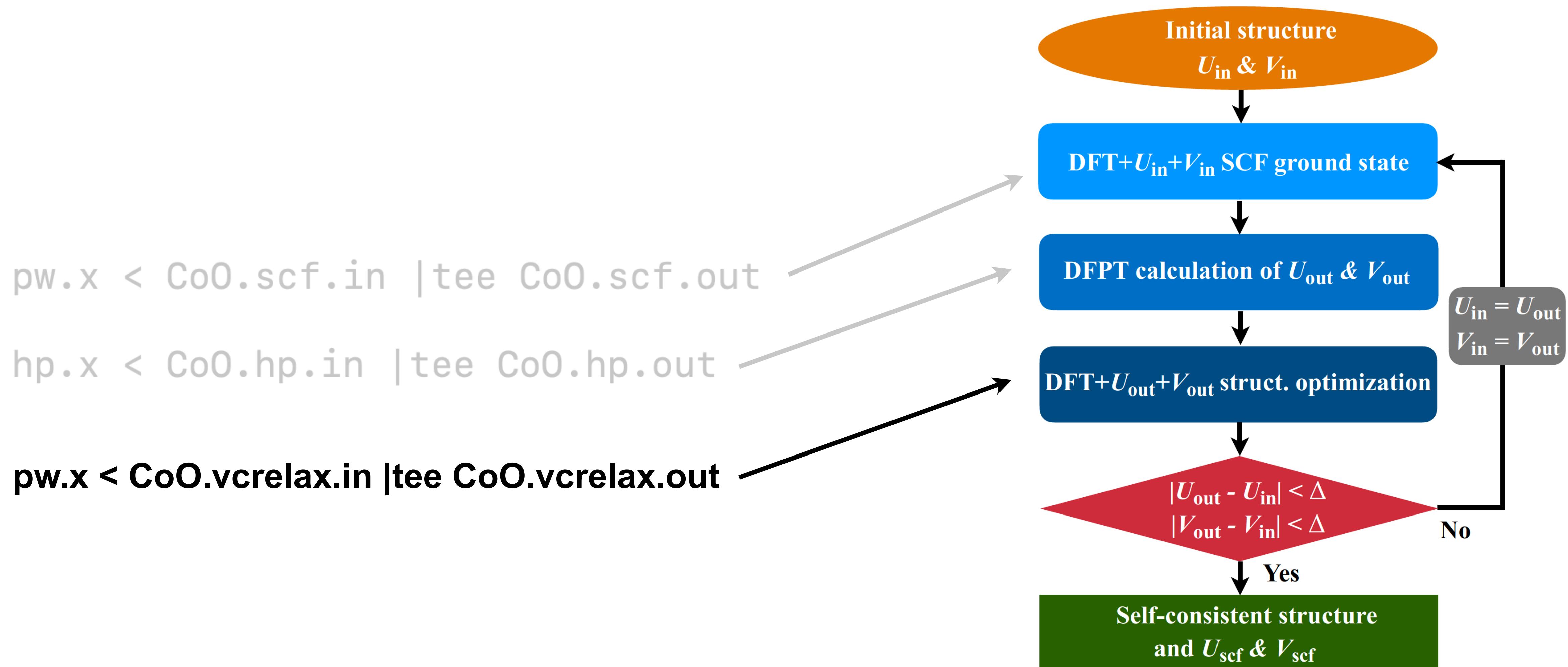
These are the output Hubbard U parameters for Co1-3d and Co2-3d states

These parameters are computed in a “one-shot” fashion (i.e. from the DFT ground state)

Input file CoO.vcrelax.in

```
&control
  calculation='vc-relax' ← Variable-cell relaxation calculation
  restart_mode='from_scratch',
  prefix='CoO'
  pseudo_dir = '../files/pseudo'
  outdir='./tmp'
  verbosity='high'
  etot_conv_thr = 1.0D-4
  forc_conv_thr = 1.0D-3 ← Convergence thresholds on the total energy and forces
/
&system
  ibrav = 0,
  celldm(1) = 8.00,
  nat = 4,
  ntyp = 3,
  ecutwfc = 50.0 ← Typically higher cutoff than for the calculation of the Hubbard parameters
  ecutrho = 400.0 (because forces and stresses converge slowly with respect to the cutoff)
  nspin = 2
  starting_magnetization(1) = 0.5,
  starting_magnetization(2) = -0.5,
  occupations = 'smearing',
  smearing = 'mv',
  degauss = 0.02
/
&electrons
  conv_thr = 1.d-10
/
&ions
  ion_dynamics = 'bfgs' ← Broyden-Fletcher-Goldfarb-Shanno (BFGS) optimization algorithm
/
&cell
  cell_dynamics = 'bfgs'
/
ATOMIC_SPECIES
Co1 58.933194 co_pbesol_v1.2.uspp.F.UPF
Co2 58.933194 co_pbesol_v1.2.uspp.F.UPF
O 15.999 O.pbesol-n-kjpaw_psl.0.1.UPF
ATOMIC_POSITIONS {crystal}
Co1 0.0000000 0.0000000 0.0000000
Co2 0.5000000 0.5000000 0.5000000
O 0.2500000 0.2500000 0.2500000
O 0.7500000 0.7500000 0.7500000
CELL_PARAMETERS {alat}
0.570726115 0.570726115 1.031099100
0.570726115 1.031099100 0.570726115
1.031099100 0.570726115 0.570726115 ← Typically denser k points mesh than for the calculation of the Hubbard parameters
(K_POINTS {automatic} (because forces and stresses converge slowly with respect to the size of the k mesh)
6 6 6 0 0 0
HUBBARD {ortho-atomic}
U Co1-3d 6.7553 ← We use the Hubbard U parameters determined in the previous step
U Co2-3d 6.7553
```

Run the calculation



Output file CoO.vcrelax.out

```
Energy error          =      1.1E-07 Ry
Gradient error        =      1.2E-07 Ry/Bohr
Cell gradient error   =      3.6E-02 kbar
Message from routine volume:
axis vectors are left-handed
```

```
bfgs converged in    6 scf cycles and    5 bfgs steps
(criteria: energy < 1.0E-04 Ry, force < 1.0E-03 Ry/Bohr, cell < 5.0E-01 kbar)
```

```
End of BFGS Geometry Optimization
```

```
Final enthalpy        =     -678.2836113097 Ry
```

```
File ./tmp/CoO.bfgs deleted, as requested
```

```
Begin final coordinates
new unit-cell volume =    251.83776 a.u.^3 (    37.31851 Ang^3 )
density =       6.66843 g/cm^3
```

```
CELL_PARAMETERS (alat= 8.0000000)
0.541886331  0.541886331  1.024861524
0.541886331  1.024861524  0.541886331
1.024861524  0.541886331  0.541886331
```



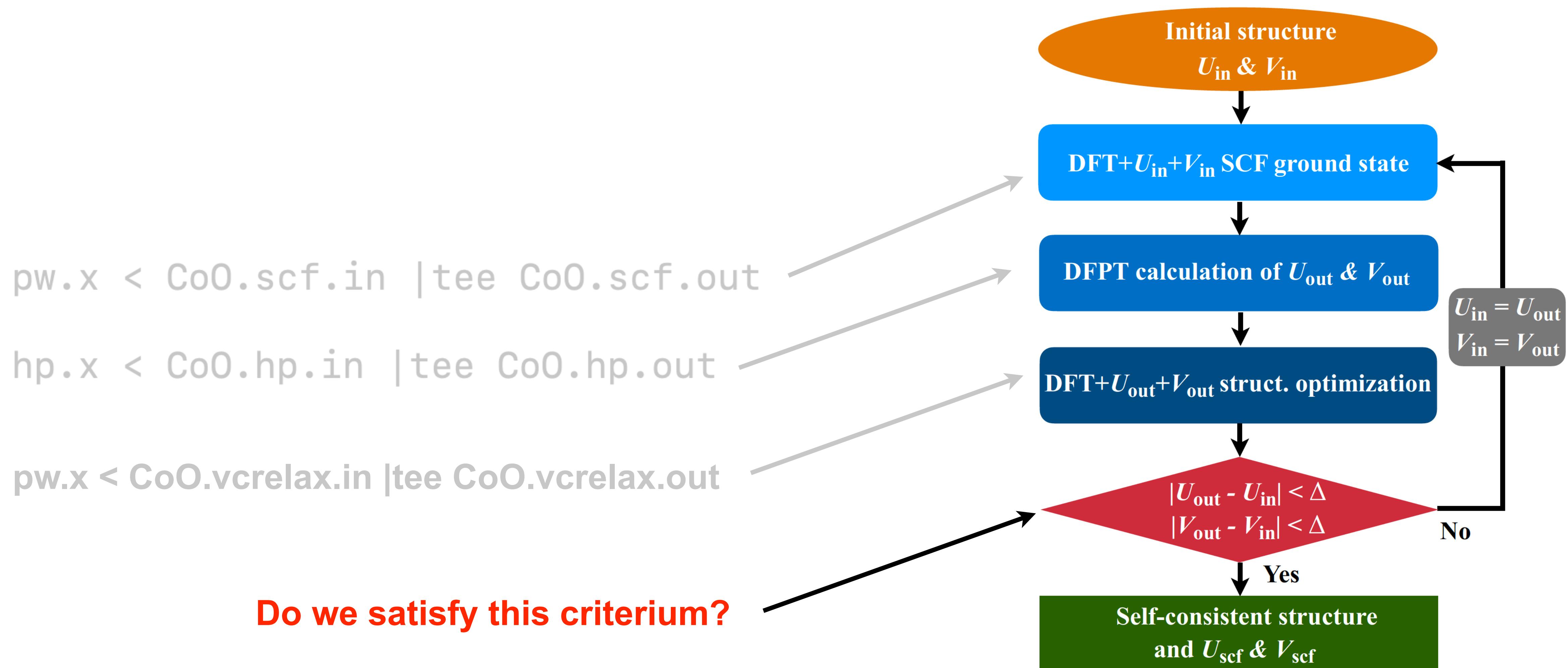
New cell parameters

```
ATOMIC_POSITIONS (crystal)
Co1           -0.0000000000  0.0000000000  -0.0000000000
Co2            0.5000000000  0.5000000000   0.5000000000
O              0.2499999831  0.2499999831   0.2499999831
O              0.750000169   0.750000169   0.750000169
End final coordinates
```



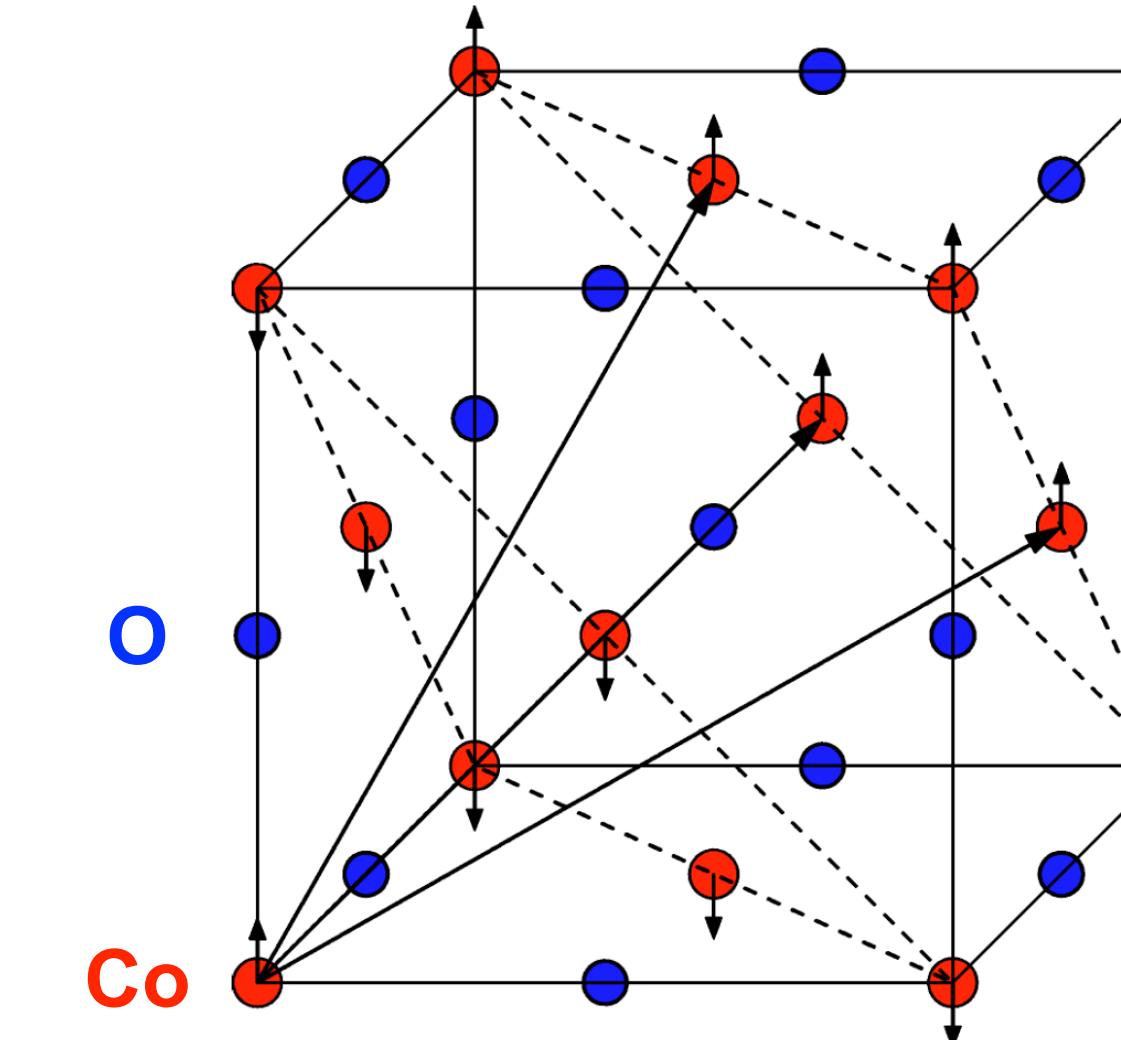
New atomic positions

Run the calculation



Input file CoO.scf.1.in

```
&control
  calculation='scf'
  restart_mode='from_scratch',
  prefix='CoO'
  pseudo_dir = ' ../../files/pseudo'
 outdir='./tmp'
  verbosity='high'
/
&system
  ibrav = 0,
  celldm(1) = 8.00,
  nat = 4,
  ntyp = 3,
  ecutwfc = 35.0
  ecutrho = 280.0
  nspin = 2
  starting_magnetization(1) =  0.5,
  starting_magnetization(2) = -0.5,
  occupations = 'smearing',
  smearing = 'mv',
  degauss = 0.02
/
&electrons
  conv_thr = 1.d-10
/
ATOMIC_SPECIES
  Co1 58.933194 co_pbesol_v1.2.uspp.F.UPF
  Co2 58.933194 co_pbesol_v1.2.uspp.F.UPF
  O   15.999  O.pbesol-n-kjpaw_psl.0.1.UPF
ATOMIC_POSITIONS {crystal}
  Co1    0.0000000    0.0000000    0.0000000
  Co2    0.5000000    0.5000000    0.5000000
  O     0.2500000    0.2500000    0.2500000
  O     0.7500000    0.7500000    0.7500000
CELL_PARAMETERS {alat}
  0.541886331  0.541886331  1.024861524
  0.541886331  1.024861524  0.541886331
  1.024861524  0.541886331  0.541886331
K_POINTS {automatic}
  3 3 3 0 0 0
HUBBARD {ortho-atomic}
  U Co1-3d 6.7553
  U Co2-3d 6.7553
```



We treat the system as a metal (i.e. with smearing) because we perform a spin-polarized calculation (fractional occupations)

New cell parameters that were determined in the previous optimization step

We use the Hubbard U parameters determined in the previous HP calculation

Input file CoO.scf.1.in

```
&control
  calculation='scf'
  restart_mode='from_scratch',
  prefix='CoO'
  pseudo_dir = '../files/pseudo'
 outdir='./tmp'
  verbosity='high'
/
&system
  ibrav = 0,
  celldm(1) = 8.00,
  nat = 4,
  ntyp = 3,
  ecutwfc = 35.0
  ecutrho = 280.0
  nspin = 2
  starting_magnetization(1) = 0.5,
  starting_magnetization(2) = -0.5,
  occupations = 'smearing',
  smearing = 'mv',
  degauss = 0.02
/
&electrons
  conv_thr = 1.d-10
/
ATOMIC_SPECIES
  Co1 58.933194 co_pbesol_v1.2.uspp.F.UPF
  Co2 58.933194 co_pbesol_v1.2.uspp.F.UPF
  O   15.999   O.pbesol-n-kjpaw_psl.0.1.UPF
ATOMIC_POSITIONS {crystal}
  Co1    0.0000000    0.0000000    0.0000000
  Co2    0.5000000    0.5000000    0.5000000
  O     0.2500000    0.2500000    0.2500000
  O     0.7500000    0.7500000    0.7500000
CELL_PARAMETERS {alat}
  0.541886331  0.541886331  1.024861524
  0.541886331  1.024861524  0.541886331
  1.024861524  0.541886331  0.541886331
K_POINTS {automatic}
  3 3 3 0 0 0
HUBBARD {ortho-atomic}
U Co1-3d 6.7553
U Co2-3d 6.7553
```

Input file CoO.scf.2.in

```
&control
  calculation='scf'
  restart_mode='from_scratch',
  prefix='CoO'
  pseudo_dir = '../files/pseudo'
 outdir='./tmp'
  verbosity='high'
/
&system
  ibrav = 0,
  celldm(1) = 8.00,
  nat = 4,
  ntyp = 3,
  ecutwfc = 35.0
  ecutrho = 280.0
  nspin = 2
  tot_magnetization = 0.00
  occupations = 'fixed',
  nbnd = 28
/
&electrons
  conv_thr = 1.d-10
  startingwfc = 'file'
  startingpot = 'file'
```

Magnetic insulator
Same as in the 1st calc.

Read wavefunctions and
density/potential from the
previous calculation

Output file CoO.scf.1.out

the Fermi energy is 14.3861 ev

! total energy = -678.47428517 Ry
estimated scf accuracy < 6.0E-11 Ry
smearing contrib. (-TS) = 0.0000000 Ry
internal energy E=TS = -678.47428517 Ry

The total energy is F=E-TS. E is the sum of the following terms:

one-electron contribution = -356.17053914 Ry
hartree contribution = 205.82368503 Ry
xc contribution = -79.61233908 Ry
ewald contribution = -430.44916468 Ry
Hubbard energy = 0.14527434 Ry
one-center paw contrib. = -18.21120163 Ry
-> PAW hartree energy AE = 0.00000000 Ry
-> PAW hartree energy PS = 0.00000000 Ry
-> PAW xc energy AE = 0.00000000 Ry
-> PAW xc energy PS = 0.00000000 Ry
-> total E_H with PAW = 205.82368503 Ry
-> total E_XC with PAW = -79.61233908 Ry

total magnetization = -0.00 Bohr mag/cell
absolute magnetization = 5.62 Bohr mag/cell

convergence has been achieved in 23 iterations

Output file CoO.scf.2.out

highest occupied, lowest unoccupied level (ev): 12.8827 15.5509

! total energy = -678.47428517 Ry
estimated scf accuracy < 6.6E-12 Ry

The total energy is the sum of the following terms:

one-electron contribution = -356.17059367 Ry
hartree contribution = 205.82374466 Ry
xc contribution = -79.61234455 Ry
ewald contribution = -430.44916468 Ry
Hubbard energy = 0.14527476 Ry
one-center paw contrib. = -18.21120169 Ry
-> PAW hartree energy AE = 0.00000000 Ry
-> PAW hartree energy PS = 0.00000000 Ry
-> PAW xc energy AE = 0.00000000 Ry
-> PAW xc energy PS = 0.00000000 Ry
-> total E_H with PAW = 205.82374466 Ry
-> total E_XC with PAW = -79.61234455 Ry

total magnetization = 0.00 Bohr mag/cell
absolute magnetization = 5.62 Bohr mag/cell

convergence has been achieved in 3 iterations

Input file CoO.hp.in

This is exactly the same as before (i.e. in the 1st step)

&inputhp

prefix = 'CoO'

outdir = './tmp'

nq1 = 2, nq2 = 2, nq3 = 2

conv_thr_chi = 1.d-6

/



The same as in the CoO.scf.in input



Size of the **q** points mesh



Convergence threshold for computing the self-consistent response matrix χ (in eV^{-1})

Computer Physics Communications
Volume 279, October 2022, 108455

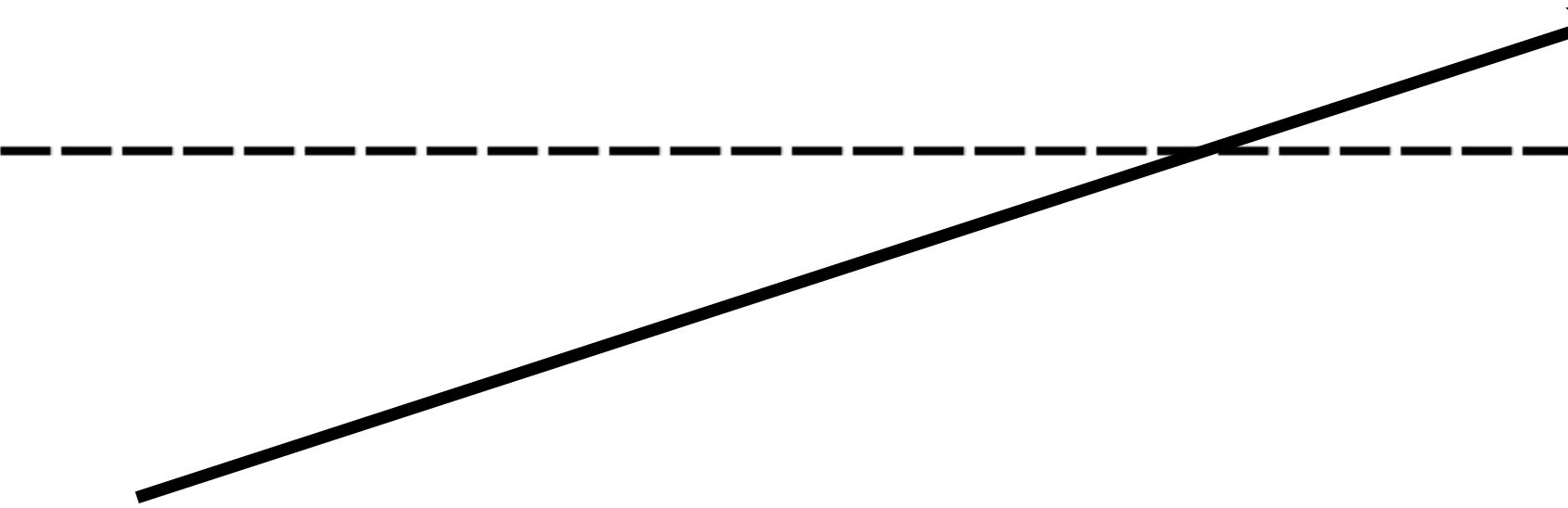
HP – A code for the calculation of Hubbard parameters using density-functional perturbation theory ★, ★★

Iurii Timrov ^a✉, Nicola Marzari ^{a, b}, Matteo Cococcioni ^c

Output file CoO.Hubbard_parameters.dat

Hubbard U parameters:

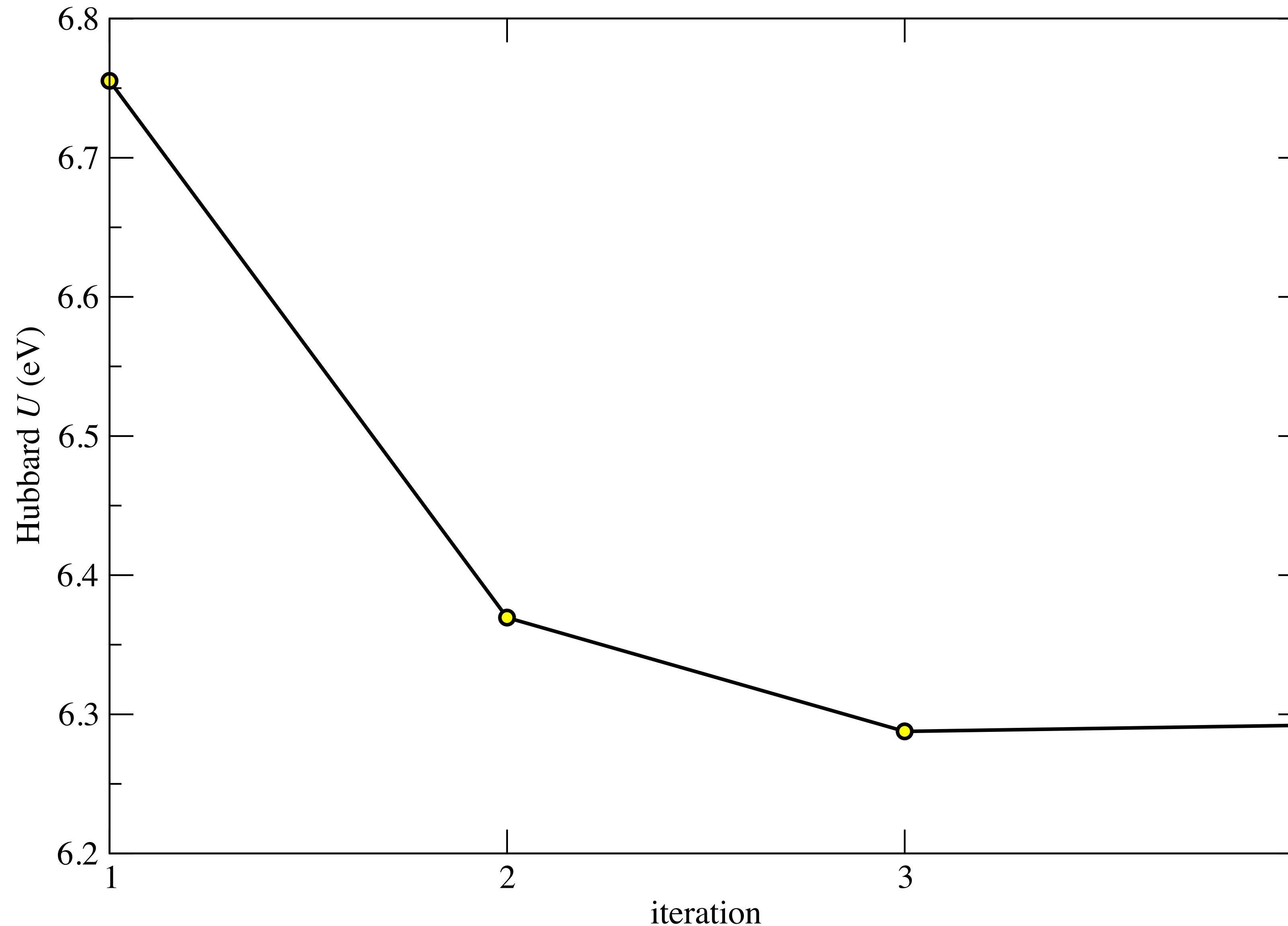
site	n.	type	label	spin	new_type	new_label	Hubbard U (eV)
1		1	Co1	1	1	Co1	6.3695
2		2	Co2	-1	1	Co1	6.3695



These are the output Hubbard U parameters for Co1-3d and Co2-3d states

Next step: vc-relax, then recalculate U again, etc. etc. until the convergence it reached

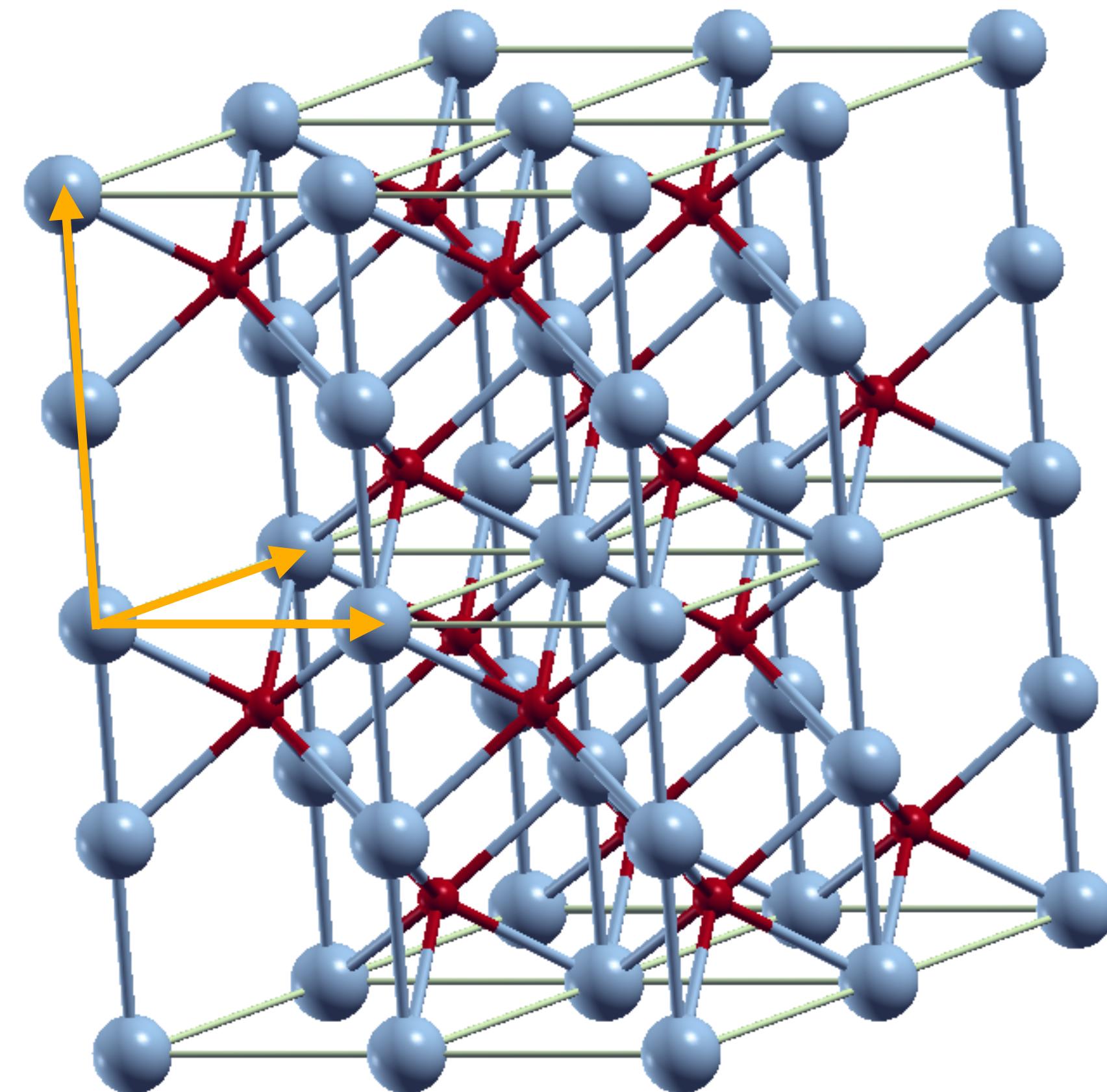
Self-consistent calculation of the Hubbard U parameter



Exercise 6

Self-consistent calculation of the Hubbard U and V parameters in MnO

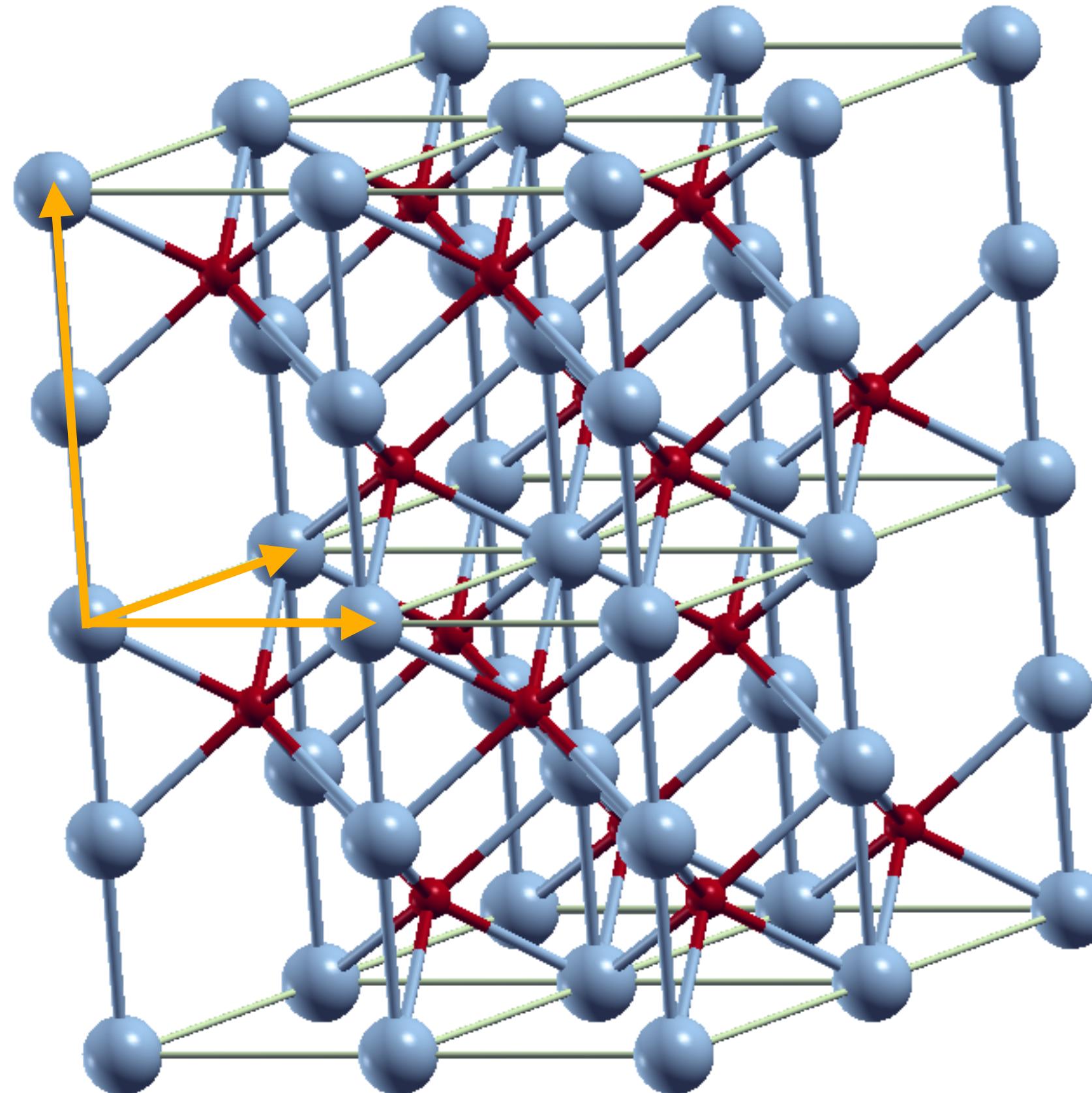
Crystal structure of h-MnO



Input file MnO.scf.in

```
&control
  calculation = 'scf',
  verbosity = 'high',
  pseudo_dir = '../..../files/pseudo'
  outdir='./tmp'
  restart_mode='from_scratch'
  verbosity = 'high',
  wf_collect = .true.
  prefix='mno',
/
&system
  ibrav= 0, celldm(1)=5.2648, nat= 4, ntyp= 3,
  nspin = 2,
  starting_magnetization(1) = 0.4,
  starting_magnetization(2) = -0.4,
  ecutwfc = 45.0,
  ecutrho = 450.0,
  nbnd = 28
  occupations='smearing',
  smearing='mv',
  degauss=0.01
/
&electrons
  mixing_beta = 0.2
  mixing_ndim = 20
  mixing_mode = 'local-TF'
  conv_thr = 1.0d-8,
  electron_maxstep = 200
/
ATOMIC_SPECIES
  Mn1 1.0 mn_pbesol_v1.5.uspp.F.UPF
  Mn2 1.0 mn_pbesol_v1.5.uspp.F.UPF
  0 1.0 O.pbesol-n-kjpaw_psl.0.1.UPF
CELL_PARAMETERS
  0.5000000 0.8660254038 0.000000000
  -0.5000000 0.8660254038 0.000000000
   0.0000000 0.000000000 1.583632480
ATOMIC_POSITIONS {crystal}
  Mn1      0.000000000 0.000000000 0.000000000
  Mn2      0.000000000 0.000000000 0.500000000
  0        0.333333333 0.333333333 0.750000000
  0        0.666666666 0.666666666 0.250000000
K_POINTS {automatic}
  4 4 3 0 0 0
```

Crystal structure of h-MnO



Band structure

Input file MnO.scf.in

```

&control
  calculation = 'scf',
  verbosity = 'high',
  pseudo_dir = '.../../files/pseudo'
 outdir='./tmp'
  restart_mode='from_scratch'
  verbosity = 'high',
  wf_collect = .true.
  prefix='mno',
/
&system
  ibrav= 0, celldm(1)=5.2648, nat= 4, ntyp= 3,
  nspin = 2,
  starting_magnetization(1) = 0.4,
  starting_magnetization(2) = -0.4,
  ecutwfc = 45.0,
  ecutrho = 450.0,
  nbnd = 28
  occupations='smearing',
  smearing='mv',
  degauss=0.01
/
&electrons
  mixing_beta = 0.2
  mixing_ndim = 20
  mixing_mode = 'local-TF'
  conv_thr = 1.0d-8,
  electron_maxstep = 200
/
ATOMIC_SPECIES
  Mn1 1.0 mn_pbessol_v1.5.uspp.F.UPF
  Mn2 1.0 mn_pbessol_v1.5.uspp.F.UPF
  0 1.0 0.pbesol-n-kjpaw_psl.0.1.UPF
CELL_PARAMETERS
  0.5000000 0.8660254038 0.000000000
  -0.5000000 0.8660254038 0.000000000
  0.0000000 0.0000000000 1.583632480
ATOMIC_POSITIONS {crystal}
Mn1      0.000000000 0.000000000 0.000000000
Mn2      0.000000000 0.000000000 0.500000000
0        0.333333333 0.333333333 0.750000000
0        0.666666666 0.666666666 0.250000000
K_POINTS {automatic}
  4 4 3 0 0 0

```

Input file MnO.bands.in

```

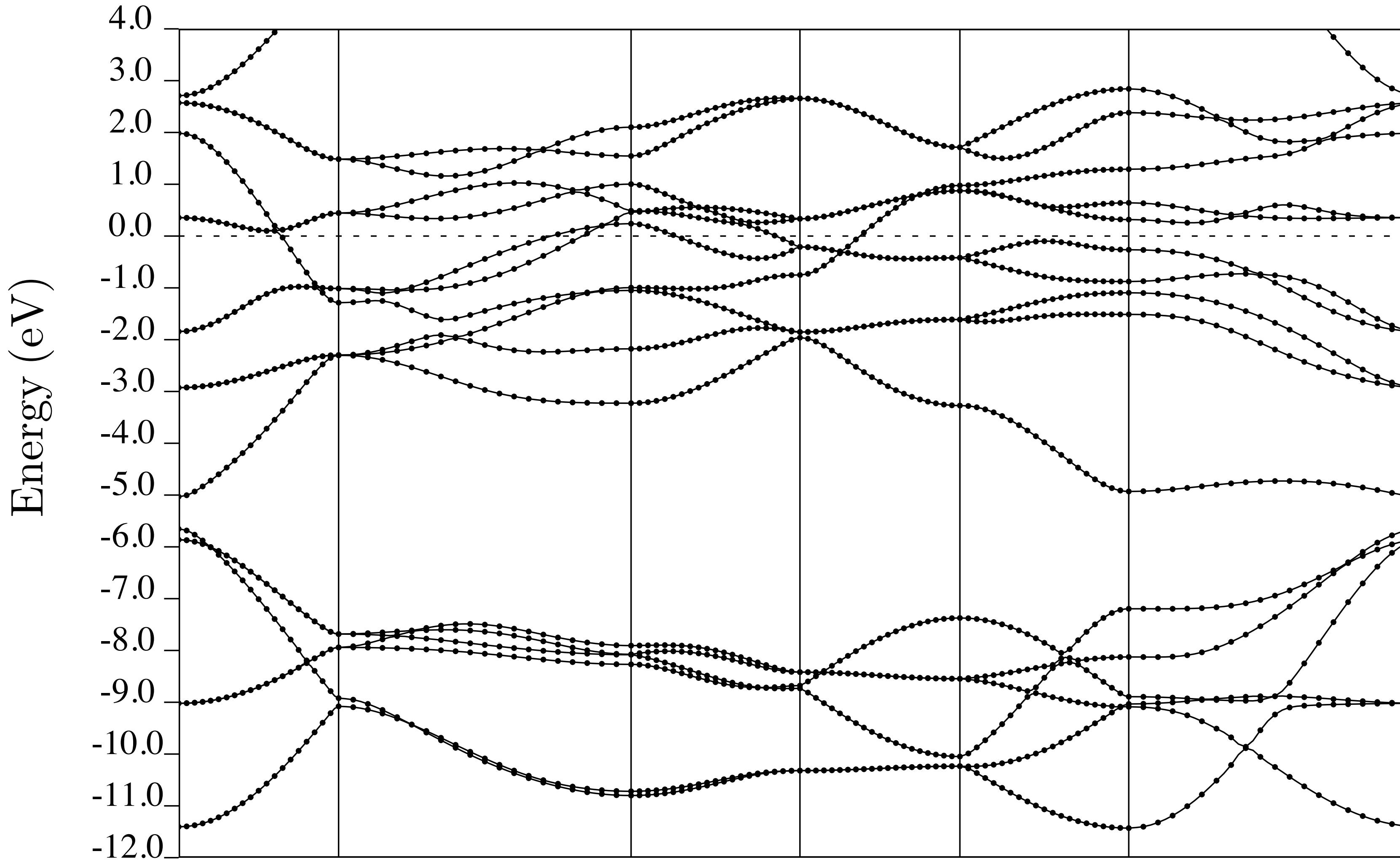
&control
  calculation = 'bands',
  verbosity = 'high',
  pseudo_dir = '../files/pseudo'
  outdir='./tmp'
  restart_mode='from_scratch'
  verbosity = 'high',
  wf_collect = .true.
  prefix='mno',
/
.
.
.
.
.

ATOMIC_POSITIONS {crystal}
Mn1      0.000000000   0.000000000   0.000000000
Mn2      0.000000000   0.000000000   0.500000000
O        0.333333333   0.333333333   0.750000000
O        0.666666666   0.666666666   0.250000000

K_POINTS crystal_b
7
0.0 0.0 0.0 20
0.0 0.0 0.5 20
0.5 0.5 0.5 20
0.66666667 0.33333333 0.5 20
0.66666667 0.33333333 0.0 20
0.5 0.5 0.0 20
0.0 0.0 0.0 1

```

Hexagonal MnO band structure (PBEsol)

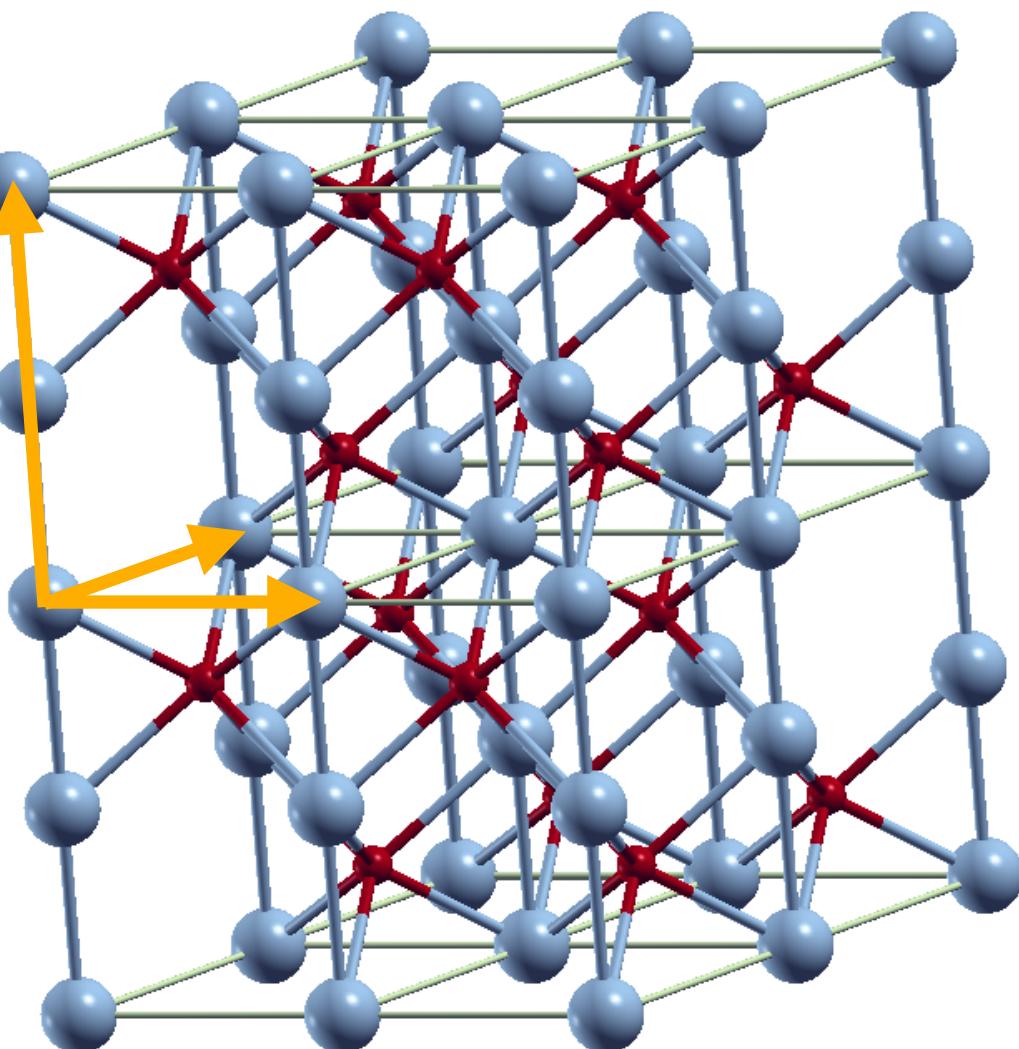


We want to run a DFT+U+V calculation computing U and V self-consistently (no structural relaxation)

Input file MnO.scf.in

```
&control
  calculation = 'scf',
  verbosity = 'high',
  pseudo_dir = '../..../files/pseudo'
  outdir='./tmp'
  restart_mode='from_scratch'
  verbosity = 'high',
  wf_collect = .true.
  prefix='mno',
/
.
.
.
.

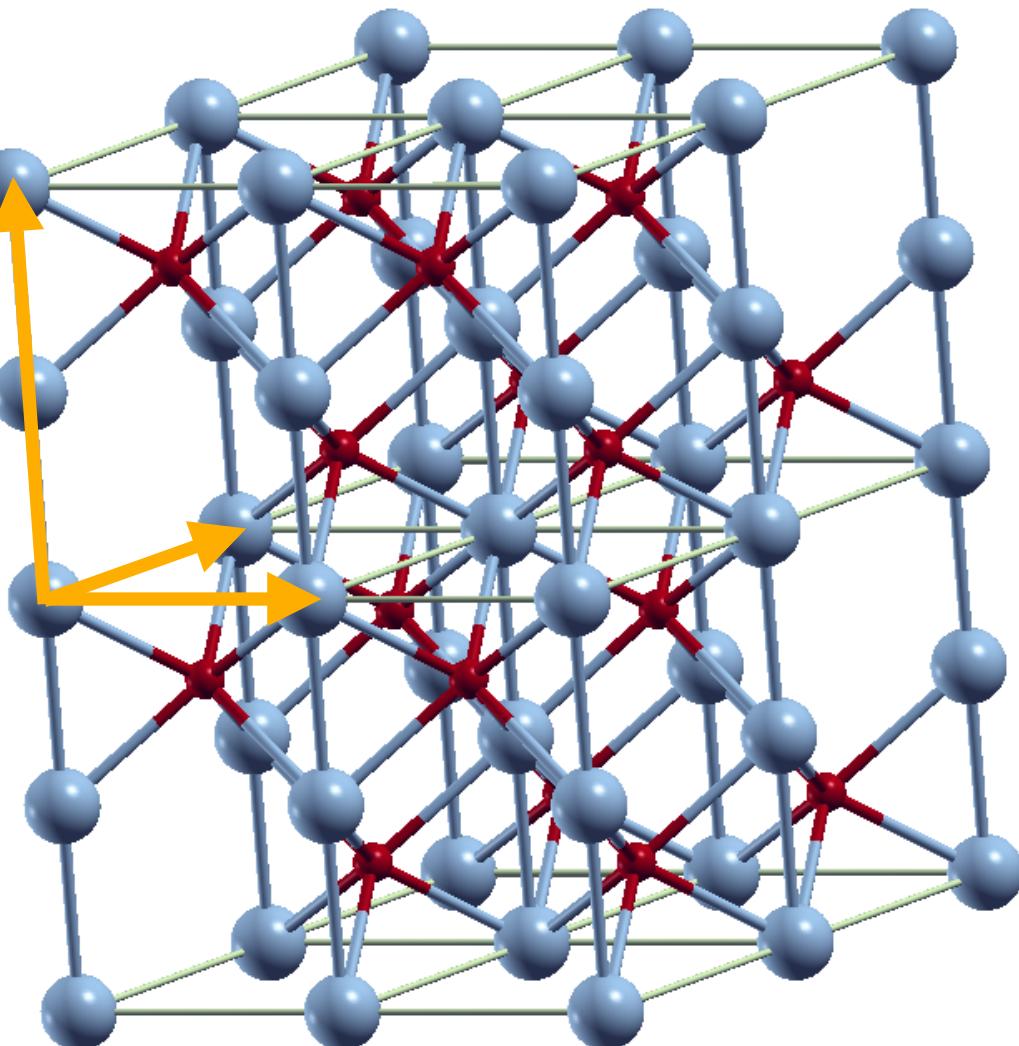
CELL_PARAMETERS
  0.5000000 0.8660254038 0.000000000
  -0.5000000 0.8660254038 0.000000000
   0.0000000 0.0000000000 1.583632480
ATOMIC_POSITIONS {crystal}
Mn1      0.000000000 0.000000000 0.000000000
Mn2      0.000000000 0.000000000 0.500000000
0        0.333333333 0.333333333 0.750000000
0        0.666666666 0.666666666 0.250000000
K_POINTS {automatic}
 4 4 3 0 0 0
HUBBARD ortho-atomic
V Mn1-3d Mn1-3d 1 1 2.0
V Mn2-3d Mn2-3d 2 2 2.0
V Mn1-3d 0-2p 1 12 1.0
V Mn2-3d 0-2p 2 3 1.0
V 0-2p 0-2p 3 3 1.d-5
V Mn1-3d Mn2-3d 1 2 0.2
```



Input file MnO.scf.in

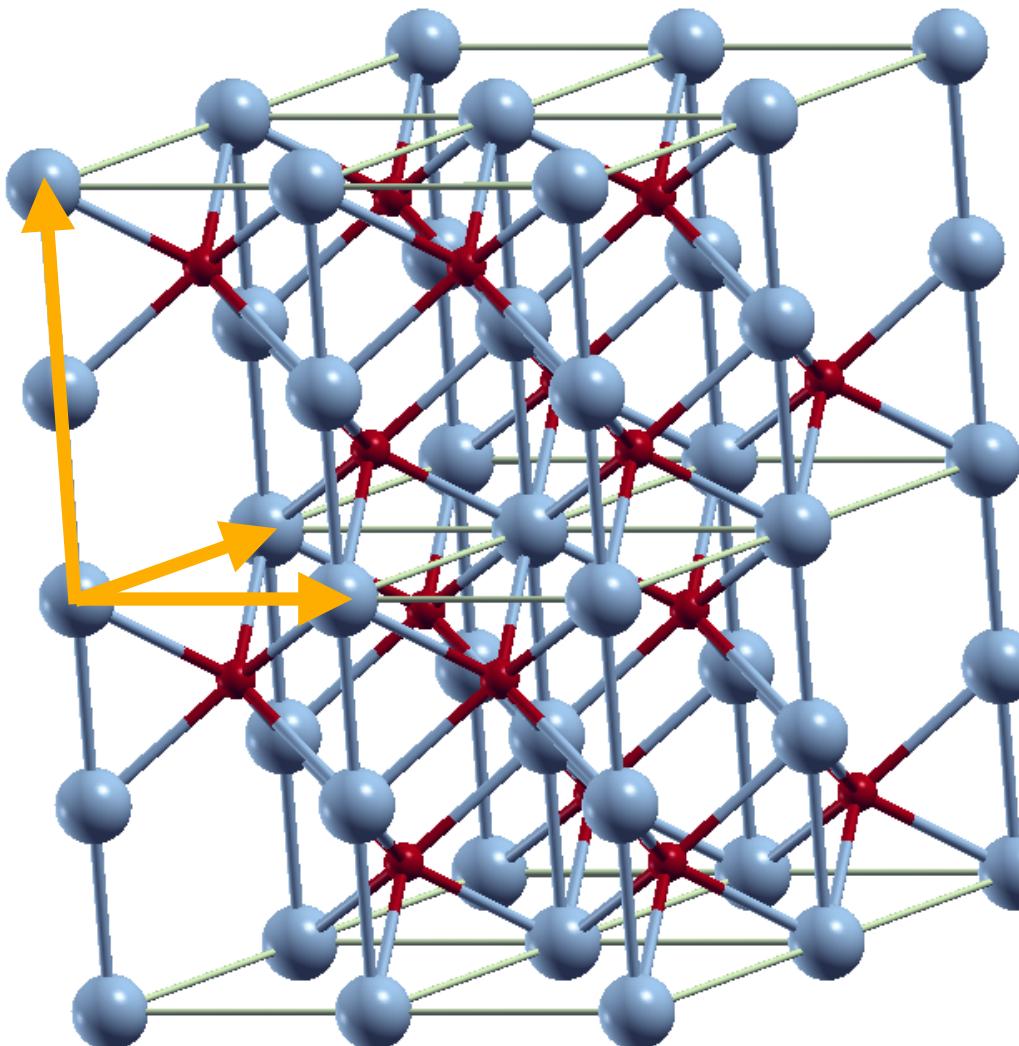
```
&control
  calculation = 'scf',
  verbosity = 'high',
  pseudo_dir = '../files/pseudo'
  outdir='./tmp'
  restart_mode='from_scratch'
  verbosity = 'high',
  wf_collect = .true.
  prefix='mno',
/
.
.
.
.

CELL_PARAMETERS
  0.5000000 0.8660254038 0.000000000
  -0.5000000 0.8660254038 0.000000000
   0.0000000 0.0000000000 1.583632480
ATOMIC_POSITIONS {crystal}
Mn1      0.000000000 0.000000000 0.000000000
Mn2      0.000000000 0.000000000 0.500000000
0        0.333333333 0.333333333 0.750000000
0        0.666666666 0.666666666 0.250000000
K_POINTS {automatic}
  4 4 3 0 0 0
HUBBARD ortho-atomic
V Mn1-3d Mn1-3d 1 1 2.0
V Mn2-3d Mn2-3d 2 2 2.0
V Mn1-3d 0-2p 1 12 1.0
V Mn2-3d 0-2p 2 3 1.0
V 0-2p 0-2p 3 3 1.d-5
V Mn1-3d Mn2-3d 1 2 0.2
```



Input file MnO.scf.in

```
&control
  calculation = 'scf',
  verbosity = 'high',
  pseudo_dir = '../files/pseudo'
  outdir='./tmp'
  restart_mode='from_scratch'
  verbosity = 'high',
  wf_collect = .true.
  prefix='mno',
/
.
.
.
CELL_PARAMETERS
  0.5000000 0.8660254038 0.000000000
  -0.5000000 0.8660254038 0.000000000
   0.0000000 0.0000000000 1.583632480
ATOMIC_POSITIONS {crystal}
Mn1      0.000000000 0.000000000 0.000000000
Mn2      0.000000000 0.000000000 0.500000000
0        0.333333333 0.333333333 0.750000000
0        0.666666666 0.666666666 0.250000000
K_POINTS {automatic}
  4 4 3 0 0 0
HUBBARD ortho-atomic
V Mn1-3d Mn1-3d 1 1 2.0
V Mn2-3d Mn2-3d 2 2 2.0
V Mn1-3d 0-2p 1 12 1.0
V Mn2-3d 0-2p 2 3 1.0
V 0-2p 0-2p 3 3 1.d-5
V Mn1-3d Mn2-3d 1 2 0.2
```

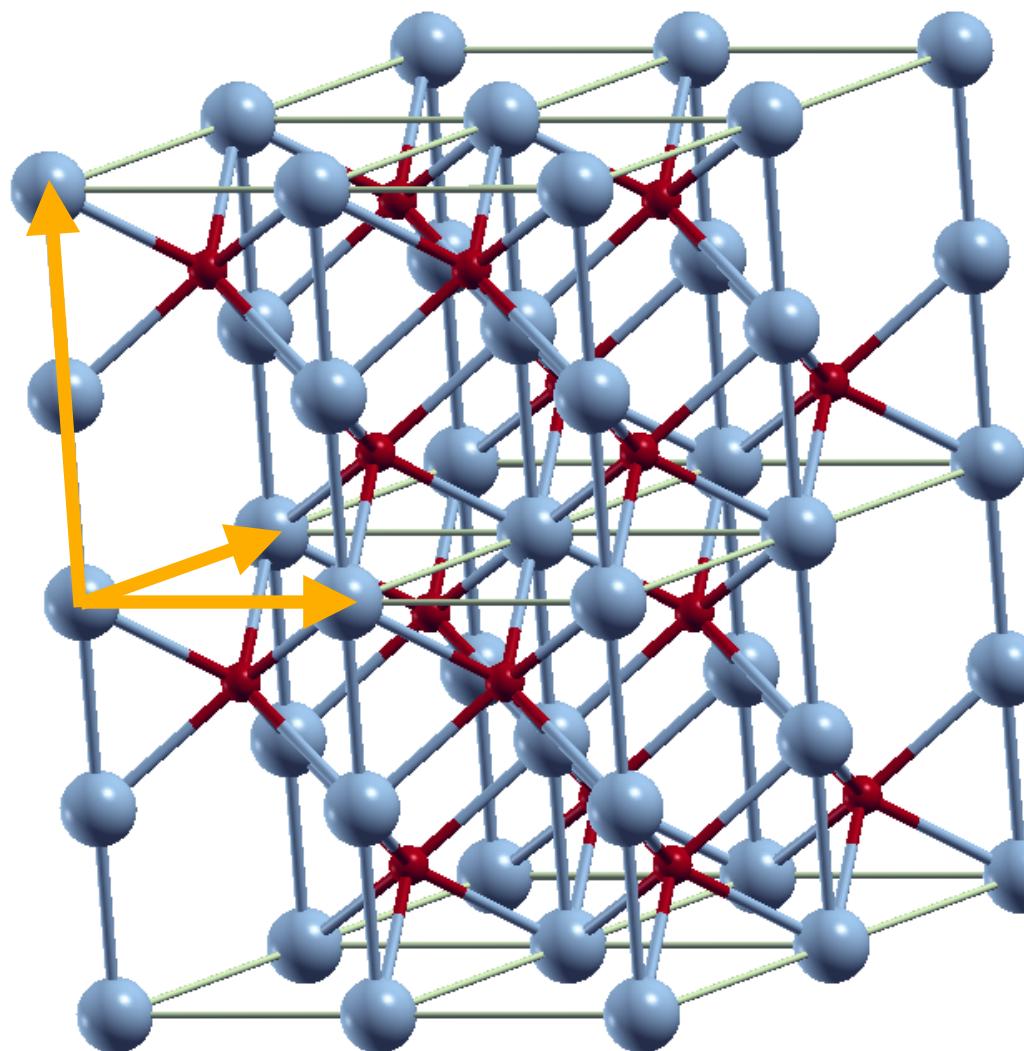


HUBBARD ortho-atomic

V Mn1-3d Mn1-3d 1 1 2.0
V Mn2-3d Mn2-3d 2 2 2.0
V Mn1-3d 0-2p 1 12 1.0
V Mn2-3d 0-2p 2 3 1.0
V 0-2p 0-2p 3 3 1.d-5
V Mn1-3d Mn2-3d 1 2 0.2

Input file MnO.scf.in

```
&control
  calculation = 'scf',
  verbosity = 'high',
  pseudo_dir = '../files/pseudo'
  outdir='./tmp'
  restart_mode='from_scratch'
  verbosity = 'high',
  wf_collect = .true.
  prefix='mno',
/
.
.
.
CELL_PARAMETERS
  0.5000000 0.8660254038 0.000000000
  -0.5000000 0.8660254038 0.000000000
   0.0000000 0.0000000000 1.583632480
ATOMIC_POSITIONS {crystal}
Mn1      0.000000000 0.000000000 0.000000000
Mn2      0.000000000 0.000000000 0.500000000
0        0.333333333 0.333333333 0.750000000
0        0.666666666 0.666666666 0.250000000
K_POINTS {automatic}
  4 4 3 0 0 0
HUBBARD ortho-atomic
V Mn1-3d Mn1-3d 1 1 2.0
V Mn2-3d Mn2-3d 2 2 2.0
V Mn1-3d 0-2p 1 12 1.0
V Mn2-3d 0-2p 2 3 1.0
V 0-2p 0-2p 3 3 1.d-5
V Mn1-3d Mn2-3d 1 2 0.2
```



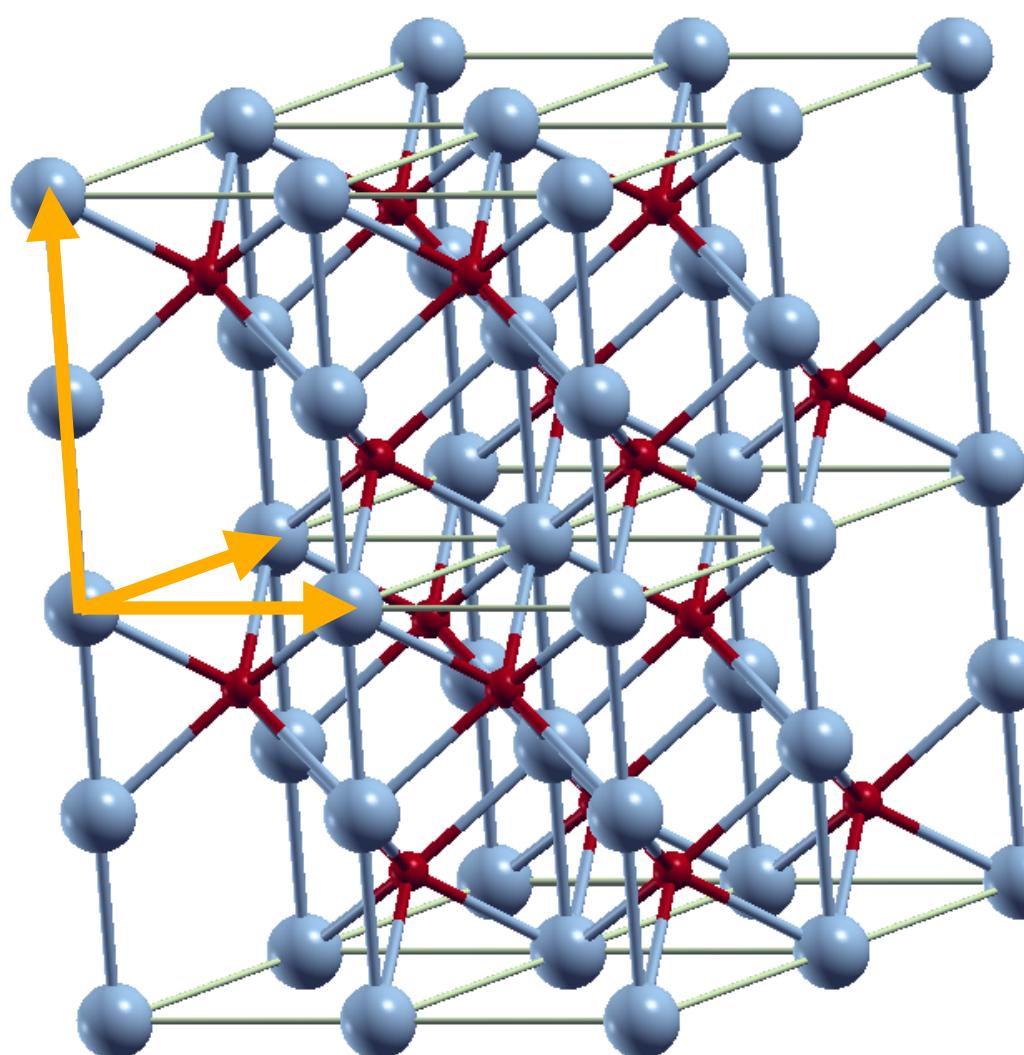
HUBBARD ortho-atomic

```
V Mn1-3d Mn1-3d 1 1 2.0
V Mn2-3d Mn2-3d 2 2 2.0
V Mn1-3d 0-2p 1 12 1.0
V Mn2-3d 0-2p 2 3 1.0
V 0-2p 0-2p 3 3 1.d-5
V Mn1-3d Mn2-3d 1 2 0.2
```

On-site U on Mn

Input file MnO.scf.in

```
&control
  calculation = 'scf',
  verbosity = 'high',
  pseudo_dir = '../files/pseudo'
  outdir='./tmp'
  restart_mode='from_scratch'
  verbosity = 'high',
  wf_collect = .true.
  prefix='mno',
/
.
.
.
CELL_PARAMETERS
  0.5000000 0.8660254038 0.000000000
  -0.5000000 0.8660254038 0.000000000
   0.0000000 0.0000000000 1.583632480
ATOMIC_POSITIONS {crystal}
Mn1      0.000000000 0.000000000 0.000000000
Mn2      0.000000000 0.000000000 0.500000000
0        0.333333333 0.333333333 0.750000000
0        0.666666666 0.666666666 0.250000000
K_POINTS {automatic}
  4 4 3 0 0 0
HUBBARD ortho-atomic
V Mn1-3d Mn1-3d 1 1 2.0
V Mn2-3d Mn2-3d 2 2 2.0
V Mn1-3d 0-2p 1 12 1.0
V Mn2-3d 0-2p 2 3 1.0
V 0-2p 0-2p 3 3 1.d-5
V Mn1-3d Mn2-3d 1 2 0.2
```



HUBBARD ortho-atomic

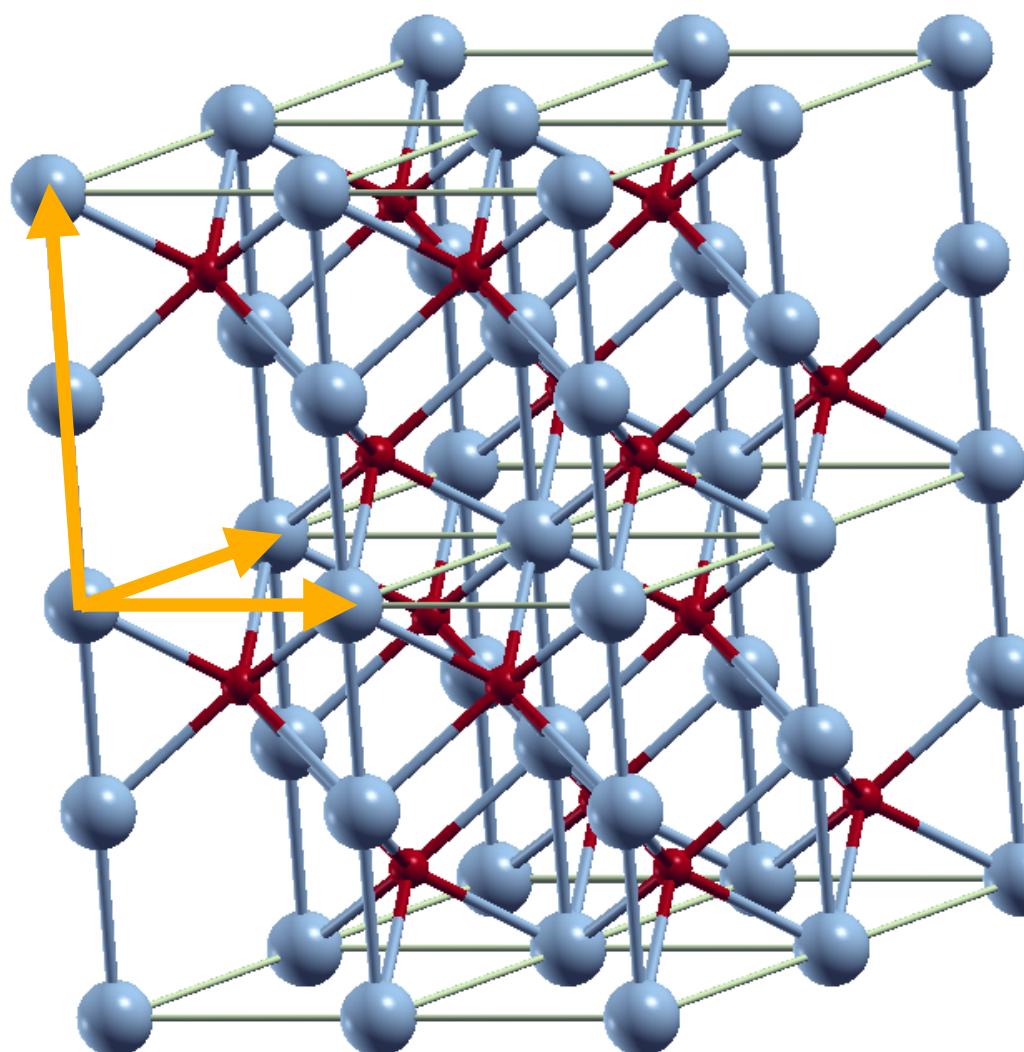
```
V Mn1-3d Mn1-3d 1 1 2.0
V Mn2-3d Mn2-3d 2 2 2.0
V Mn1-3d 0-2p 1 12 1.0
V Mn2-3d 0-2p 2 3 1.0
V 0-2p 0-2p 3 3 1.d-5
V Mn1-3d Mn2-3d 1 2 0.2
```

On-site U on Mn

On-site U on O (small)

Input file MnO.scf.in

```
&control
  calculation = 'scf',
  verbosity = 'high',
  pseudo_dir = '../files/pseudo'
  outdir='./tmp'
  restart_mode='from_scratch'
  verbosity = 'high',
  wf_collect = .true.
  prefix='mno',
/
.
.
.
CELL_PARAMETERS
  0.5000000 0.8660254038 0.000000000
  -0.5000000 0.8660254038 0.000000000
   0.0000000 0.0000000000 1.583632480
ATOMIC_POSITIONS {crystal}
Mn1      0.000000000 0.000000000 0.000000000
Mn2      0.000000000 0.000000000 0.500000000
0        0.333333333 0.333333333 0.750000000
0        0.666666666 0.666666666 0.250000000
K_POINTS {automatic}
  4 4 3 0 0 0
HUBBARD ortho-atomic
V Mn1-3d Mn1-3d 1 1 2.0
V Mn2-3d Mn2-3d 2 2 2.0
V Mn1-3d 0-2p 1 12 1.0
V Mn2-3d 0-2p 2 3 1.0
V 0-2p 0-2p 3 3 1.d-5
V Mn1-3d Mn2-3d 1 2 0.2
```



HUBBARD ortho-atomic

V Mn1-3d Mn1-3d 1 1 2.0
V Mn2-3d Mn2-3d 2 2 2.0
V Mn1-3d 0-2p 1 12 1.0
V Mn2-3d 0-2p 2 3 1.0
V 0-2p 0-2p 3 3 1.d-5
V Mn1-3d Mn2-3d 1 2 0.2

On-site U on Mn

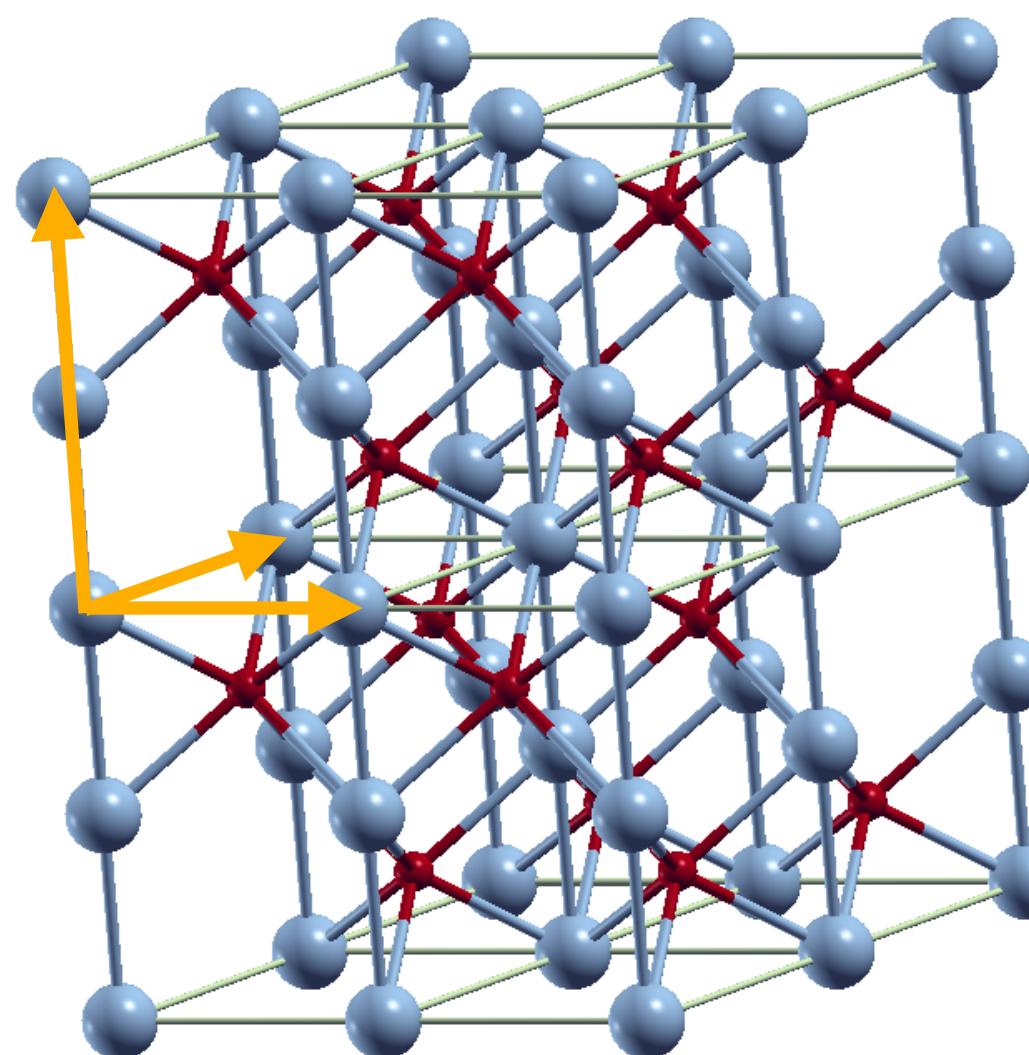
inter-site V: Mn-O n.n.

On-site U on O (small)

Input file MnO.scf.in

```
&control
  calculation = 'scf',
  verbosity = 'high',
  pseudo_dir = '../files/pseudo'
  outdir='./tmp'
  restart_mode='from_scratch'
  verbosity = 'high',
  wf_collect = .true.
  prefix='mno',
/
.
.
.
CELL_PARAMETERS
  0.5000000 0.8660254038 0.000000000
  -0.5000000 0.8660254038 0.000000000
   0.0000000 0.0000000000 1.583632480
ATOMIC_POSITIONS {crystal}
Mn1      0.000000000 0.000000000 0.000000000
Mn2      0.000000000 0.000000000 0.500000000
0        0.333333333 0.333333333 0.750000000
0        0.666666666 0.666666666 0.250000000
K_POINTS {automatic}
  4 4 3 0 0 0
```

```
HUBBARD ortho-atomic
V Mn1-3d Mn1-3d 1 1 2.0
V Mn2-3d Mn2-3d 2 2 2.0
V Mn1-3d 0-2p 1 12 1.0
V Mn2-3d 0-2p 2 3 1.0
V 0-2p 0-2p 3 3 1.d-5
V Mn1-3d Mn2-3d 1 2 0.2
```



HUBBARD ortho-atomic

V Mn1-3d Mn1-3d 1 1 2.0
V Mn2-3d Mn2-3d 2 2 2.0
V Mn1-3d 0-2p 1 12 1.0
V Mn2-3d 0-2p 2 3 1.0
V 0-2p 0-2p 3 3 1.d-5
V Mn1-3d Mn2-3d 1 2 0.2

On-site U on Mn

inter-site V: Mn-O n.n.

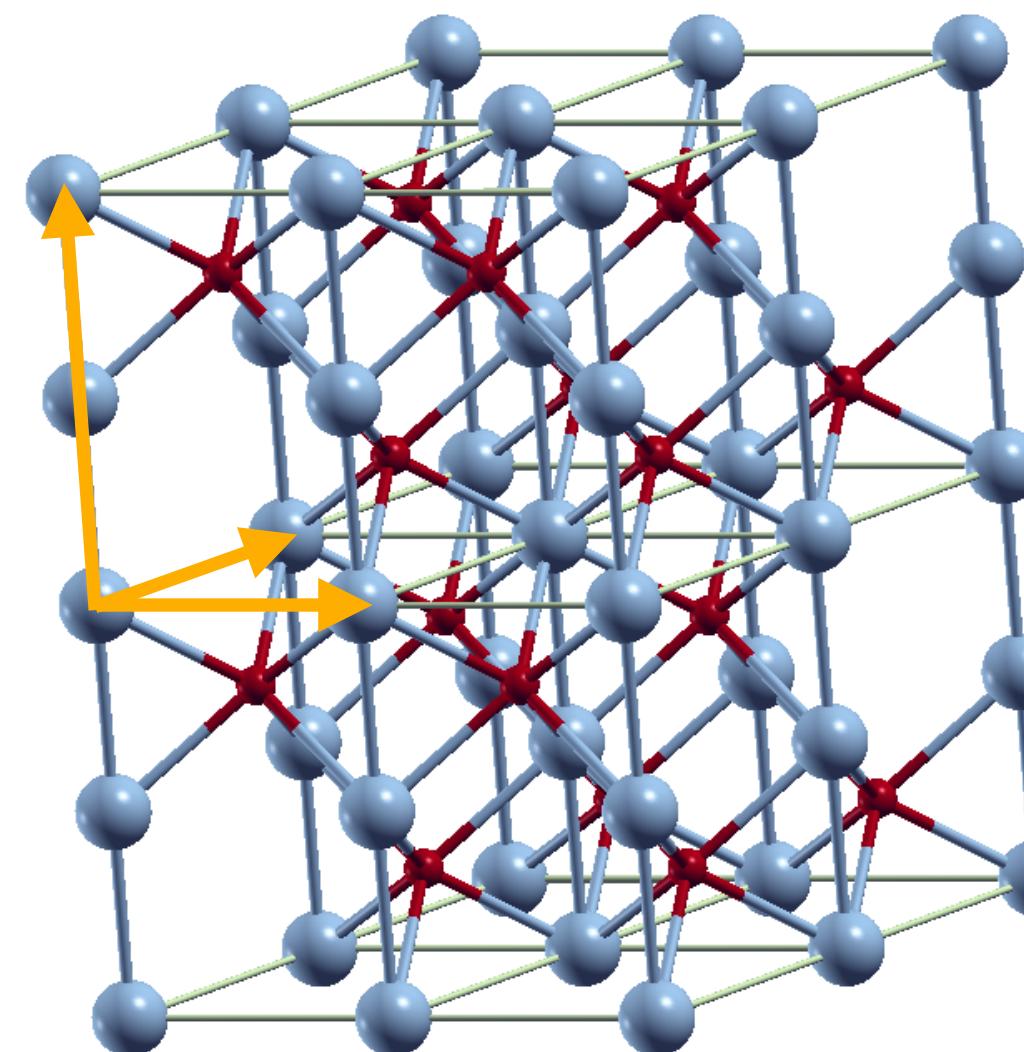
On-site U on O (small)

inter-site V: Mn-Mn n.n.n.

Input file MnO.scf.in

```
&control
  calculation = 'scf',
  verbosity = 'high',
  pseudo_dir = '../files/pseudo'
  outdir='./tmp'
  restart_mode='from_scratch'
  verbosity = 'high',
  wf_collect = .true.
  prefix='mno',
/
.
.
.
CELL_PARAMETERS
  0.5000000 0.8660254038 0.000000000
  -0.5000000 0.8660254038 0.000000000
   0.0000000 0.0000000000 1.583632480
ATOMIC_POSITIONS {crystal}
Mn1      0.000000000 0.000000000 0.000000000
Mn2      0.000000000 0.000000000 0.500000000
0        0.333333333 0.333333333 0.750000000
0        0.666666666 0.666666666 0.250000000
K_POINTS {automatic}
  4 4 3 0 0 0
```

```
HUBBARD ortho-atomic
V Mn1-3d Mn1-3d 1 1 2.0
V Mn2-3d Mn2-3d 2 2 2.0
V Mn1-3d 0-2p 1 12 1.0
V Mn2-3d 0-2p 2 3 1.0
V 0-2p 0-2p 3 3 1.d-5
V Mn1-3d Mn2-3d 1 2 0.2
```



HUBBARD ortho-atomic

V Mn1-3d Mn1-3d 1 1 2.0
V Mn2-3d Mn2-3d 2 2 2.0
V Mn1-3d 0-2p 1 12 1.0
V Mn2-3d 0-2p 2 3 1.0
V 0-2p 0-2p 3 3 1.d-5
V Mn1-3d Mn2-3d 1 2 0.2

On-site U on Mn

inter-site V: Mn-0 n.n.

On-site U on O (small)

inter-site V: Mn-Mn n.n.n.

How do we determine these numbers?

Input file MnO.scf.in

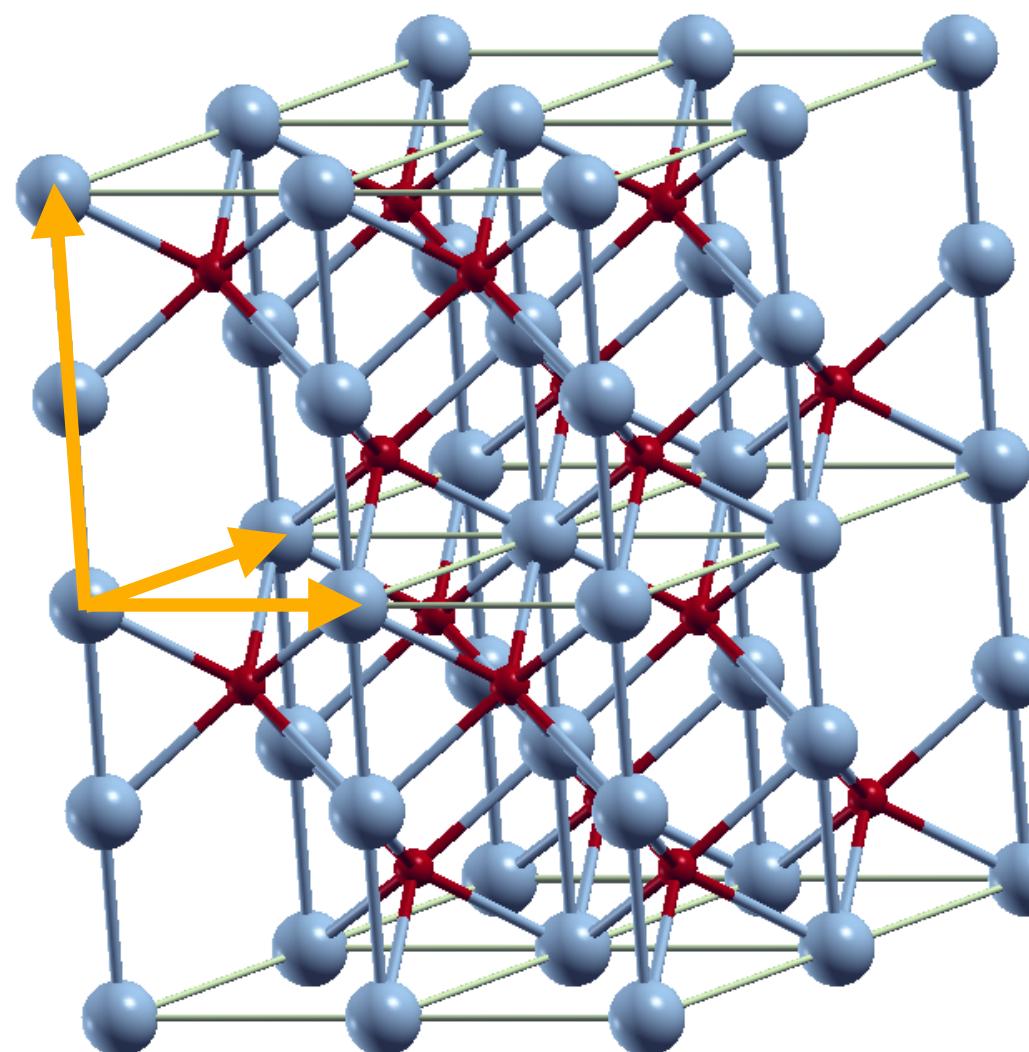
```
&control
  calculation = 'scf',
  verbosity = 'high',
  pseudo_dir = '../files/pseudo'
  outdir='./tmp'
  restart_mode='from_scratch'
  verbosity = 'high',
  wf_collect = .true.
  prefix='mno',
/
.
.
.
.

CELL_PARAMETERS
  0.5000000 0.8660254038 0.000000000
  -0.5000000 0.8660254038 0.000000000
   0.0000000 0.0000000000 1.583632480

ATOMIC_POSITIONS {crystal}
Mn1      0.000000000 0.000000000 0.000000000
Mn2      0.000000000 0.000000000 0.500000000
0        0.333333333 0.333333333 0.750000000
0        0.666666666 0.666666666 0.250000000

K_POINTS {automatic}
  4 4 3 0 0 0
```

```
HUBBARD ortho-atomic
V Mn1-3d Mn1-3d 1 1 2.0
V Mn2-3d Mn2-3d 2 2 2.0
V Mn1-3d 0-2p 1 12 1.0
V Mn2-3d 0-2p 2 3 1.0
V 0-2p 0-2p 3 3 1.d-5
V Mn1-3d Mn2-3d 1 2 0.2
```



HUBBARD ortho-atomic

```
V Mn1-3d Mn1-3d 1 1 2.0
V Mn2-3d Mn2-3d 2 2 2.0
V Mn1-3d 0-2p 1 12 1.0
V Mn2-3d 0-2p 2 3 1.0
V 0-2p 0-2p 3 3 1.d-5
V Mn1-3d Mn2-3d 1 2 0.2
```

Input file MnO.hp.in

```
&inputhp
  prefix='mno',
  outdir='../files/pseudo'
  outdir='./tmp'
  nq1 = 2, nq2 = 2, nq3 = 1,
  conv_thr_chi = 1.0d-7,
  alpha_mix(1) = 0.05
  docc_thr = 1.0d-4
  iverbosity = 2
  determine_num_pert_only = .false.
  niter_max = 200
/
```

On-site U on Mn

inter-site V: Mn-O n.n.

On-site U on O (small)

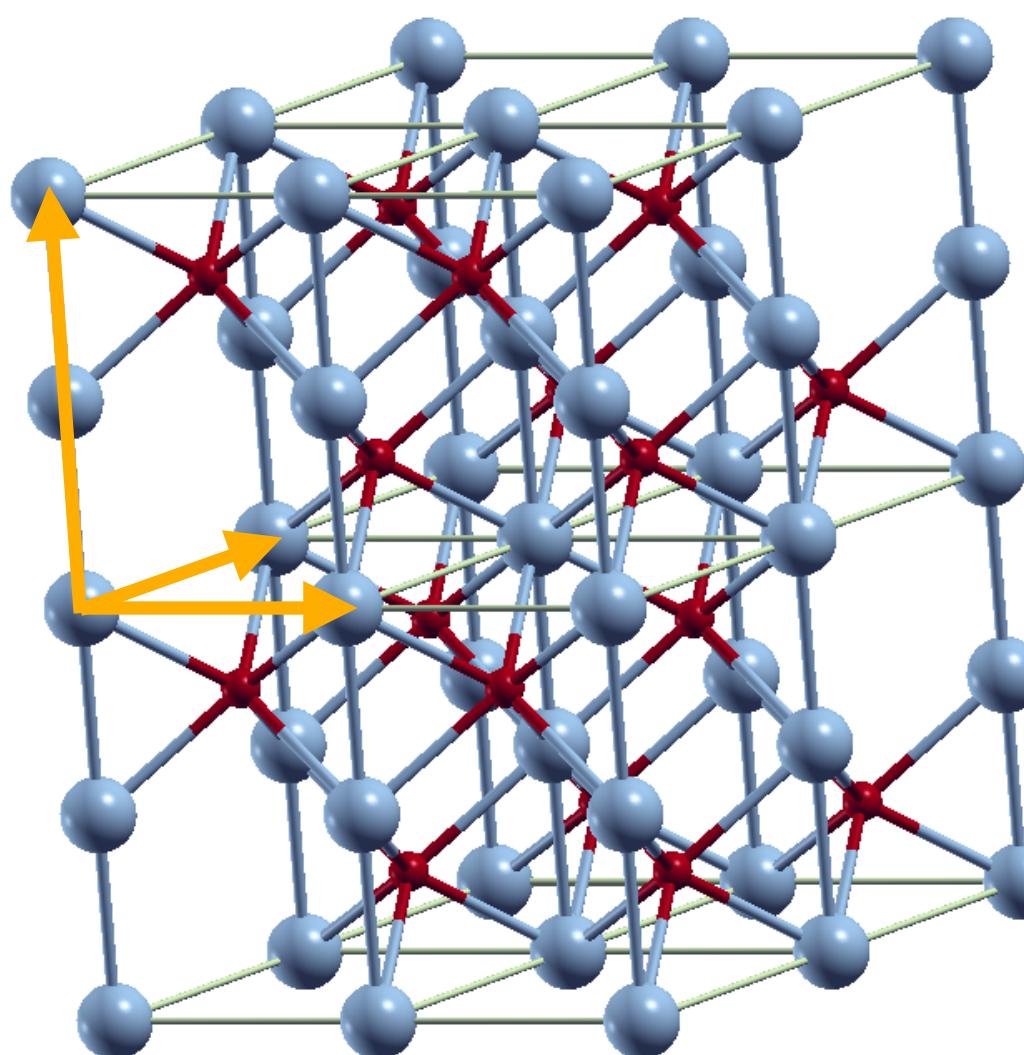
inter-site V: Mn-Mn n.n.n.

How do we determine these numbers?

Input file MnO.scf.in

```
&control
  calculation = 'scf',
  verbosity = 'high',
  pseudo_dir = '../files/pseudo'
  outdir='./tmp'
  restart_mode='from_scratch'
  verbosity = 'high',
  wf_collect = .true.
  prefix='mno',
/
.
.
.
.

CELL_PARAMETERS
  0.5000000 0.8660254038 0.000000000
  -0.5000000 0.8660254038 0.000000000
   0.0000000 0.0000000000 1.583632480
ATOMIC_POSITIONS {crystal}
Mn1      0.000000000 0.000000000 0.000000000
Mn2      0.000000000 0.000000000 0.500000000
0        0.333333333 0.333333333 0.750000000
0        0.666666666 0.666666666 0.250000000
K_POINTS {automatic}
  4 4 3 0 0 0
HUBBARD ortho-atomic
V Mn1-3d Mn1-3d 1 1 2.0
V Mn2-3d Mn2-3d 2 2 2.0
V Mn1-3d 0-2p 1 12 1.0
V Mn2-3d 0-2p 2 3 1.0
V 0-2p 0-2p 3 3 1.d-5
V Mn1-3d Mn2-3d 1 2 0.2
```



Input file MnO.hp.in

```
&inputhp
  prefix='mno',
  outdir='../files/pseudo'
  outdir='./tmp'
  nq1 = 2, nq2 = 2, nq3 = 1,
  conv_thr_chi = 1.0d-7,
  alpha_mix(1) = 0.05
  docc_thr = 1.0d-4
  iverbosity = 2
  determine_num_pert_only = .false.
  niter_max = 200
/
```

We could run a preliminary hp calculation with `determine_num_pert_only = .true.` and `hp.x` will tell us

HUBBARD ortho-atomic

V Mn1-3d Mn1-3d 1 1 2.0
V Mn2-3d Mn2-3d 2 2 2.0
V Mn1-3d 0-2p 1 12 1.0
V Mn2-3d 0-2p 2 3 1.0
V 0-2p 0-2p 3 3 1.d-5
V Mn1-3d Mn2-3d 1 2 0.2

On-site U on Mn

inter-site V: Mn-0 n.n.

On-site U on O (small)
inter-site V: Mn-Mn n.n.n.

How do we determine these numbers?

How to determine neighbour numbers?

File mno.Hubbard_parameters.dat

Atom 1	Atom 2	Distances Distance (Bohr)
1 Mn1	1 Mn1	0.000000
1 Mn1	48 0	3.685648
1 Mn1	24 0	3.685648
1 Mn1	12 0	3.685648
1 Mn1	43 0	3.685648
1 Mn1	19 0	3.685648
1 Mn1	55 0	3.685648
1 Mn1	2 Mn1	4.168754
1 Mn1	45 Mn1	5.264800
1 Mn1	33 Mn1	5.264800
1 Mn1	21 Mn1	5.264800
2 Mn1	2 Mn1	0.000000
2 Mn1	47 0	3.685648
2 Mn1	23 0	3.685648
2 Mn1	3 0	3.685648
2 Mn1	24 0	3.685648
2 Mn1	12 0	3.685648
2 Mn1	48 0	3.685648
2 Mn1	1 Mn1	4.168754
2 Mn1	46 Mn1	5.264800
2 Mn1	34 Mn1	5.264800
2 Mn1	22 Mn1	5.264800

How to determine neighbour numbers?

File mno.Hubbard_parameters.dat

Atom 1	Atom 2	Distances Distance (Bohr)	
1 Mn1	1 Mn1	0.000000	
1 Mn1	48 0	3.685648	
1 Mn1	24 0	3.685648	
1 Mn1	12 0	3.685648	
1 Mn1	43 0	3.685648	HUBBARD ortho-atomic
1 Mn1	19 0	3.685648	V Mn1-3d Mn1-3d 1 1 4.0
1 Mn1	55 0	3.685648	V Mn2-3d Mn2-3d 2 2 4.0
1 Mn1	2 Mn1	4.168754	V Mn1-3d 0-2p 1 12 1.0
1 Mn1	45 Mn1	5.264800	V Mn2-3d 0-2p 2 3 1.0
1 Mn1	33 Mn1	5.264800	V 0-2p 0-2p 3 3 1.d-5
1 Mn1	21 Mn1	5.264800	V Mn1-3d Mn2-3d 1 2 0.2
2 Mn1	2 Mn1	0.000000	
2 Mn1	47 0	3.685648	
2 Mn1	23 0	3.685648	
2 Mn1	3 0	3.685648	
2 Mn1	24 0	3.685648	
2 Mn1	12 0	3.685648	
2 Mn1	48 0	3.685648	
2 Mn1	1 Mn1	4.168754	
2 Mn1	46 Mn1	5.264800	
2 Mn1	34 Mn1	5.264800	
2 Mn1	22 Mn1	5.264800	

How to determine neighbour numbers?

File mno.Hubbard_parameters.dat

Atom 1	Atom 2	Distances Distance (Bohr)	HUBBARD ortho-atomic
1 Mn1	1 Mn1	0.000000	V Mn1-3d Mn1-3d 1 1 4.0
1 Mn1	48 0	3.685648	V Mn2-3d Mn2-3d 2 2 4.0
1 Mn1	24 0	3.685648	V Mn1-3d 0-2p 1 12 1.0
1 Mn1	12 0	3.685648	V Mn2-3d 0-2p 2 3 1.0
1 Mn1	43 0	3.685648	V 0-2p 0-2p 3 3 1.d-5
1 Mn1	19 0	3.685648	V Mn1-3d Mn2-3d 1 2 0.2
1 Mn1	55 0	3.685648	
1 Mn1	2 Mn1	4.168754	
1 Mn1	45 Mn1	5.264800	
1 Mn1	33 Mn1	5.264800	
1 Mn1	21 Mn1	5.264800	
2 Mn1	2 Mn1	0.000000	
2 Mn1	47 0	3.685648	
2 Mn1	23 0	3.685648	
2 Mn1	3 0	3.685648	
2 Mn1	24 0	3.685648	
2 Mn1	12 0	3.685648	
2 Mn1	48 0	3.685648	
2 Mn1	1 Mn1	4.168754	
2 Mn1	46 Mn1	5.264800	
2 Mn1	34 Mn1	5.264800	
2 Mn1	22 Mn1	5.264800	

How to determine neighbour numbers?

File mno.Hubbard_parameters.dat

Atom 1	Atom 2	Distances Distance (Bohr)
1 Mn1	1 Mn1	0.000000
1 Mn1	48 0	3.685648
1 Mn1	24 0	3.685648
1 Mn1	12 0	3.685648
1 Mn1	43 0	3.685648
1 Mn1	19 0	3.685648
1 Mn1	55 0	3.685648
1 Mn1	2 Mn1	4.168754
1 Mn1	45 Mn1	5.264800
1 Mn1	33 Mn1	5.264800
1 Mn1	21 Mn1	5.264800
2 Mn1	2 Mn1	0.000000
2 Mn1	47 0	3.685648
2 Mn1	23 0	3.685648
2 Mn1	3 0	3.685648
2 Mn1	24 0	3.685648
2 Mn1	12 0	3.685648
2 Mn1	48 0	3.685648
2 Mn1	1 Mn1	4.168754
2 Mn1	46 Mn1	5.264800
2 Mn1	34 Mn1	5.264800
2 Mn1	22 Mn1	5.264800

HUBBARD ortho-atomic
V Mn1-3d Mn1-3d 1 1 4.0
V Mn2-3d Mn2-3d 2 2 4.0
V Mn1-3d 0-2p 1 12 1.0
V Mn2-3d 0-2p 2 3 1.0
V 0-2p 0-2p 3 3 1.d-5
V Mn1-3d Mn2-3d 1 2 0.2

How to determine neighbour numbers?

File mno.Hubbard_parameters.dat

Atom 1	Atom 2	Distances Distance (Bohr)
1 Mn1	1 Mn1	0.000000
1 Mn1	48 0	3.685648
1 Mn1	24 0	3.685648
1 Mn1	12 0	3.685648
1 Mn1	43 0	3.685648
1 Mn1	19 0	3.685648
1 Mn1	55 0	3.685648
1 Mn1	2 Mn1	4.168754
1 Mn1	45 Mn1	5.264800
1 Mn1	33 Mn1	5.264800
1 Mn1	21 Mn1	5.264800
2 Mn1	2 Mn1	0.000000
2 Mn1	47 0	3.685648
2 Mn1	23 0	3.685648
2 Mn1	3 0	3.685648
2 Mn1	24 0	3.685648
2 Mn1	12 0	3.685648
2 Mn1	48 0	3.685648
2 Mn1	1 Mn1	4.168754
2 Mn1	46 Mn1	5.264800
2 Mn1	34 Mn1	5.264800
2 Mn1	22 Mn1	5.264800

HUBBARD ortho-atomic
V Mn1-3d Mn1-3d 1 1 4.0
V Mn2-3d Mn2-3d 2 2 4.0
V Mn1-3d 0-2p 1 12 1.0
V Mn2-3d 0-2p 2 3 1.0
V 0-2p 0-2p 3 3 1.d-5
V Mn1-3d Mn2-3d 1 2 0.2

Calculation of U and V from the DFT ground state (metallic)

Input file MnO.scf.UV.in

```
&control
  calculation = 'scf',
  verbosity = 'high',
  pseudo_dir = '../files/pseudo'
 outdir='./tmp'
  restart_mode='from_scratch'
  verbosity = 'high',
  prefix='MnO',
/
&system
  ibrav = 0,
  celldm(1) = 5.2648,
  nat = 4,
  ntyp = 3,
  nspin = 2,
  starting_magnetization(1) = 0.4,
  starting_magnetization(2) = -0.4,
  ecutwfc = 45.0,
  ecutrho = 450.0,
  nbnd = 28
  occupations = 'smearing',
  smearing = 'mv',
  degauss = 0.01
/
&electrons
  mixing_beta = 0.2
  mixing_ndim = 20
  mixing_mode = 'local-TF'
  conv_thr = 1.0d-8,
  electron_maxstep = 200
/
ATOMIC_SPECIES
  Mn1 1.0 mn_pbesol_v1.5.uspp.F.UPF
  Mn2 1.0 mn_pbesol_v1.5.uspp.F.UPF
  O 1.0 O.pbesol-n-kjpaw_psl.0.1.UPF
CELL_PARAMETERS
  0.5000000 0.8660254038 0.000000000
  -0.5000000 0.8660254038 0.000000000
  0.0000000 0.000000000 1.583632480
ATOMIC_POSITIONS {crystal}
Mn1    0.00000000  0.00000000  0.000000000
Mn2    0.00000000  0.00000000  0.500000000
O      0.33333333  0.33333333  0.750000000
O      0.66666666  0.66666666  0.250000000
K_POINTS {automatic}
  4 4 3 0 0 0
HUBBARD ortho-atomic
V Mn1-3d Mn1-3d 1 1 1.d-4
V Mn2-3d Mn2-3d 2 2 1.d-4
V Mn1-3d 0-2p   1 3 1.d-4
V Mn2-3d 0-2p   2 3 1.d-4
```

Input file MnO.hp.in

```
&inpathp
  prefix='MnO',
  outdir='./tmp'
  nq1 = 2, nq2 = 2, nq3 = 1,
  conv_thr_chi = 1.0d-7,
  alpha_mix(1) = 0.05
  docc_thr = 1.0d-4
  iverbosity = 2
  determine_num_pert_only = .false.
  niter_max = 200
/
```

```
pw.x < MnO.scf.UV.in |tee MnO.scf.UV.out
hp.x < MnO.hp.in |tee MnO.hp.out
```

We set some small initial value
just to activate the Hubbard machinery in the code

Calculation of U and V from the DFT ground state (metallic)

Input file MnO.scf.UV.in

```
&control
  calculation = 'scf',
  verbosity = 'high',
  pseudo_dir = '../files/pseudo'
 outdir='./tmp'
  restart_mode='from_scratch'
  verbosity = 'high',
  prefix='MnO',
/
&system
  ibrav = 0,
  celldm(1) = 5.2648,
  nat = 4,
  ntyp = 3,
  nspin = 2,
  starting_magnetization(1) = 0.4,
  starting_magnetization(2) = -0.4,
  ecutwfc = 45.0,
  ecutrho = 450.0,
  nbnd = 28
  occupations = 'smearing',
  smearing = 'mv',
  degauss = 0.01
/
&electrons
  mixing_beta = 0.2
  mixing_ndim = 20
  mixing_mode = 'local-TF'
  conv_thr = 1.0d-8,
  electron_maxstep = 200
/
ATOMIC_SPECIES
  Mn1 1.0 mn_pbesol_v1.5.uspp.F.UPF
  Mn2 1.0 mn_pbesol_v1.5.uspp.F.UPF
  O 1.0 O.pbesol-n-kjpaw_psl.0.1.UPF
CELL_PARAMETERS
  0.5000000 0.8660254038 0.000000000
  -0.5000000 0.8660254038 0.000000000
  0.0000000 0.000000000 1.583632480
ATOMIC_POSITIONS {crystal}
Mn1    0.00000000  0.00000000  0.000000000
Mn2    0.00000000  0.00000000  0.500000000
O     0.33333333  0.33333333  0.750000000
O     0.66666666  0.66666666  0.250000000
K_POINTS {automatic}
  4 4 3 0 0 0
HUBBARD ortho-atomic
V Mn1-3d Mn1-3d 1 1 1.d-4
V Mn2-3d Mn2-3d 2 2 1.d-4
V Mn1-3d 0-2p   1 3 1.d-4
V Mn2-3d 0-2p   2 3 1.d-4
```

Input file MnO.hp.in

```
&inpuhp
  prefix='MnO',
  outdir='./tmp'
  nq1 = 2, nq2 = 2, nq3 = 1,
  conv_thr_chi = 1.0d-7,
  alpha_mix(1) = 0.05
  docc_thr = 1.0d-4
  iverbosity = 2
  determine_num_pert_only = .false.
  niter_max = 200
/
```

```
pw.x < MnO.scf.UV.in |tee MnO.scf.UV.out
hp.x < MnO.hp.in |tee MnO.hp.out
```

We set some small initial value
just to activate the Hubbard machinery in the code

Calculation of U and V from the DFT+ U + V ground state (insulating)

Calculation of U and V from the DFT+ U + V ground state (insulating)

```
pw.x < Mn0.scf.UV.in | tee Mn0.scf.UV.out
```

Calculation of U and V from the DFT+ U + V ground state (insulating)

```
pw.x < Mn0.scf.UV.in | tee Mn0.scf.UV.out
```

```
nstates=`grep 'number of Kohn-Sham states' Mn0.scf.UV.out | awk '{print $5}'`
```

```
totmagn=`grep 'total magnetization' Mn0.scf.UV.out | tail -1 | awk '{print $4}'`
```

Calculation of U and V from the DFT+ U + V ground state (insulating)

```
pw.x < Mn0.scf.UV.in | tee Mn0.scf.UV.out
```

```
nstates=`grep 'number of Kohn-Sham states' Mn0.scf.UV.out | awk '{print $5}'`  
totmagn=`grep 'total magnetization' Mn0.scf.UV.out | tail -1 | awk '{print $4}'`  
  
&system  
    ibrav= 0, celldm(1)=5.2648, nat= 4, ntyp= 3,  
    nspin = 2,  
    starting_magnetization(1) = 0.4,  
    starting_magnetization(2) = -0.4,  
    ecutwfc = 45,  
    ecutrho = 450,  
    nbnd = 28  
    occupations='fixed',  
    smearing='mv',  
    degauss=0.01  
    nbnd = $nstates  
    tot_magnetization = $totmagn  
/  
&electrons  
    mixing_beta = 0.2  
    mixing_ndim = 20  
    mixing_mode = 'local-TF'  
    conv_thr = 1.0d-8,  
    electron_maxstep = 200  
    startingpot = 'file'  
    startingwfc = 'file'  
/
```

Build a Mn0.scf.UV.2.in with:

Calculation of U and V from the DFT+ U + V ground state (insulating)

```
pw.x < Mn0.scf.UV.in | tee Mn0.scf.UV.out
```

```
nstates=`grep 'number of Kohn-Sham states' Mn0.scf.UV.out | awk '{print $5}'`  
totmagn=`grep 'total magnetization' Mn0.scf.UV.out | tail -1 | awk '{print $4}'`  
  
Build a Mn0.scf.UV.2.in with:  
  
&system  
    ibrav= 0, celldm(1)=5.2648, nat= 4, ntyp= 3,  
    nspin = 2,  
    starting_magnetization(1) = 0.4,  
    starting_magnetization(2) = -0.4,  
    ecutwfc = 45,  
    ecutrho = 450,  
    nbnd = 28  
    occupations='fixed',  
    smearing='mv',  
    degauss=0.01  
    nbnd = $nstates  
    tot_magnetization = $totmagn  
/  
&electrons  
    mixing_beta = 0.2  
    mixing_ndim = 20  
    mixing_mode = 'local-TF'  
    conv_thr = 1.0d-8,  
    electron_maxstep = 200  
    startingpot = 'file'  
    startingwfc = 'file'  
/  
pw.x < Mn0.scf.UV.2.in | tee Mn0.scf.UV.2.out
```

Calculation of U and V from the DFT+ U + V ground state (insulating)

```
pw.x < Mn0.scf.UV.in | tee Mn0.scf.UV.out
```

```
nstates=`grep 'number of Kohn-Sham states' Mn0.scf.UV.out | awk '{print $5}'`  
totmagn=`grep 'total magnetization' Mn0.scf.UV.out | tail -1 | awk '{print $4}'`
```

```
&system  
  ibrav= 0, celldm(1)=5.2648, nat= 4, ntyp= 3,  
  nspin = 2,  
  starting_magnetization(1) = 0.4,  
  starting_magnetization(2) = -0.4,  
  ecutwfc = 45,  
  ecutrho = 450,  
  nbnd = 28  
  occupations='fixed',  
  smearing='mv',  
  degauss=0.01  
  nbnd = $nstates  
  tot_magnetization = $totmagn  
/  
&electrons  
  mixing_beta = 0.2  
  mixing_ndim = 20  
  mixing_mode = 'local-TF'  
  conv_thr = 1.0d-8,  
  electron_maxstep = 200  
  startingpot = 'file'  
  startingwfc = 'file'  
/
```

```
pw.x < Mn0.scf.UV.2.in | tee Mn0.scf.UV.2.out
```

```
hp.x < Mn0.hp.in | tee Mn0.hp.out
```

Results

File MnO.Hubbard_parameters.dat

Hubbard V parameters:
(adapted for a supercell 3x3x3)

Atom 1	Atom 2	Distance (Bohr)	Hubbard V (eV)
--------	--------	-----------------	----------------

1 Mn1	1 Mn1	0.00000	5.7430
1 Mn1	48 0	3.685648	0.3537
1 Mn1	24 0	3.685648	0.3537
1 Mn1	12 0	3.685648	0.3537
1 Mn1	43 0	3.685648	0.3537
1 Mn1	19 0	3.685648	0.3537
1 Mn1	55 0	3.685648	0.3537
1 Mn1	2 Mn1	4.168754	0.2557

New calculation:

2 Mn1	2 Mn1	0.00000	5.7430
2 Mn1	47 0	3.685648	0.3537
2 Mn1	23 0	3.685648	0.3537
2 Mn1	3 0	3.685648	0.3537
2 Mn1	24 0	3.685648	0.3537
2 Mn1	12 0	3.685648	0.3537
2 Mn1	48 0	3.685648	0.3537
2 Mn1	1 Mn1	4.168754	0.2557

3 0	3 0	0.00000	8.6179
3 0	2 Mn1	3.685648	0.3537
3 0	57 Mn1	3.685648	0.3537
3 0	90 Mn1	3.685648	0.3537
3 0	66 Mn1	3.685648	0.3537
3 0	93 Mn1	3.685648	0.3537
3 0	69 Mn1	3.685648	0.3537

Results

File MnO.Hubbard_parameters.dat

Hubbard V parameters:
(adapted for a supercell 3x3x3)

Atom 1	Atom 2	Distance (Bohr)	Hubbard V (eV)
1 Mn1	1 Mn1	0.000000	5.7430
1 Mn1	48 0	3.685648	0.3537
1 Mn1	24 0	3.685648	0.3537
1 Mn1	12 0	3.685648	0.3537
1 Mn1	43 0	3.685648	0.3537
1 Mn1	19 0	3.685648	0.3537
1 Mn1	55 0	3.685648	0.3537
1 Mn1	2 Mn1	4.168754	0.2557
·	·		
2 Mn1	2 Mn1	0.000000	5.7430
2 Mn1	47 0	3.685648	0.3537
2 Mn1	23 0	3.685648	0.3537
2 Mn1	3 0	3.685648	0.3537
2 Mn1	24 0	3.685648	0.3537
2 Mn1	12 0	3.685648	0.3537
2 Mn1	48 0	3.685648	0.3537
2 Mn1	1 Mn1	4.168754	0.2557
·	·		
3 0	3 0	0.000000	8.6179
3 0	2 Mn1	3.685648	0.3537
3 0	57 Mn1	3.685648	0.3537
3 0	90 Mn1	3.685648	0.3537
3 0	66 Mn1	3.685648	0.3537
3 0	93 Mn1	3.685648	0.3537
3 0	69 Mn1	3.685648	0.3537

New calculation:

HUBBARD ortho-atomic
V Mn1-3d Mn1-3d 1 1 **5.74**
V Mn2-3d Mn2-3d 2 2 **5.74**
V Mn1-3d 0-2p 1 12 **0.3537**
V Mn2-3d 0-2p 2 3 **0.3537**
V 0-2p 0-2p 3 3 1.d-5
V Mn1-3d Mn2-3d 1 2 **0.2557**

Results

File MnO.Hubbard_parameters.dat

Hubbard V parameters:
(adapted for a supercell 3x3x3)

Atom 1	Atom 2	Distance (Bohr)	Hubbard V (eV)
--------	--------	-----------------	----------------

1 Mn1	1 Mn1	0.00000	5.7430
1 Mn1	48 0	3.685648	0.3537
1 Mn1	24 0	3.685648	0.3537
1 Mn1	12 0	3.685648	0.3537
1 Mn1	43 0	3.685648	0.3537
1 Mn1	19 0	3.685648	0.3537
1 Mn1	55 0	3.685648	0.3537
1 Mn1	2 Mn1	4.168754	0.2557

2 Mn1	2 Mn1	0.00000	5.7430
2 Mn1	47 0	3.685648	0.3537
2 Mn1	23 0	3.685648	0.3537
2 Mn1	3 0	3.685648	0.3537
2 Mn1	24 0	3.685648	0.3537
2 Mn1	12 0	3.685648	0.3537
2 Mn1	48 0	3.685648	0.3537
2 Mn1	1 Mn1	4.168754	0.2557

3 0	3 0	0.00000	8.6179
3 0	2 Mn1	3.685648	0.3537
3 0	57 Mn1	3.685648	0.3537
3 0	90 Mn1	3.685648	0.3537
3 0	66 Mn1	3.685648	0.3537
3 0	93 Mn1	3.685648	0.3537
3 0	69 Mn1	3.685648	0.3537

New calculation:

HUBBARD ortho-atomic
V Mn1-3d Mn1-3d 1 1 **5.74**
V Mn2-3d Mn2-3d 2 2 **5.74**
V Mn1-3d 0-2p 1 12 **0.3537**
V Mn2-3d 0-2p 2 3 **0.3537**
V 0-2p 0-2p 3 3 1.d-5
V Mn1-3d Mn2-3d 1 2 **0.2557**

Not used

Results: second and third steps

New files mno.Hubbard_parameters.dat

Hubbard V parameters:
(adapted for a supercell 3x3x3)

Atom 1	Atom 2	Distance (Bohr)	Hubbard V (eV)
1 Mn1	1 Mn1	0.000000	5.2612
1 Mn1	48 0	3.685648	0.2980
1 Mn1	24 0	3.685648	0.2980
1 Mn1	12 0	3.685648	0.2980
1 Mn1	43 0	3.685648	0.2980
1 Mn1	19 0	3.685648	0.2980
1 Mn1	55 0	3.685648	0.2980
1 Mn1	2 Mn1	4.168754	0.2685

Results: second and third steps

New files mno.Hubbard_parameters.dat

Hubbard V parameters:
(adapted for a supercell 3x3x3)

Atom 1	Atom 2	Distance (Bohr)	Hubbard V (eV)
1 Mn1	1 Mn1	0.000000	5.2612
1 Mn1	48 0	3.685648	0.2980
1 Mn1	24 0	3.685648	0.2980
1 Mn1	12 0	3.685648	0.2980
1 Mn1	43 0	3.685648	0.2980
1 Mn1	19 0	3.685648	0.2980
1 Mn1	55 0	3.685648	0.2980
1 Mn1	2 Mn1	4.168754	0.2685

Hubbard V parameters:
(adapted for a supercell 3x3x3)

Atom 1	Atom 2	Distance (Bohr)	Hubbard V (eV)
1 Mn1	1 Mn1	0.000000	5.3149
1 Mn1	48 0	3.685648	0.3031
1 Mn1	24 0	3.685648	0.3031
1 Mn1	12 0	3.685648	0.3031
1 Mn1	43 0	3.685648	0.3031
1 Mn1	19 0	3.685648	0.3031
1 Mn1	55 0	3.685648	0.3031
1 Mn1	2 Mn1	4.168754	0.2698

Results: second and third steps

New files mno.Hubbard_parameters.dat

Hubbard V parameters:
(adapted for a supercell 3x3x3)

Atom 1	Atom 2	Distance (Bohr)	Hubbard V (eV)
1 Mn1	1 Mn1	0.000000	5.2612
1 Mn1	48 0	3.685648	0.2980
1 Mn1	24 0	3.685648	0.2980
1 Mn1	12 0	3.685648	0.2980
1 Mn1	43 0	3.685648	0.2980
1 Mn1	19 0	3.685648	0.2980
1 Mn1	55 0	3.685648	0.2980
1 Mn1	2 Mn1	4.168754	0.2685

Hubbard V parameters:
(adapted for a supercell 3x3x3)

Atom 1	Atom 2	Distance (Bohr)	Hubbard V (eV)
1 Mn1	1 Mn1	0.000000	5.3149
1 Mn1	48 0	3.685648	0.3031
1 Mn1	24 0	3.685648	0.3031
1 Mn1	12 0	3.685648	0.3031
1 Mn1	43 0	3.685648	0.3031
1 Mn1	19 0	3.685648	0.3031
1 Mn1	55 0	3.685648	0.3031
1 Mn1	2 Mn1	4.168754	0.2698

Hubbard V parameters:
(adapted for a supercell 3x3x3)

Atom 1	Atom 2	Distance (Bohr)	Hubbard V (eV)
1 Mn1	1 Mn1	0.000000	5.3087
1 Mn1	48 0	3.685648	0.3025
1 Mn1	24 0	3.685648	0.3025
1 Mn1	12 0	3.685648	0.3025
1 Mn1	43 0	3.685648	0.3025
1 Mn1	19 0	3.685648	0.3025
1 Mn1	55 0	3.685648	0.3025
1 Mn1	2 Mn1	4.168754	0.2694

Results: second and third steps

New files mno.Hubbard_parameters.dat

Hubbard V parameters:
(adapted for a supercell 3x3x3)

Atom 1	Atom 2	Distance (Bohr)	Hubbard V (eV)
1 Mn1	1 Mn1	0.000000	5.2612
1 Mn1	48 0	3.685648	0.2980
1 Mn1	24 0	3.685648	0.2980
1 Mn1	12 0	3.685648	0.2980
1 Mn1	43 0	3.685648	0.2980
1 Mn1	19 0	3.685648	0.2980
1 Mn1	55 0	3.685648	0.2980
1 Mn1	2 Mn1	4.168754	0.2685

Hubbard V parameters:
(adapted for a supercell 3x3x3)

Atom 1	Atom 2	Distance (Bohr)	Hubbard V (eV)
1 Mn1	1 Mn1	0.000000	5.3149
1 Mn1	48 0	3.685648	0.3031
1 Mn1	24 0	3.685648	0.3031
1 Mn1	12 0	3.685648	0.3031
1 Mn1	43 0	3.685648	0.3031
1 Mn1	19 0	3.685648	0.3031
1 Mn1	55 0	3.685648	0.3031
1 Mn1	2 Mn1	4.168754	0.2698

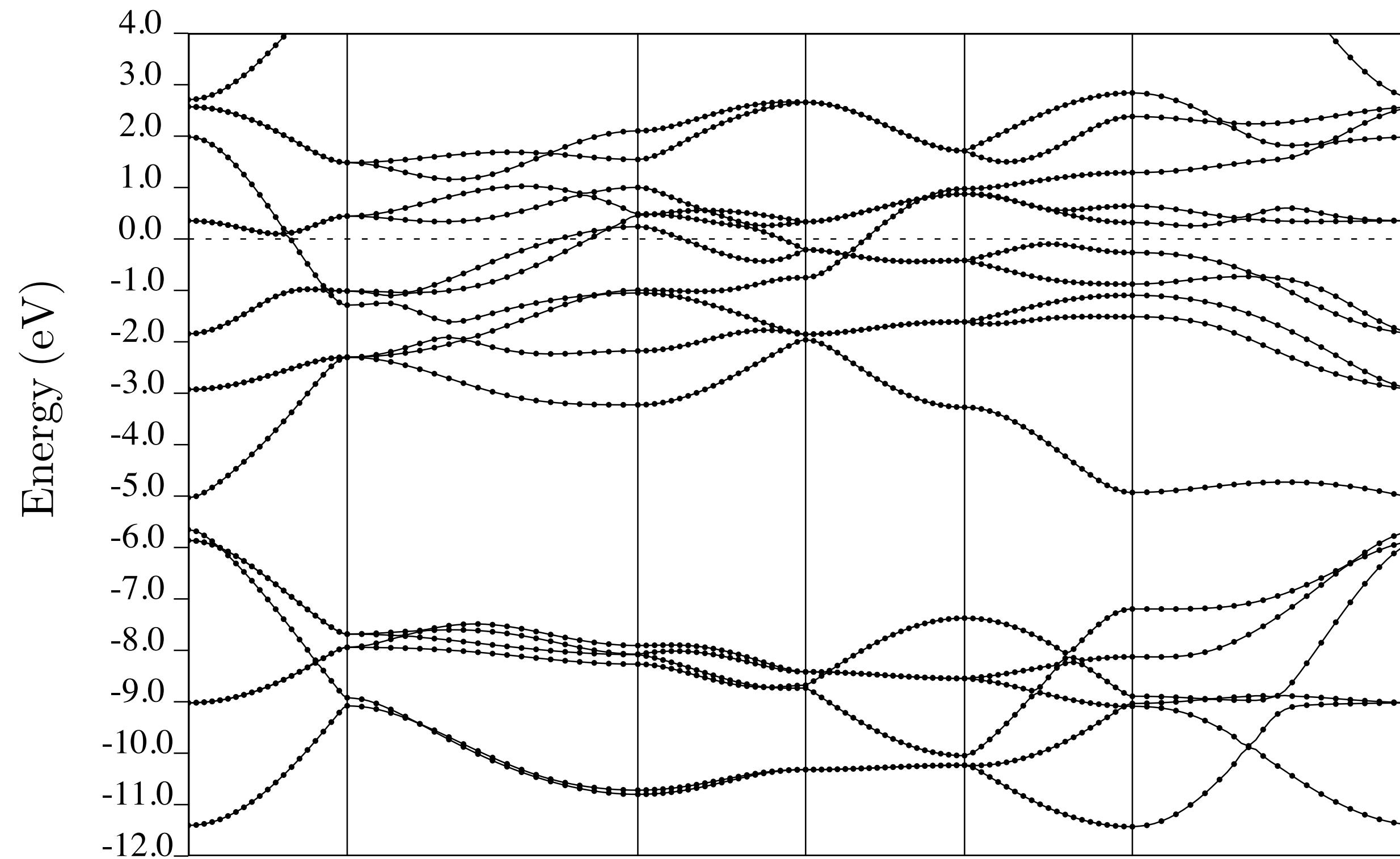
Hubbard V parameters:
(adapted for a supercell 3x3x3)

Atom 1	Atom 2	Distance (Bohr)	Hubbard V (eV)
1 Mn1	1 Mn1	0.000000	5.3087
1 Mn1	48 0	3.685648	0.3025
1 Mn1	24 0	3.685648	0.3025
1 Mn1	12 0	3.685648	0.3025
1 Mn1	43 0	3.685648	0.3025
1 Mn1	19 0	3.685648	0.3025
1 Mn1	55 0	3.685648	0.3025
1 Mn1	2 Mn1	4.168754	0.2694

Convergence has been reached!

Energy bands

PBEsol



PBEsol+U+V

