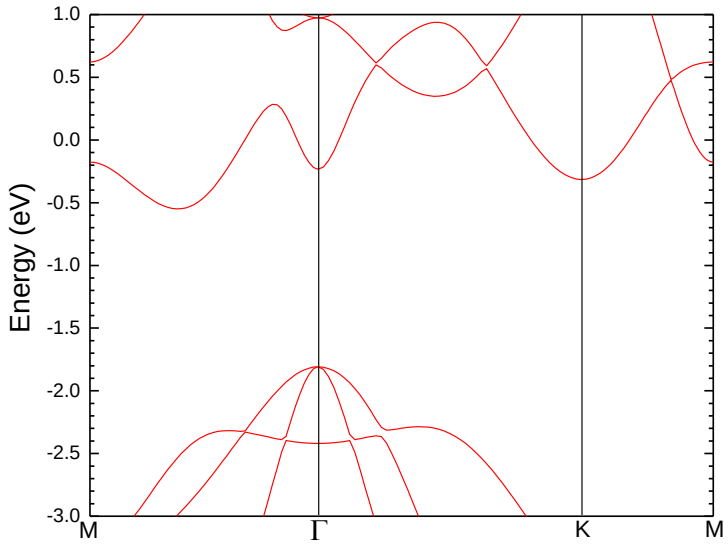
Solution for excercise sheet 4

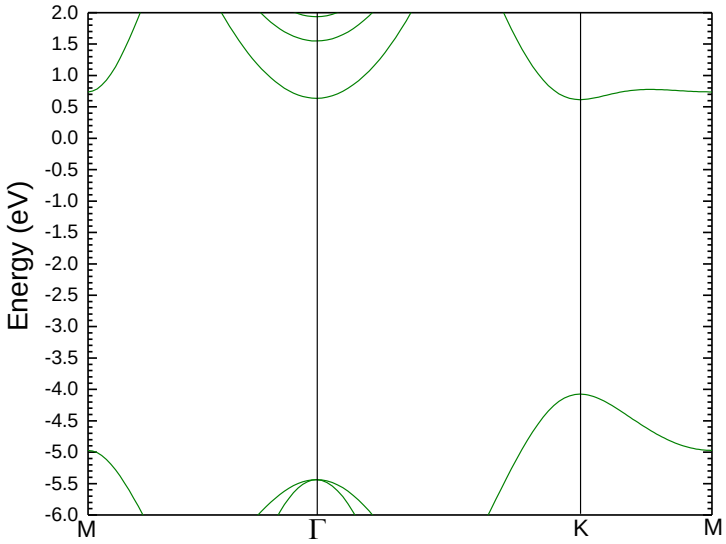
Exercise 1: Band alignment between monolayer boron nitride and antimonene

(a)

```
     atom    1 type  1   force =     0.00000000    0.00000000    0.00006528
     atom    2 type  1   force =    -0.00000000   -0.00000000   -0.00006528

     Total force =     0.000092     Total SCF correction =     0.000004


     Computing stress (Cartesian axis) and pressure


     negative rho (up, down):  4.386E-07 0.000E+00
          total   stress  (Ry/bohr**3)                   (kbar)     P=   -0.12
  -0.00000006  -0.00000000   0.00000000         -0.01     -0.00      0.00
  -0.00000000  -0.00000006   0.00000000         -0.00     -0.01      0.00
   0.00000000   0.00000000  -0.00000224          0.00      0.00     -0.33


     bfgs converged in  12 scf cycles and  11 bfgs steps
     (criteria: energy <  1.0E-04 Ry, force <  1.0E-03Ry/Bohr, cell <  1.0E-02kbar)

     End of BFGS Geometry Optimization

     Final enthalpy =    -363.8062938778 Ry
Begin final coordinates
     new unit-cell volume =   1979.95766 a.u.^3 (   293.39945 Ang^3 )
     density =      1.37824 g/cm^3

CELL_PARAMETERS (angstrom)
   4.115753297  -0.000000000   0.000000000
  -2.057876648   3.564346911   0.000000000
   0.000000000   0.000000000  20.000000000

ATOMIC_POSITIONS (angstrom)
Sb       0.000000000   0.000000000  -0.820132609
Sb       2.057876951   1.188115637   0.820132609
End final coordinates
```

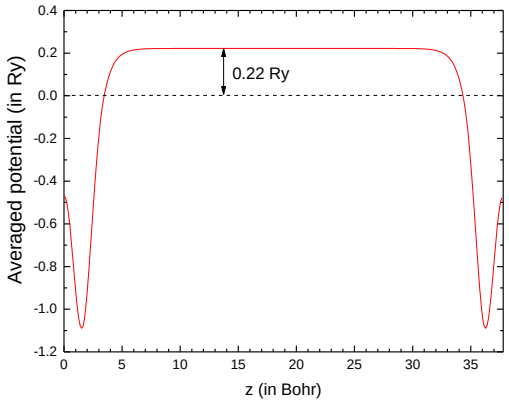


(b)

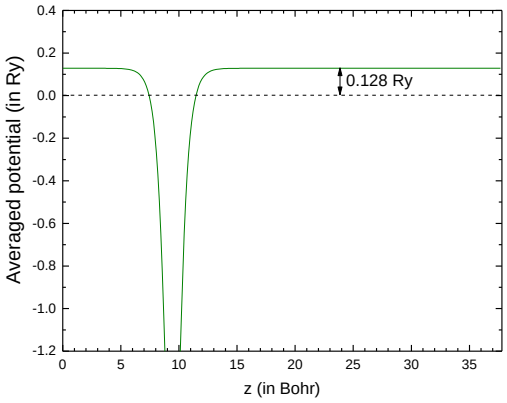


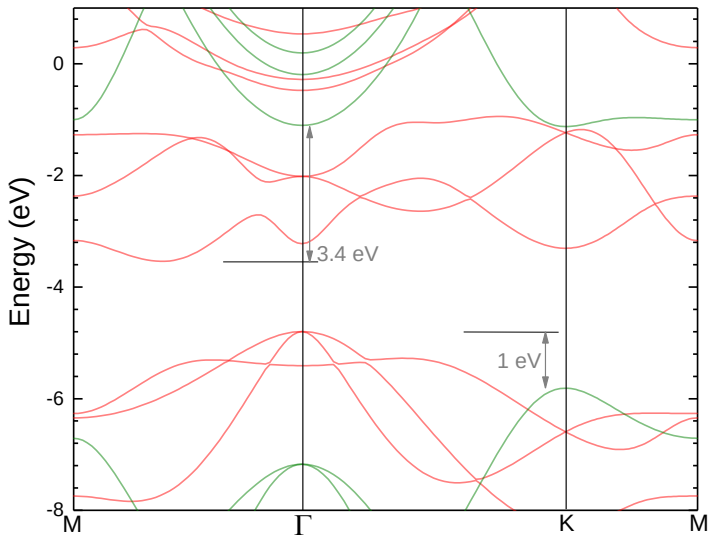
(c)

Antimonene



Boron nitride





Valence band maximum: In Antimonene

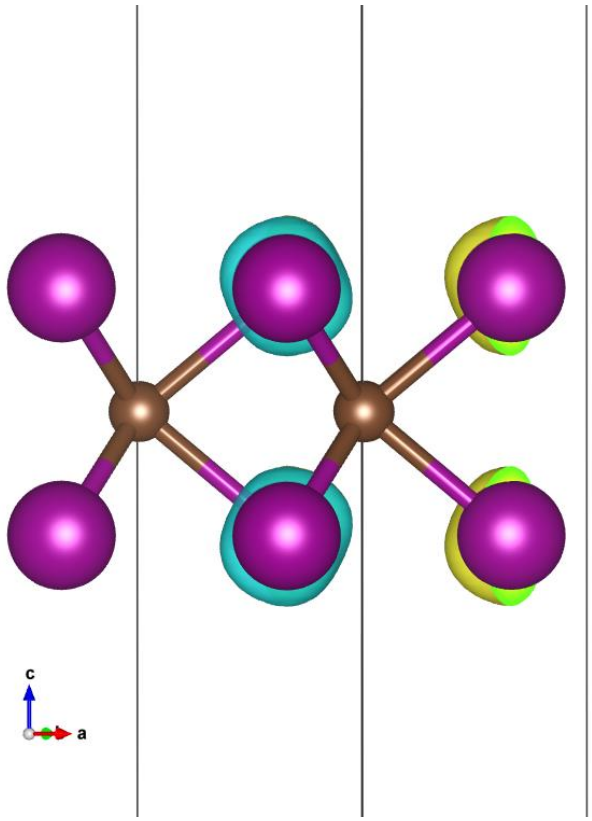
Conduction band minimum: In Antimonene

Valence band offset: 1 eV
Conduction band offset: 3.4 eV

Exercise 2: Magnetism in two-dimensional Mn_2C.

(a)

```
     atom    3 type  1   force =     0.00000000   -0.00001129    0.00000003
     atom    4 type  1   force =     0.00000000   -0.00001129   -0.00000003
     atom    5 type  2   force =     0.00000000   -0.00001140    0.00000012
     atom    6 type  2   force =     0.00000000   -0.00001140   -0.00000012

     Total force =     0.000039     Total SCF correction =     0.000025
     SCF correction compared to forces is large: reduce conv_thr to get better values


     Computing stress (Cartesian axis) and pressure

          total   stress  (Ry/bohr**3)                   (kbar)     P=   -0.36
  -0.00000001   0.00000000   0.00000000         -0.00      0.00      0.00
   0.00000000  -0.00000011   0.00000000          0.00     -0.02      0.00
   0.00000000   0.00000000  -0.00000731          0.00      0.00     -1.08

     Message from routine bfgs:
     history already reset at previous step: stopping

     bfgs converged in   7 scf cycles and   6 bfgs steps
     (criteria: energy <  1.0E-04 Ry, force <  4.0E-04Ry/Bohr, cell <  1.0E-02kbar)

     End of BFGS Geometry Optimization

     Final enthalpy =    -893.5242173025 Ry
Begin final coordinates
     new unit-cell volume =   1597.36006 a.u.^3 (   236.70434 Ang^3 )
     density =      1.70976 g/cm^3

CELL_PARAMETERS (angstrom)
   2.635968696   0.000000000   0.000000000
   0.000000000   4.489892795   0.000000000
   0.000000000   0.000000000  20.000000000

ATOMIC_POSITIONS (crystal)
C        0.000000000   0.007905982   0.500000000
C        0.500000000   0.507906089   0.500000000
Mn1      0.000000000   0.662713624   0.562508527
Mn1      0.000000000   0.662713624  -0.562508527
Mn2      0.500000000   0.162713674   0.562508515
Mn2      0.500000000   0.162713674  -0.562508515
End final coordinates
```



Yelelow: Spin up density > Spin down density
Blue: Spin-down density > spin up density

(b) Ferromagnetic:

```
     Forces acting on atoms (cartesian axes, Ry/au):

     atom    1 type  2   force =     0.00000000    0.00000000    0.00000000
     atom    2 type  1   force =    -0.00000000   -0.00000000   -0.00000282
     atom    3 type  1   force =    -0.00000000   -0.00000000    0.00000282

     Total force =     0.000004     Total SCF correction =     0.000018
     SCF correction compared to forces is large: reduce conv_thr to get better values


     Computing stress (Cartesian axis) and pressure


     negative rho (up, down):  0.000E+00 1.667E-03
          total   stress  (Ry/bohr**3)                   (kbar)     P=   -0.24
   0.00000005   0.00000000  -0.00000000          0.01      0.00     -0.00
   0.00000000   0.00000005  -0.00000000          0.00      0.01     -0.00
   0.00000000   0.00000000  -0.00000490          0.00      0.00     -0.72


     bfgs converged in   9 scf cycles and   8 bfgs steps
     (criteria: energy <  1.0E-04 Ry, force <  4.0E-04Ry/Bohr, cell <  1.0E-02kbar)

     End of BFGS Geometry Optimization

     Final enthalpy =    -446.7517616189 Ry
Begin final coordinates
     new unit-cell volume =    763.37200 a.u.^3 (   113.12006 Ang^3 )
     density =      1.78884 g/cm^3

CELL_PARAMETERS (angstrom)
   2.555580086  -0.000000000   0.000000000
  -1.277790043   2.213197276   0.000000000
   0.000000000   0.000000000  20.000000000

ATOMIC_POSITIONS (crystal)
C        0.000000000   0.000000000   0.500000000
Mn       0.333333333   0.666666667   0.562066321
Mn       0.333333333   0.666666667  -0.562066321
End final coordinates
```

Non-magnetic

```
     Forces acting on atoms (cartesian axes, Ry/au):

     atom    1 type  2   force =     0.00000000    0.00000000    0.00000000
     atom    2 type  1   force =     0.00000000    0.00000000   -0.00000612
     atom    3 type  1   force =    -0.00000000   -0.00000000    0.00000612

     Total force =     0.000009     Total SCF correction =     0.000001
     SCF correction compared to forces is large: reduce conv_thr to get better values


     Computing stress (Cartesian axis) and pressure

          total   stress  (Ry/bohr**3)                   (kbar)     P=   -0.24
  -0.00000007  -0.00000000  -0.00000000         -0.01     -0.00     -0.00
  -0.00000000  -0.00000007  -0.00000000         -0.00     -0.01     -0.00
  -0.00000000  -0.00000000  -0.00000474         -0.00     -0.00     -0.70

     Message from routine bfgs:
     history already reset at previous step: stopping

     bfgs converged in   9 scf cycles and   8 bfgs steps
     (criteria: energy <  1.0E-04 Ry, force <  4.0E-04Ry/Bohr, cell <  1.0E-02kbar)

     End of BFGS Geometry Optimization

     Final enthalpy =    -446.7488843657 Ry
Begin final coordinates
     new unit-cell volume =    765.87178 a.u.^3 (   113.49049 Ang^3 )
     density =      1.78300 g/cm^3

CELL_PARAMETERS (angstrom)
   2.559760998  -0.000000000   0.000000000
  -1.279880499   2.216818052   0.000000000
   0.000000000   0.000000000  20.000000000

ATOMIC_POSITIONS (crystal)
C        0.000000000   0.000000000   0.500000000
Mn       0.333333333   0.666666667   0.560840357
Mn       0.333333333   0.666666667  -0.560840357
End final coordinates
```

Comparing the calculated final enthalpies per atom in the unit cell from the three initial spin orders, the AFM spin order appears to be the most stable (remember that the primitive cell of the AFM phase is twice as large as those of the FM and NM phases).

(c)

No U:

```
     the Fermi energy is     0.7649 ev

!    total energy              =    -893.52421923 Ry
     Harris-Foulkes estimate   =    -893.52421924 Ry
     estimated scf accuracy    <          4.3E-12 Ry

     The total energy is the sum of the following terms:

     one-electron contribution =   -5691.55007668 Ry
     hartree contribution      =    2845.70145346 Ry
     xc contribution           =    -153.12175032 Ry
     ewald contribution        =    2105.44582279 Ry
     smearing contrib. (-TS)   =       0.00033151 Ry

     total magnetization       =    -0.00 Bohr mag/cell
     absolute magnetization    =     9.41 Bohr mag/cell

     convergence has been achieved in  25 iterations
```

U=5 V:

```
     the Fermi energy is     1.0492 ev

!    total energy              =    -892.51938428 Ry
     Harris-Foulkes estimate   =    -892.51938428 Ry
     estimated scf accuracy    <          5.4E-10 Ry

     The total energy is the sum of the following terms:

     one-electron contribution =   -5706.53230210 Ry
     hartree contribution      =    2853.98774664 Ry
     xc contribution           =    -154.10661764 Ry
     ewald contribution        =    2113.34961854 Ry
     Hubbard energy            =       0.78238790 Ry
     smearing contrib. (-TS)   =      -0.00021761 Ry

     total magnetization       =     0.00 Bohr mag/cell
     absolute magnetization    =    15.58 Bohr mag/cell

     convergence has been achieved in  24 iterations

     negative rho (up, down):  0.000E+00 1.029E-05
```

(d)

Noncollinear spin:

```
     the Fermi energy is     0.7770 ev

!    total energy              =    -893.52217737 Ry
     Harris-Foulkes estimate   =    -893.52217737 Ry
     estimated scf accuracy    <          7.8E-10 Ry

     The total energy is the sum of the following terms:

     one-electron contribution =   -5707.51846248 Ry
     hartree contribution      =    2853.77959077 Ry
     xc contribution           =    -153.13291566 Ry
     ewald contribution        =    2113.34961854 Ry
     smearing contrib. (-TS)   =      -0.00000853 Ry

     total magnetization       =     0.00     0.00    -0.00 Bohr mag/cell
     absolute magnetization    =     9.34 Bohr mag/cell
```

Noncollinear spin+spin-orbit coupling:

```
     the Fermi energy is     0.7759 ev

!    total energy              =    -893.53700692 Ry
     Harris-Foulkes estimate   =    -893.53700692 Ry
     estimated scf accuracy    <          9.2E-10 Ry

     The total energy is the sum of the following terms:

     one-electron contribution =   -5707.53313365 Ry
     hartree contribution      =    2853.77923877 Ry
     xc contribution           =    -153.13271785 Ry
     ewald contribution        =    2113.34961854 Ry
     smearing contrib. (-TS)   =      -0.00001273 Ry

     total magnetization       =     0.00     0.00     0.00 Bohr mag/cell
     absolute magnetization    =     9.33 Bohr mag/cell

     convergence has been achieved in  36 iterations
```

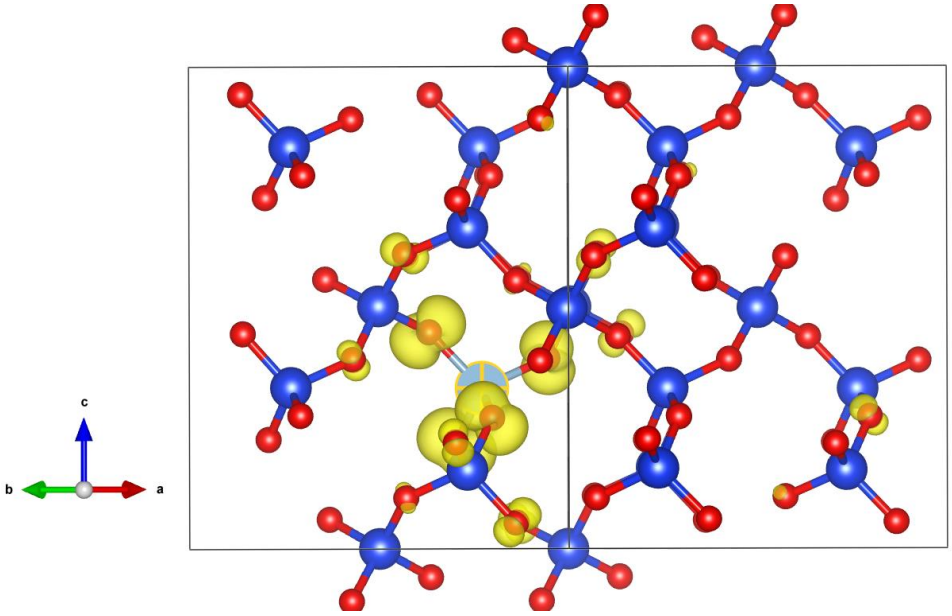
Inclusion of spin-orbit coupling slightly decreases the predicted total energy of the system.

Time per step:

AFM-2	Noncollinear spin	Noncollinear spin+SOI
~15 s	~55 s	~70 s

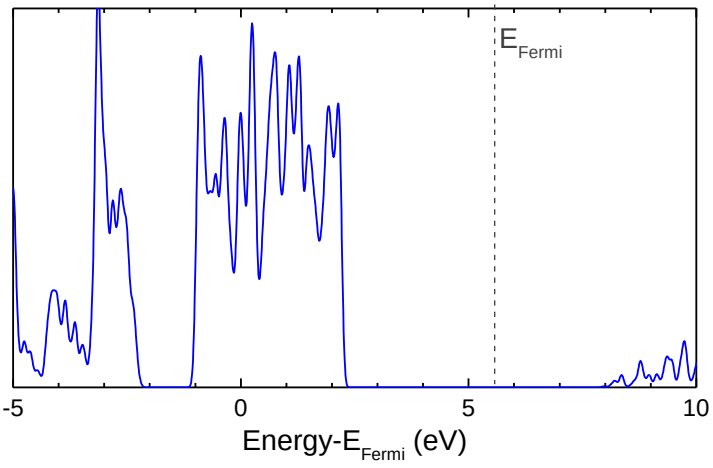
Extra-Exercise: Aluminum-doped SiO_2

(a)

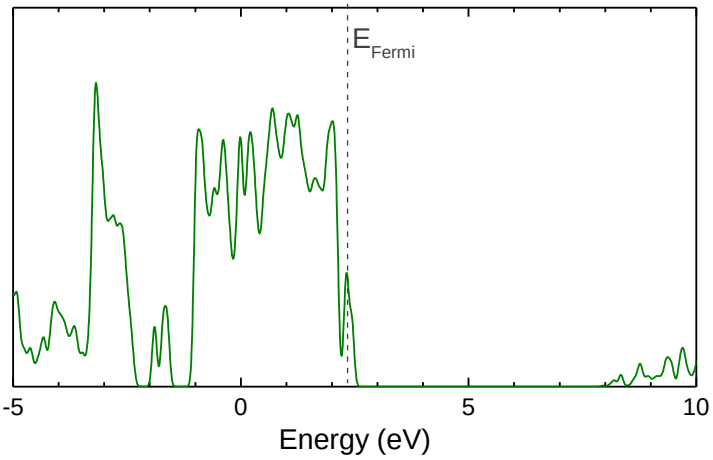


Total spin: 1.03 μ_B/cell

(b) Undoped SiO_2



Doped SiO_2



(c)

	Charge 0
Total energy of doped SiO_2, $E_{tot}^{SiO2:Al}$	-1781.37 Ry
Total energy of pristine SiO_2, E_{tot}^{SiO2}	-1784.86 Ry
Chemical potential of Si atom, μ_{Si}	-9.55266 Ry
Chemical potential of Al atom, μ_{Al}	-6.66477 Ry
Formation energy	0.21 Ry = 2.863 eV