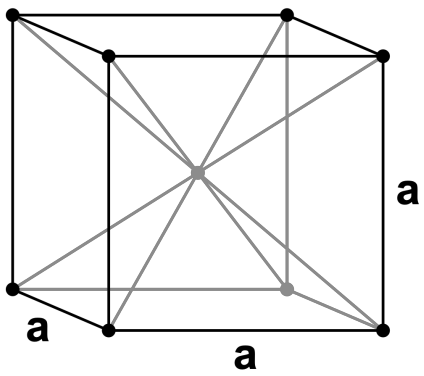
Exercises

Metal: Bulk sodium (Na)

- bcc

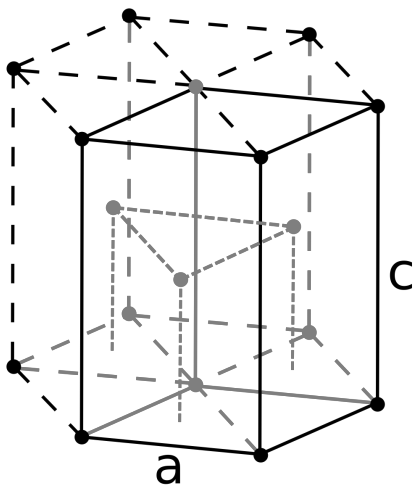


taken from https://en.wikipedia.org

```
0 0 0 0 0 0
4.00000 10.0000 1 1 1
229 1
7.900000 7.900000 7.900000 90.000 90.000 90.000
12 12 12 1 1 1
0 0
0.000000d0 0.000000d0 0.000000d0 1 0 1
11 0.5000 22.99 6 1 0.2
0 0 0 0 0
0 1
20 20 0 84200.00 0
6 1
0 20 0.60
0.20 0.30 0.20 0.20 0.20
300.00 4 1 0.50D-09
-10.0002 0.50D+03 0
ggapbe 1
2.00
101
4 4 4
4 4 4
6
1
0
2
0
0
0 0.000
```

Metal: Bulk magnesium (Mg)

- hcp

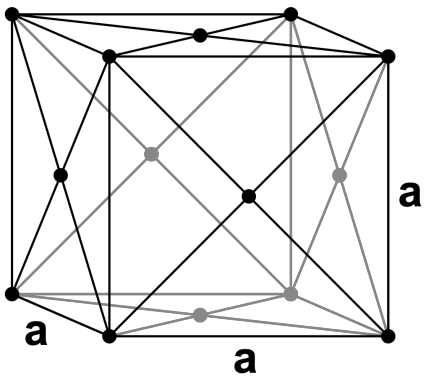


taken from https://en.wikipedia.org

```
0 0 0 0 0 0
4.0000 08.0000 1 2 2
194 0
6.10000000 6.10000000 9.60000000 90.0d0 90.0d0 120.0d0
12 12 8 1 1 1
0 0
 0.3333333333333  0.666666666667  0.2500000000 1 0 1
-0.3333333333333 -0.666666666667 -0.2500000000 1 0 1
12 0.2000 24.31 6 1 0.0
0 0 0 0 0
0 1
50 50 0 36000.00 0
6 1
0 30 0.6
0.2 0.3 0.20 0.20 0.20
30.00 1 1 0.10D-9
-10.0020 0.50D+05 0
ggapbe 1
1.00 3
101
2 2 2
2 2 2
8
1
0
2
0
0
0 0.0
```


Metal: Bulk aluminum (Al)

- fcc

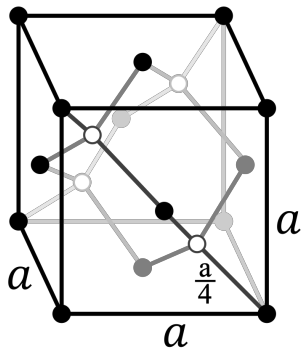


taken from https://en.wikipedia.org

```
0 0 0 0 0 0
4.00000 8.0000 1 1 1
221 2
7.5 7.5 7.5 90.000 90.000 90.000
12 12 12 1 1 1
0 0
0.000000d0 0.000000d0 0.000000d0 1 0 1
13 0.5000 26.98 6 1 0.2
0 0 0 0 0
0 1
30 30 0 84200.00 0
6 1
0 20 0.60
0.20 0.30 0.20 0.20 0.20
300.00 4 1 0.50D-09
-0.0020 0.50D+03 0
ggapbe 1
2.00
101
4 4 4
4 4 4
6
1
0
2
0
0
0 0.000
```

Semiconductor: Bulk silicon (Si)

- space group 227
- diamond structure
- atomic number 14



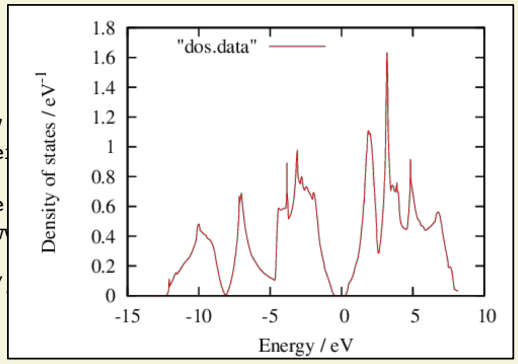
taken from https://en.wikipedia.org

- Band gap?

```
0 0 0 0 0 0
4.00000 8.0000 1 2 2
227 2
10.300000 10.300000 10.300000 90.000 90.000 90.000
08 08 08 1 1 1
0 0
0.000000d0 0.000000d0 0.000000d0 1 0 1
0.250000d0 0.250000d0 0.250000d0 1 0 1
14 0.5000 28.09 6 1 0.2
0 0 0 0 0
0 1
20 20 0 84200.00 0
6 1
0 20 0.60
0.20 0.30 0.20 0.20 0.20
300.00 4 1 0.50D-09
0.0002 0.50D+03 0
ggapbe 1
2.00
102
4 4 4
4 4 4
8
1
0
2
0
0
0 0.000
```


Semiconductor: Bulk silicon (Si)

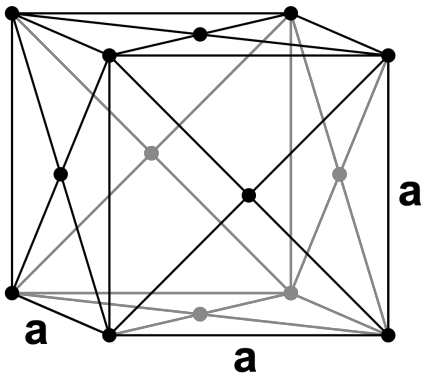
```
$ gnuplot

          G N U P L O T
          Version 4.2 patchlevel 6
          last modified Sep 2009
          System: Linux 2.6.32-642.11.1.el6.x86_64

          Copyright (C) 1986 - 1993, 1998, 2004, 2007
          Thomas Williams, Colin Kelley and many othe

          Type `help` to access the on-line reference
          The gnuplot FAQ is available from http://ww

          Send bug reports and suggestions to <http:/


Terminal type set to 'x11'
gnuplot> plot "dos.data" with lines
gnuplot>
```



- Calculated band gap ~ 0.6 eV
- c.f. Experimental band gap ~ 1 eV

Ferromagnet: Bulk nickel (Ni)

- fcc



taken from https://en.wikipedia.org

- Spin polarization?

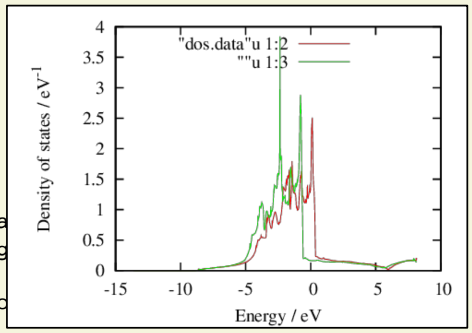
```
0 0 0 0 0 0
5.00000 15.0000 1 1 1
221 2
6.700000 6.700000 6.700000 90.000 90.000 90.000
12 12 12 1 1 1
0 0
0.000000d0 0.000000d0 0.000000d0 1 0 1
28 0.5000 58.69 6 1 0.1
0 0 0 0 0
0 1
30 30 0 84200.00 0
6 1
0 20 0.30
0.20 0.30 0.20 0.20 0.20
300.00 4 1 0.50D-09
-0.0020 0.50D+03 0
ggapbe 2
2.00
101
4 4 4
4 4 4
10
1
0
2
0
0 0.000
```


Spin polarization

```
$ head dos.data
    -13.5948134416      0.0000000000      0.0000000000      0.0000000000      0.0000000000
    -13.5839288832      0.0000000000      0.0000000000      0.0000000000      0.0000000000
    -13.5730443248      0.0[illegible]000      [illegible]      0.0000000000      0.0000000000
    -13.5621597664      0.0[illegible]000      [illegible]      0.0000000000      0.0000000000
    -13.5512752080      0.0[illegible]000      [illegible]      0.0000000000      0.0000000000
    -13.5403906496      0.0000000000      0.0000000000      0.0000000000      0.0000000000
    -13.5295060912      0.0000000000      0.0000000000      0.0000000000      0.0000000000
```

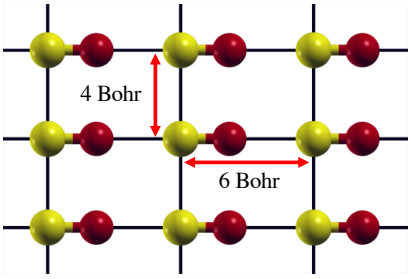
up down

```
$ gnuplot

          G N U P L O T
          Version 4.2 patchlevel 6
          last modified Sep 2009
          System: Linux 2.6.32-642.11.1.el6.x86_64

          Copyright (C) 1986 - 1993, 1998, 2004, 2007 -
          Thomas Williams, Colin Kelley and many others

          Type `help` to access the on-line reference ma
          The gnuplot FAQ is available from http://www.g

          Send bug reports and suggestions to <http://sc


Terminal type set to 'x11'
gnuplot> plot "dos.data" using 1:2 with lines, "" using 1:3 with lines
gnuplot>
```



Diatomic molecule: Carbon monoxide (CO)

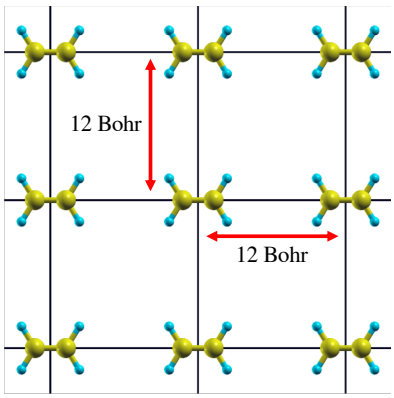
- cuboid unit cell
- no van der Waals




```
0 0 0 0 0 0
5.5000 20.0000 2 2 2
1 0
6.0000 4.0000 4.0000 90.0 90.0 90.0
1 1 1 1 1 1
1 0
0.0000000000 0.0000000000 0.0000000000 1 1 1 0.0 0.0 0
2.2000000000 0.0000000000 0.0000000000 1 1 2 0.0 0.0 0
6 0.1500 12.01 3 1 0.d0
8 0.1500 16.00 3 1 0.d0
0 0 0 0 0
0 1
200 200 0 57200.00 0
3 1
0 8 0.8
0.60 0.50 0.60 0.70 1.00
30.00 2 1 0.10D-08 1.d-06
0.0010 0.10D+02 0
ggapbe 1
1.00 3
102
0 0 0
0 0 0
8
1
0
2 0 0 0
0
0
0 0.0
```


Hydrocarbon: Ethylene (C_2H_4)

- Ethylene (C_2H_4)



- Structure relaxation
- Force criterion:

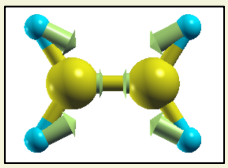
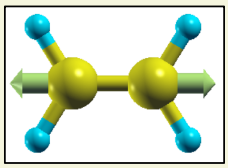
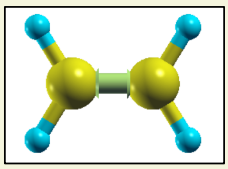
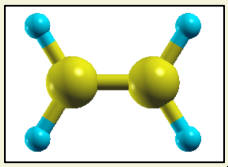
5×10^{-4} Hartree/Bohr

```
0 0 0 0 0 0
5.0000 15.0000 2 6 6
1 0
12.0000 12.0000 12.0000 90.0 90.0 90.0
1 1 1 1 1 1
1 0
 1.2627229833  0.0000000000 0.0000000000 1 1 1
 2.3483288468  1.7534586685 0.0000000000 1 1 2
 2.3483288468 -1.7534586685 0.0000000000 1 1 2
-1.2627229833  0.0000000000 0.0000000000 1 1 1
-2.3483288468  1.7534586685 0.0000000000 1 1 2
-2.3483288468 -1.7534586685 0.0000000000 1 1 2
6 0.1500 12.01 3 1 0.d0
1 0.1500 1.008 3 1 0.d0
0 0 0 0 0
0 1
100 200 0 57200.00 0
3 1
0 8 0.8
0.60 0.50 0.60 0.70 1.00
300.00 4 1 0.10D-08 1.d-06
0.0010 0.05D-02 0
ggapbe 1
1.00 3
102
0 0 0
0 0 0
10
1
0
2 0 0 0
0
```

Structure relaxation of C_2H_4

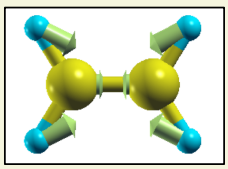
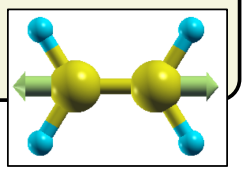
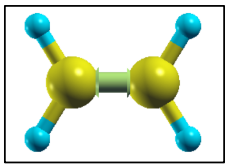
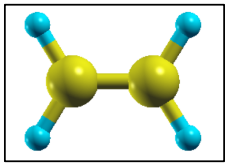
coordinates forces

```
$ grep MD: nfout_1
MD:    1
MD:      1  C     1.262723     0.000000     0.000000  -0.00109   0.00000   0.00000
MD:      2  H     2.348329     1.753459     0.000000  -0.00124  -0.00063   0.00000
MD:      3  H     2.348329    -1.753459     0.000000  -0.00124   0.00063  -0.00000
MD:      4  C    -1.262723     0.000000     0.000000   0.00109  -0.00000   0.00000
MD:      5  H    -2.348329     1.753459     0.000000   0.00124  -0.00063   0.00000
MD:      6  H    -2.348329    -1.753459     0.000000   0.00124   0.00063  -0.00000
MD:    2
MD:      1  C     1.259460     0.000000     0.000001   0.00200  -0.00000  -0.00000
MD:      2  H     2.344603     1.751556     0.000000  -0.00085  -0.00008   0.00000
MD:      3  H     2.344603    -1.751556    -0.000000  -0.00085   0.00008   0.00000
MD:      4  C    -1.259456    -0.000000     0.000000  -0.00200   0.00000  -0.00000
MD:      5  H    -2.344603     1.751557     0.000000   0.00085  -0.00008   0.00000
MD:      6  H    -2.344603    -1.751557    -0.000000   0.00085   0.00008   0.00000
MD:    3
MD:      1  C     1.262349     0.000000     0.000000  -0.00219   0.00000   0.00000
MD:      2  H     2.343376     1.751441     0.000000  -0.00034   0.00046   0.00000
MD:      3  H     2.343376    -1.751441     0.000000  -0.00034  -0.00046   0.00000
MD:      4  C    -1.262347     0.000000     0.000000   0.00219  -0.00000   0.00000
MD:      5  H    -2.343375     1.751441     0.000000   0.00034   0.00046   0.00000
MD:      6  H    -2.343374    -1.751441    -0.000000   0.00034  -0.00046   0.00000
MD:    4
MD:      1  C     1.260579    -0.000000    -0.000000   0.00002   0.00000   0.00000
MD:      2  H     2.341738     1.752212     0.000000  -0.00040   0.00022  -0.00000
MD:      3  H     2.341738    -1.752212     0.000000  -0.00040  -0.00022  -0.00000
MD:      4  C    -1.260578     0.000000    -0.000000  -0.00002  -0.00000  -0.00000
MD:      5  H    -2.341735     1.752211     0.000000   0.00040   0.00022  -0.00000
MD:      6  H    -2.341735    -1.752211    -0.000000   0.00040  -0.00022  -0.00000
```

Structure relaxation of C_2H_4

```
$ grep -A1 f_max nfout_1
   NIT      TotalEnergy      f_max      f_rms       edel       vdel       fdel
     1     -13.90231646   0.001395   0.001300   0.32D-09   0.80D-07   0.32D-09
--
   NIT      TotalEnergy      f_max      f_rms       edel       vdel       fdel
     2     -13.90233259   0.002005   0.001351   0.44D-10   0.45D-07   0.44D-10
--
   NIT      TotalEnergy      f_max      f_rms       edel       vdel       fdel
     3     -13.90233634   0.002190   0.001348   0.11D-08   0.13D-06   0.11D-08
--
   NIT      TotalEnergy      f_max      f_rms       edel       vdel       fdel
     4     -13.90234327   0.000451   0.000368   0.17D-08   0.14D-06   0.17D-08
```

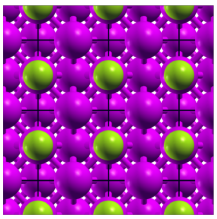
- Structure relaxation stops when

  maximal force < 0.0005 Hartree/Bohr

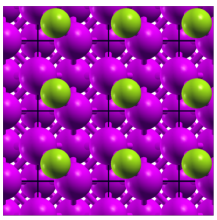
Adatom on a metal surface

- Cl / Al(100)

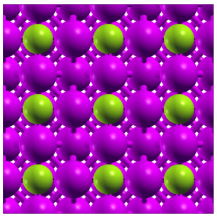
top



bridge



hollow



```
1 0 0 0 0 0
4.000 10.0000 2 7 7
1 0
CARTESIAN
7.6534000000  0.0000000000 00.0000000000
0.0000000000  7.6534000000 00.0000000000
0.0000000000 00.0000000000 30.6136000000
4 4 1 2 2 1
1 0
0.0000000000 3.8267000000  4.0000000000 1 1 2
0.0000000000 3.8267000000  0.0000000000 1 1 1
3.8267000000 0.0000000000  0.0000000000 1 1 1
0.0000000000 0.0000000000 -3.8267000000 1 0 1
3.8267000000 3.8267000000 -3.8267000000 1 0 1
0.0000000000 3.8267000000 -7.6534000000 1 0 1
3.8267000000 0.0000000000 -7.6534000000 1 0 1
13 0.15 26.98150000 3 1 0.00000000
17 0.15 35.45270000 3 1 0.00000000
0 0 0 0 0
0 1
100 200 0 57200.00 0
3 1
0 20 0.8
0.60 0.50 0.60 0.70 1.00
600.00 4 1 0.10D-08 1.d-06
-0.0020 0.10D-02 0
ggapbe 1
1.00 3
102
0 0 0
0 0 0
16
```


Vibrational mode analysis

- nfinp_2
- relaxed structure

```
1 0 0 0 0 0
4.000 10.0000 2 7 7
1 0
CARTESIAN
7.6534000000  0.0000000000 00.0000000000
0.0000000000  7.6534000000 00.0000000000
0.0000000000 00.0000000000 30.6136000000
4 4 1 2 2 1
1 0
-0.000000251836 3.826701578025  4.049619608896 1 1 2
-0.000001836163 3.826699462952 -0.045772180307 1 1 1
 3.826699127649 0.000000430959 -0.233606043422 1 1 1
 0.000000000000 0.000000000000 -3.826700000000 1 0 1
 3.826700000000 3.826700000000 -3.826700000000 1 0 1
 0.000000000000 3.826700000000 -7.653400000000 1 0 1
 3.826700000000 0.000000000000 -7.653400000000 1 0 1
13 0.15 26.98150000 3 1 0.00000000
17 0.15 35.45270000 3 1 0.00000000
1 0 0 0 0
0 1
100 200 0 57200.00 0
3 1
0 20 0.8
0.60 0.50 0.60 0.70 1.00
600.00 3 1 0.10D-08 1.d-06
-0.0020 0.10D-02 0
ggapbe 1
1.00 3
102
0 0 0
0 0 0
16
```

Vibrational mode analysis

Make nfvibrate.data and submit qsub2.csh

```
  1  1.0d0
   1   0.0000000000     0.0000000000     0.000000000000

  1  1.0d0
   1   0.1000000000     0.0000000000     0.000000000000

  1 -1.0d0
   1   0.1000000000     0.0000000000     0.000000000000

  1  1.0d0
   1   0.0000000000     0.1000000000     0.000000000000

  1 -1.0d0
   1   0.0000000000     0.1000000000     0.000000000000

  1  1.0d0
   1   0.0000000000     0.0000000000     0.100000000000

  1 -1.0d0
   1   0.0000000000     0.0000000000     0.100000000000
```

- number of atoms to displace
- index of atom
- factor for displacements
- displacements

Vibrational mode analysis

Make MD_2.dat

```
7  3
36 27 27 27 27 27 27
   2
     1      0.100000     3.826702     4.049620  -0.00006  0.00000  0.00075
     2     -0.000002     3.826699    -0.045772  -0.00043  0.00000 -0.00031
     3      3.826699     0.000000    -0.233606   0.00033 -0.00000  0.00024
     4      0.000000     0.000000    -3.826700   0.00021 -0.00000  0.00030
     5      3.826700     3.826700    -3.826700  -0.00005  0.00000  0.00031
     6      0.000000     3.826700    -7.653400   0.00020  0.00000 -0.00156
     7      3.826700     0.000000    -7.653400  -0.00021 -0.00000  0.00028
   3
     1     -0.100000     3.826702     4.049620   0.00006  0.00000  0.00076
     2     -0.000002     3.826699    -0.045772   0.00043  0.00000 -0.00031
     3      3.826699     0.000000    -0.233606  -0.00033 -0.00000  0.00025
     4      0.000000     0.000000    -3.826700  -0.00021 -0.00000  0.00030
     5      3.826700     3.826700    -3.826700   0.00005  0.00000  0.00031
     6      0.000000     3.826700    -7.653400  -0.00020  0.00000 -0.00156
     7      3.826700     0.000000    -7.653400   0.00021 -0.00000  0.00028
(continued)
```

```
$ ls ../../../tools/Vibration
GiF.f90  Makefile  PlotMolVib      PlotMolVib.o  Tests      duplicate.f90  gif
GiF.o    Original  PlotMolVib.f90  Refs          duplicate  duplicate.o
$ ../../../tools/Vibration/gif < MD_2.dat > MD_2.out
```