Lab report 2: phonon calculation of bulk Si and AlAs

1. Exercise one

a. Calculate total energy of bulk Si and report energy

si.scf.out
total energy = -15.85438131 Ry

b. Calculate Gamma point phonon frequency of bulk Si and report phonon frequency at Gamma

si.phG.out

```
     Dielectric constant in cartesian axis

(     13.998253693      -0.000000000      -0.000000000 )
(     -0.000000000      13.998253693      -0.000000000 )
(     -0.000000000      -0.000000000      13.998253693 )

     Effective charges (d Force / dE) in cartesian axis without acoustic sum rule applied (asr)

          Effective charges (d Force / dE) in cartesian axis with asr applied:
          atom    1  Si    Mean Z*:       -0.00000
     E*x (       -0.00000       -0.00000        0.00000 )
     E*y (       -0.00000       -0.00000        0.00000 )
     E*z (        0.00000        0.00000       -0.00000 )
          atom    2  Si    Mean Z*:        0.00000
     E*x (        0.00000        0.00000       -0.00000 )
     E*y (        0.00000        0.00000       -0.00000 )
     E*z (       -0.00000       -0.00000        0.00000 )

     Diagonalizing the dynamical matrix

     q = (    0.000000000   0.000000000   0.000000000 )

 **************************************************************************
     freq (    1) =       0.088873 [THz] =       2.964471 [cm-1]
     freq (    2) =       0.088873 [THz] =       2.964471 [cm-1]
     freq (    3) =       0.088873 [THz] =       2.964471 [cm-1]
     freq (    4) =      15.549157 [THz] =     518.664042 [cm-1]
     freq (    5) =      15.549157 [THz] =     518.664042 [cm-1]
     freq (    6) =      15.549157 [THz] =     518.664042 [cm-1]
 **************************************************************************
```

dyn.G

```
     Diagonalizing the dynamical matrix

     q = (    0.000000000   0.000000000   0.000000000 )

 **************************************************************************
     freq (    1) =       0.088873 [THz] =       2.964471 [cm-1]
( -0.696529  0.000000  0.114392 -0.000000  0.041975 -0.000000 )
( -0.696529  0.000000  0.114392 -0.000000  0.041975 -0.000000 )
     freq (    2) =       0.088873 [THz] =       2.964471 [cm-1]
( -0.067381  0.000000 -0.158644  0.000000 -0.685778  0.000000 )
( -0.067381  0.000000 -0.158644  0.000000 -0.685778  0.000000 )
     freq (    3) =       0.088873 [THz] =       2.964471 [cm-1]
(  0.101524  0.000000  0.679519  0.000000 -0.167171  0.000000 )
(  0.101524  0.000000  0.679519  0.000000 -0.167171  0.000000 )
     freq (    4) =      15.549157 [THz] =     518.664042 [cm-1]
( -0.411199  0.000000 -0.571990  0.000000  0.061182  0.000000 )
(  0.411199  0.000000  0.571990  0.000000 -0.061182  0.000000 )
     freq (    5) =      15.549157 [THz] =     518.664042 [cm-1]
( -0.080177  0.000000  0.131458 -0.000000  0.690138 -0.000000 )
(  0.080177 -0.000000 -0.131458  0.000000 -0.690138  0.000000 )
     freq (    6) =      15.549157 [THz] =     518.664042 [cm-1]
( -0.569638  0.000000  0.394394  0.000000 -0.141302  0.000000 )
(  0.569638  0.000000 -0.394394  0.000000  0.141302  0.000000 )
 **************************************************************************
```

2. Exercise two

a. Calculate total energy of AlAs and report energy

alas.scf.out
total energy = -16.98632170 Ry

b. Calculate Gamma point phonon frequency of AlAs and report phonon frequency at Gamma

alas.phG.out

```
     Dielectric constant in cartesian axis

     (      9.091766604      -0.000000000      -0.000000000 )
     (     -0.000000000       9.091766604       0.000000000 )
     (     -0.000000000       0.000000000       9.091766604 )

     Effective charges (d Force / dE) in cartesian axis without acoustic sum rule applied (asr)

        Effective charges (d Force / dE) in cartesian axis with asr applied:
        atom    1  Al    Mean Z*:       2.09004
     E*x (       2.09004       0.00000       0.00000 )
     E*y (       0.00000       2.09004      -0.00000 )
     E*z (       0.00000       0.00000       2.09004 )
        atom    2  As    Mean Z*:      -2.09004
     E*x (      -2.09004      -0.00000      -0.00000 )
     E*y (      -0.00000      -2.09004       0.00000 )
     E*z (      -0.00000      -0.00000      -2.09004 )

     Diagonalizing the dynamical matrix

     q = (    0.000000000   0.000000000   0.000000000 )

 **************************************************************************
     freq (    1) =       0.148956 [THz] =       4.968626 [cm-1]
     freq (    2) =       0.148956 [THz] =       4.968626 [cm-1]
     freq (    3) =       0.148956 [THz] =       4.968626 [cm-1]
     freq (    4) =      12.384087 [THz] =     413.088681 [cm-1]
     freq (    5) =      12.384087 [THz] =     413.088681 [cm-1]
     freq (    6) =      12.384087 [THz] =     413.088681 [cm-1]
 **************************************************************************
```

dyn.G

```
     Diagonalizing the dynamical matrix

     q = (    0.000000000   0.000000000   0.000000000 )

 **************************************************************************
     freq (    1) =       0.148956 [THz] =       4.968626 [cm-1]
 ( -0.535164  0.000000  0.002244  0.000000 -0.462196  0.000000 )
 ( -0.535131  0.000000  0.002244  0.000000 -0.462168  0.000000 )
     freq (    2) =       0.148956 [THz] =       4.968626 [cm-1]
 (  0.115330  0.000000 -0.684104  0.000000 -0.136860  0.000000 )
 (  0.115323  0.000000 -0.684063  0.000000 -0.136851  0.000000 )
     freq (    3) =       0.148956 [THz] =       4.968626 [cm-1]
 ( -0.447581  0.000000 -0.178960  0.000000  0.517373 -0.000000 )
 ( -0.447554  0.000000 -0.178949  0.000000  0.517342 -0.000000 )
     freq (    4) =      12.384087 [THz] =     413.088681 [cm-1]
 (  0.906096  0.000000  0.034405  0.000000  0.250977  0.000000 )
 ( -0.326332  0.000000 -0.012391  0.000000 -0.090390  0.000000 )
     freq (    5) =      12.384087 [THz] =     413.088681 [cm-1]
 ( -0.116901  0.000000 -0.770153  0.000000  0.527619  0.000000 )
 (  0.042102  0.000000  0.277372  0.000000 -0.190023  0.000000 )
     freq (    6) =      12.384087 [THz] =     413.088681 [cm-1]
 (  0.224738  0.000000 -0.539318  0.000000 -0.737436  0.000000 )
 ( -0.080940  0.000000  0.194236  0.000000  0.265589  0.000000 )
 **************************************************************************
```

c. Apply Acoustic sum rule and LO-TO splitting then report phonon frequency at Gamma

alas.dynmat.out

#	mode	[cm-1]	[THz]	IR
	1	0.00	0.0000	0.0000
	2	0.00	0.0000	0.0000
	3	0.00	0.0000	0.0000
	4	374.24	11.2195	5.3672
	5	374.24	11.2195	5.3672
	6	410.67	12.3115	5.3672

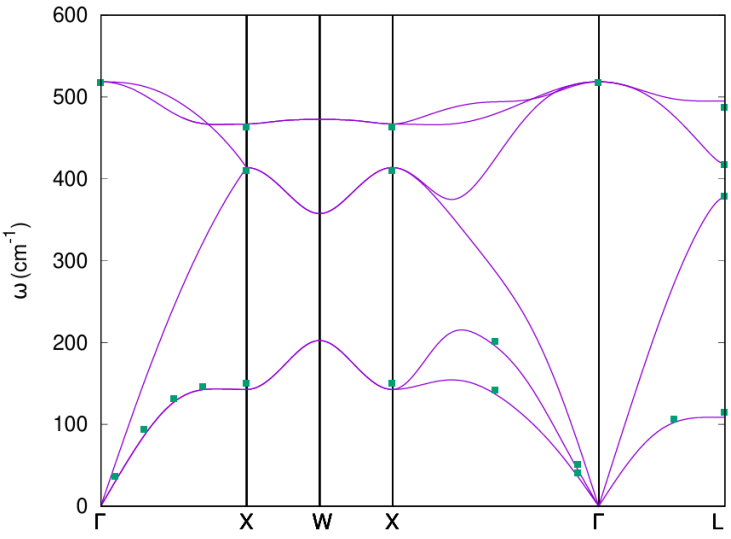
3. Exercise three (Bulk Si)

a. Calculate phonon frequency at uniform grid 4x4x4

si.freq

```
&plot nbnd=   6, nks=   8 /
        0.000000  0.000000  0.000000
  0.0000    0.0000    0.0000  518.6779  518.6779  518.6779
       -0.250000  0.250000 -0.250000
 94.5487   94.5487  233.0106  489.8554  500.8858  500.8858
        0.500000 -0.500000  0.500000
108.6634  108.6634  377.2493  418.6630  495.1119  495.1119
        0.000000  0.500000  0.000000
127.0369  127.0369  243.5610  480.0542  480.0542  497.5688
        0.750000 -0.250000  0.750000
139.7615  198.3612  322.5409  418.7902  473.0484  486.0663
        0.500000  0.000000  0.500000
136.8300  195.4058  286.5263  425.3250  479.5034  494.1714
        0.000000 -1.000000  0.000000
142.6706  142.6706  413.8565  413.8565  467.1091  467.1091
       -0.500000 -1.000000  0.000000
202.4693  202.4693  357.6096  357.6096  472.6910  472.6910
```

b. Calculate phonon dispersion and plot phonon dispersion



c. Calculate phonon density of states and plot phonon density of states