Excercise sheet 8

Exercise 1: Bethe-Salpeter Equation for absorption spectra

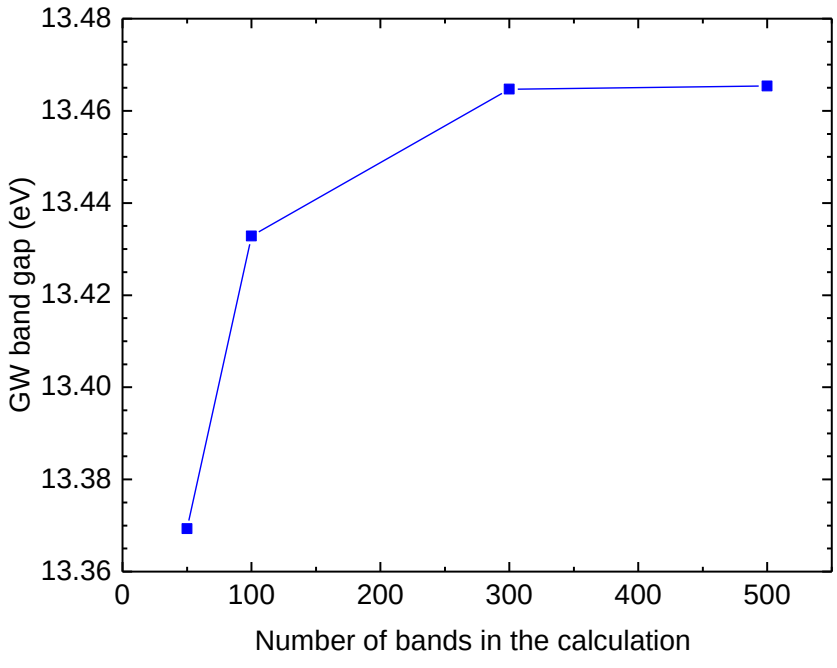
(a) Nothing to plot

(b) o.qp:

```
# QP @ K 1 - 3 : b 1 - 8
#
#    K-point      Band         Eo          E-Eo         Sc|Eo
#
     1.00000      1.00000   -15.23776     -1.85292      8.04397
    1.000000     2.000000    0.000000    -3.144548     1.946219
    1.000000     3.000000    0.000000    -3.145066     1.946338
    1.000000     4.000000    0.000000    -3.145314     1.946176
    1.000000     5.000000    8.341253     1.882751    -2.492452
     1.00000      6.00000    15.59293      2.97156     -2.65236
     1.00000      7.00000    15.59293      2.97122     -2.65237
     1.00000      8.00000    15.59293      2.97146     -2.65230
     2.00000      1.00000   -15.21222     -1.94305      8.02523
    2.000000     2.000000   -0.174744    -3.155245     1.946207
     2.00000      3.00000    -0.01604     -3.14710      1.94809
     2.00000      4.00000    -0.01604     -3.14709      1.94802
    2.000000     5.000000    8.593277     1.887607    -2.496070
     2.00000      6.00000    15.27161      2.86373     -2.64266
     2.00000      7.00000    15.69235      2.97585     -2.66460
```

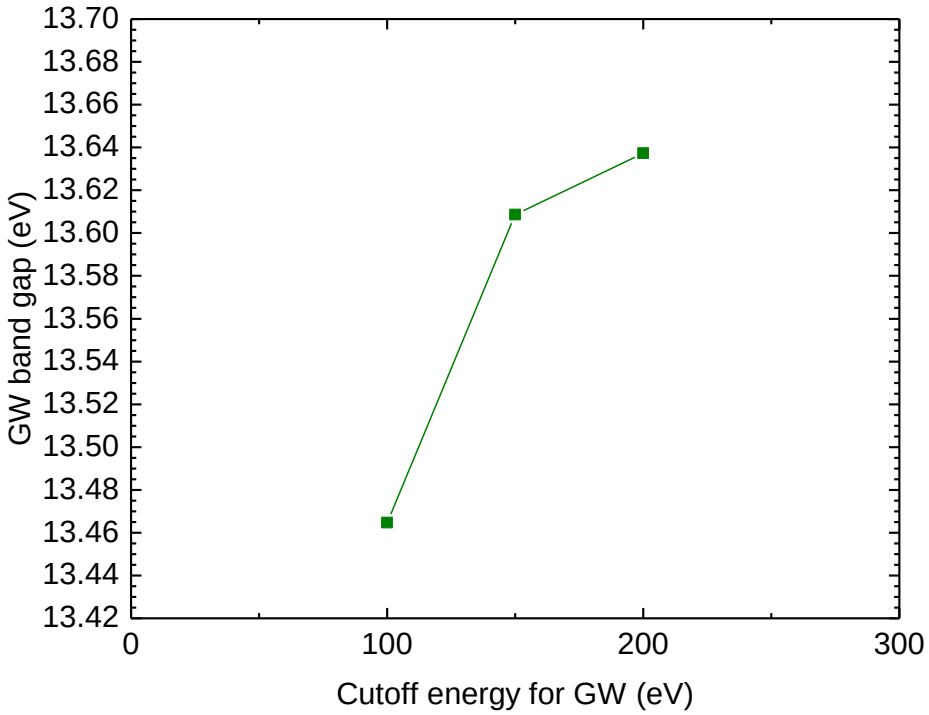
The GW band energies we are interested in is the sum of the E0 and E-E0 columns. The band gap is between the 4th and the 5th band at the Brillouin zone center (k-point 1). The GW band gap is 13.37 eV.

(c)

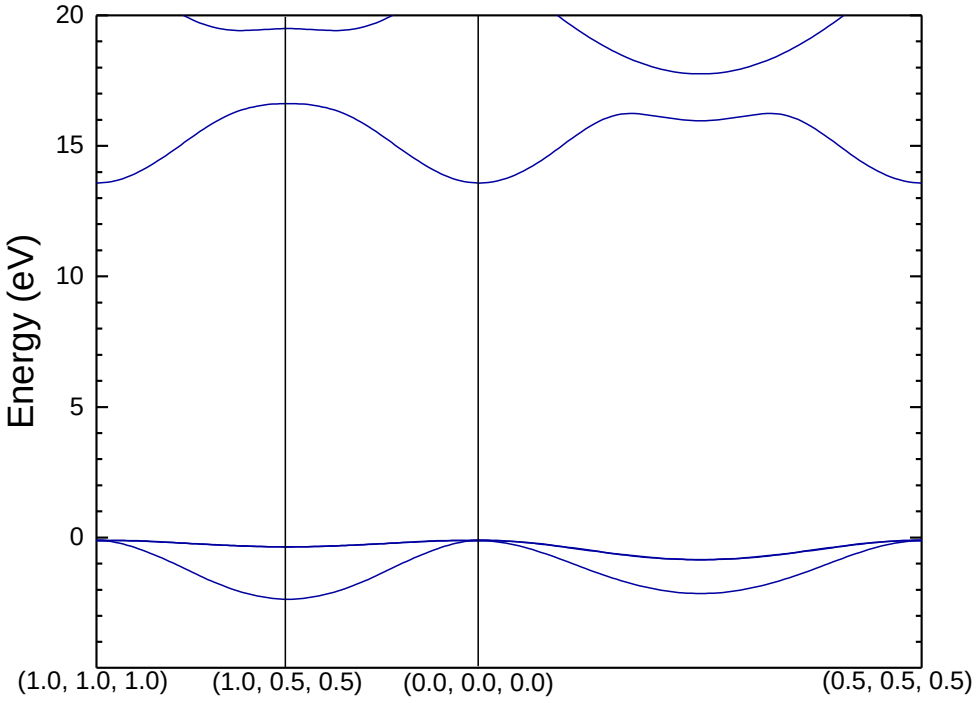


We should use at least 300 bands to ensure converged and accurate GW quasiparticle energies

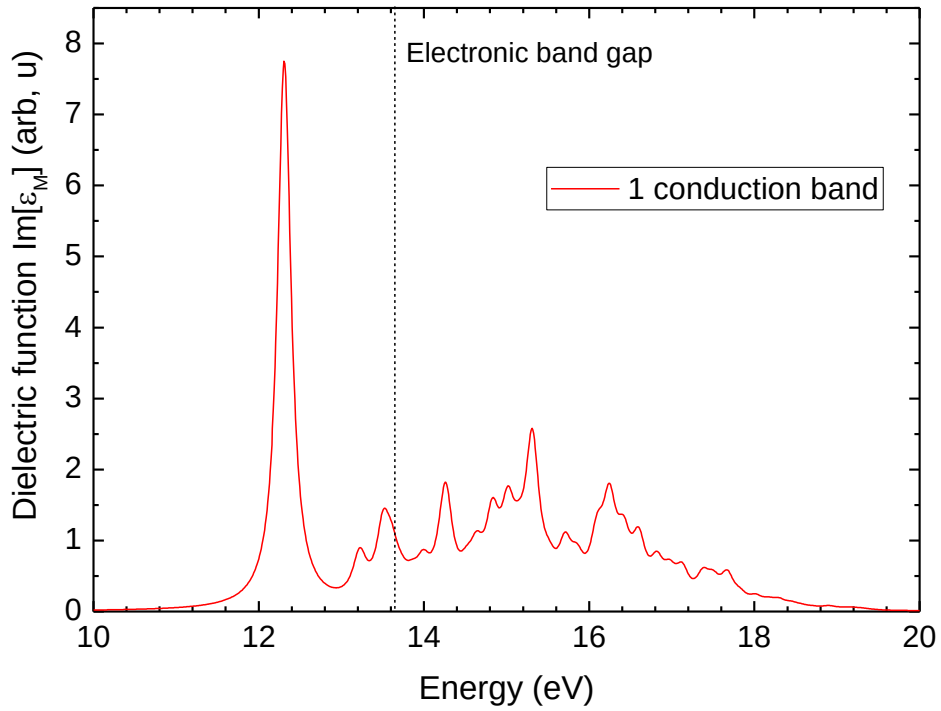
(d)



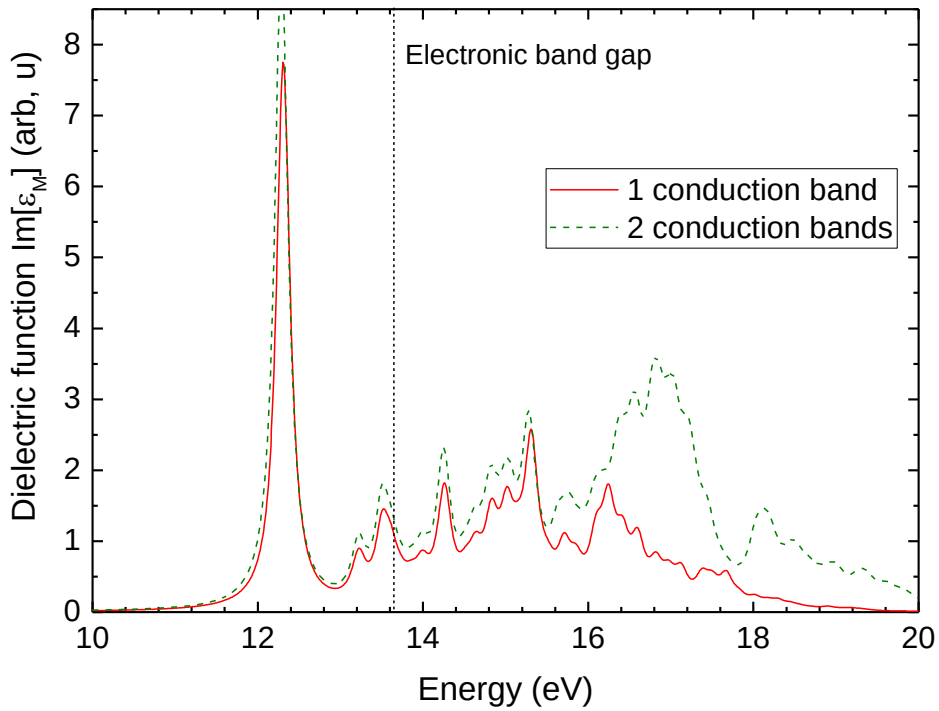
(e)



(f)


Electronic band gap
1 conduction band
Dielectric function Im[ε_M] (arb, u)
Energy (eV)
0
1
2
3
4
5
6
7
8
10
12
14
16
18
20

(g)


Electronic band gap
1 conduction band
2 conduction bands
Dielectric function Im[ε_M] (arb, u)
Energy (eV)
0
1
2
3
4
5
6
7
8
10
12
14
16
18
20

Exercise 2: Excitons in 2D BN

(a)

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

     atom    1 type  1   force =     0.00000000    0.00000000    0.00000007
     atom    2 type  2   force =    -0.00000000   -0.00000000   -0.00000007

     Total force =     0.000000     Total SCF correction =     0.000000
     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=    0.02
   0.00000023  -0.00000000  -0.00000000          0.03     -0.00     -0.00
  -0.00000000   0.00000023  -0.00000000         -0.00      0.03     -0.00
   0.00000000   0.00000000  -0.00000003          0.00      0.00     -0.00


     bfgs converged in   4 scf cycles and   3 bfgs steps
     (criteria: energy <  1.0E-04 Ry, force <  2.0E-04Ry/Bohr, cell <  1.0E-01kbar)

     End of BFGS Geometry Optimization

     Final enthalpy =     -26.8167348987 Ry
Begin final coordinates
     new unit-cell volume =    736.92293 a.u.^3 (   109.20071 Ang^3 )
     density =      0.36495 g/cm^3

CELL_PARAMETERS (angstrom)
   2.510924066  -0.000000000  -0.000000000
   1.255462033   2.174524027  -0.000000000
   0.000000000   0.000000000  19.999893010

ATOMIC_POSITIONS (crystal)
B       -0.000000000   0.000000000   0.249999996
N        0.333333333   0.333333333   0.250000004
End final coordinates
```

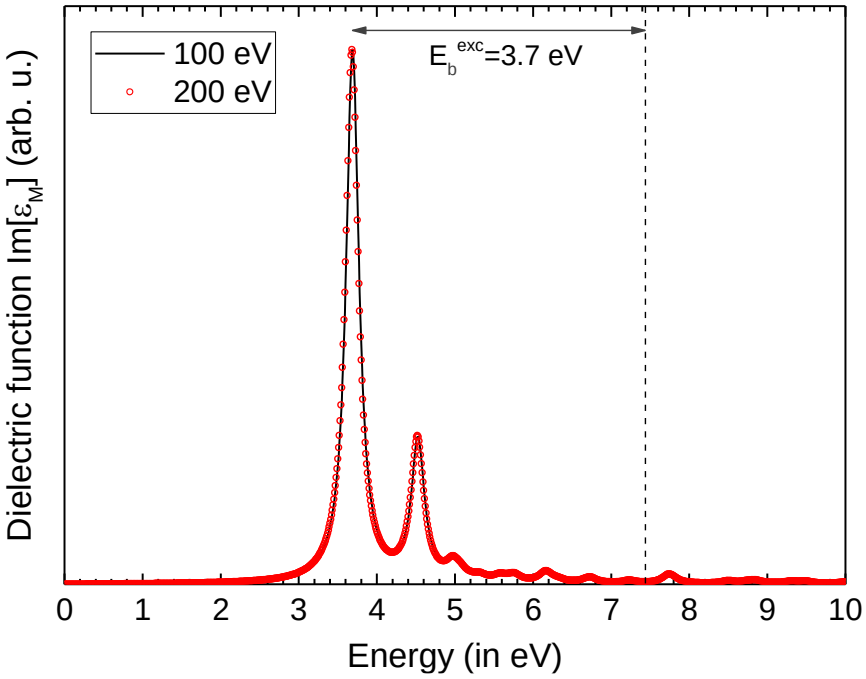
(b) o.qp:

```
# QP @ K 19 - 19 : b 3 - 6
#
#    K-point      Band         Eo          E-Eo         Sc|Eo
#
    19.00000      3.00000     -7.16203     -2.17596      3.76798
    19.00000      4.00000      0.00000     -1.25686      1.67077
    19.00000      5.00000      4.68978      1.49456     -3.48396
    19.00000      6.00000     12.40882      1.21009     -2.98503
#
```

The band gap is between band 4 and band 5 and we are interested In the difference of E.

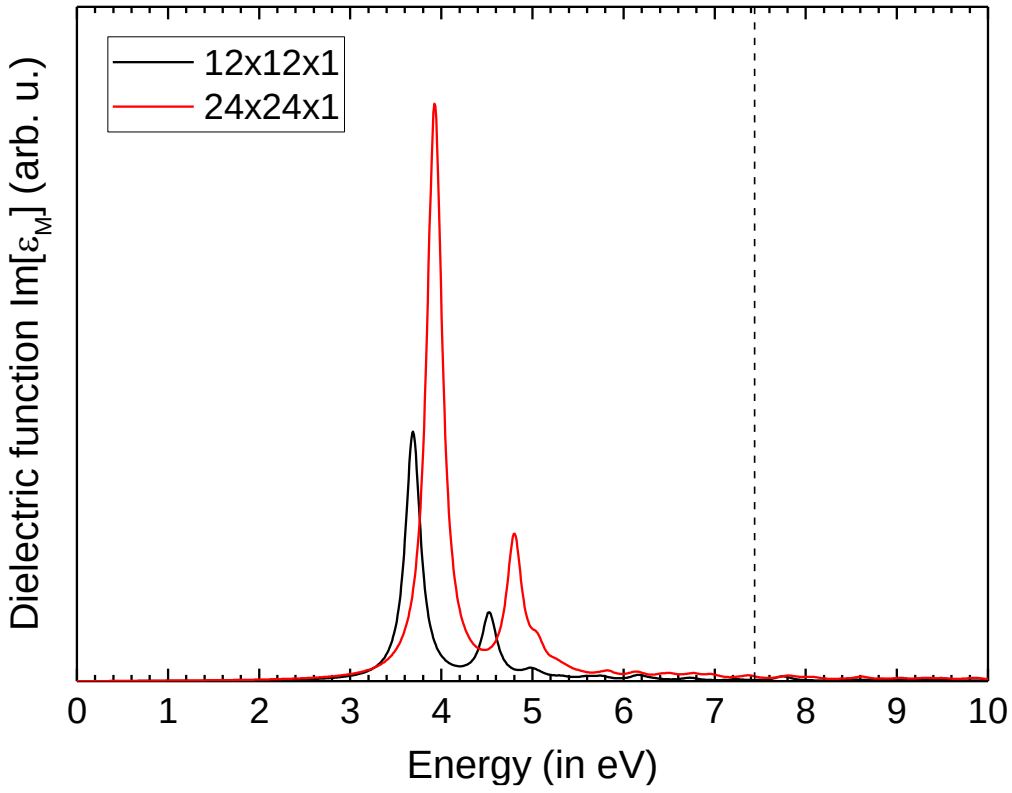
The band gap size at kpoint 19 (the K point) is then 7.44 eV

(c)



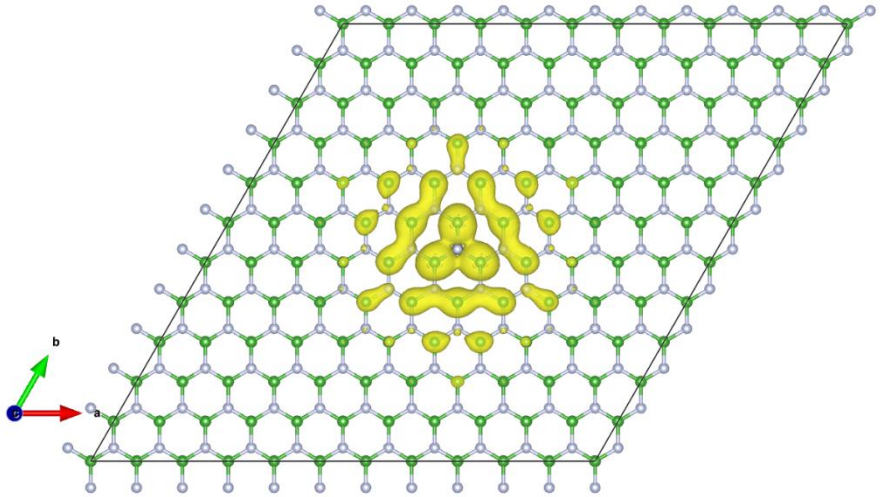
The initial cutoff of 100 eV was a good choice, as doubling the cutoff did not change the calculated dielectric function in any way.

(d)



(e) Exciton 1 (combined with exciton 2)

Electron-Hole pairs that contributes to Excitonic State 1 more than 1%
#
K-point [iku] Weight
0.08333 -0.54167 0.00000 0.14382
0.166667 -0.583333 0.000000 0.112407
0.166667 -0.500000 0.000000 0.254541
0.25000 -0.62500 0.00000 0.05102
0.250000 -0.541667 0.000000 1.000000
0.333333 -0.500000 0.000000 0.596187
#
Band_V Band_C K_V ibz Symm. K_C ibz Weight Energy
#
  4.00000 5.00000 19.00000 4.00000 19.00000 0.26439 4.68978
  4.00000 5.00000 19.00000 1.00000 19.00000 0.26438 4.68978
  4.00000 5.00000 18.00000 5.00000 18.00000 0.07390 5.23130
  4.00000 5.00000 18.00000 2.00000 18.00000 0.07390 5.23130
  4.00000 5.00000 18.00000 1.00000 18.00000 0.07389 5.23130
  4.00000 5.00000 18.00000 4.00000 18.00000 0.07389 5.23130
  4.00000 5.00000 18.00000 6.00000 18.00000 0.07389 5.23130
  4.00000 5.00000 18.00000 9.00000 18.00000 0.07389 5.23130
  4.00000 5.00000 18.00000 12.00000 18.00000 0.07389 5.23130
  4.00000 5.00000 18.00000 10.00000 18.00000 0.07389 5.23130
  4.00000 5.00000 18.00000 7.00000 18.00000 0.07389 5.23130
  4.00000 5.00000 18.00000 3.00000 18.00000 0.07389 5.23130
  4.00000 5.00000 18.00000 8.00000 18.00000 0.07388 5.23130
  4.00000 5.00000 18.00000 11.00000 18.00000 0.07387 5.23130



Exciton 3 (combined with exciton 4)

Electron-Hole pairs that contributes to Excitonic State 3 more than 1%
#
K-point [iku] Weight
0.00000 0.41667 0.00000 0.05163
0.000000 -0.500000 0.000000 0.207184
0.08333 -0.54167 0.00000 0.44644
0.166667 -0.583333 0.000000 0.109708
0.166667 -0.500000 0.000000 0.563717
0.250000 -0.541667 0.000000 0.509684
0.333333 -0.500000 0.000000 1.000000
#

# Band_V	Band_C	K_V ibz	Symm.	K_C ibz	Weight	Energy
4.00000	5.00000	19.00000	1.00000	19.00000	0.33999	4.68978
4.00000	5.00000	19.00000	4.00000	19.00000	0.33998	4.68978
4.00000	5.00000	16.00000	5.00000	16.00000	0.06391	5.38693
4.00000	5.00000	16.00000	3.00000	16.00000	0.06390	5.38693
4.00000	5.00000	16.00000	1.00000	16.00000	0.06390	5.38693
4.00000	5.00000	16.00000	6.00000	16.00000	0.06390	5.38693
4.00000	5.00000	16.00000	2.00000	16.00000	0.06390	5.38693
4.00000	5.00000	16.00000	4.00000	16.00000	0.06389	5.38693
4.00000	5.00000	7.00000	1.00000	7.00000	0.04698	5.71072
4.00000	5.00000	7.00000	2.00000	7.00000	0.04697	5.71072
4.00000	5.00000	7.00000	3.00000	7.00000	0.04697	5.71072
4.00000	5.00000	18.00000	5.00000	18.00000	0.02889	5.23130
4.00000	5.00000	18.00000	3.00000	18.00000	0.02888	5.23130
4.00000	5.00000	18.00000	2.00000	18.00000	0.02887	5.23130