Solid States - TP2

May 20, 2022

1 Question 1

According to the VASP wiki, GGA stand for “Generalized Gradient Approximation” and PE stand for “Perdew-Burke-Ernzerhof” (a GGA fonctionnal)

2 Question 2

```
PAW_PBE C 08Apr2002
```

I assume that PBE mean Perdew-Burke-Ernzerhof, so it is consistant with the previous answer

3 Question 3

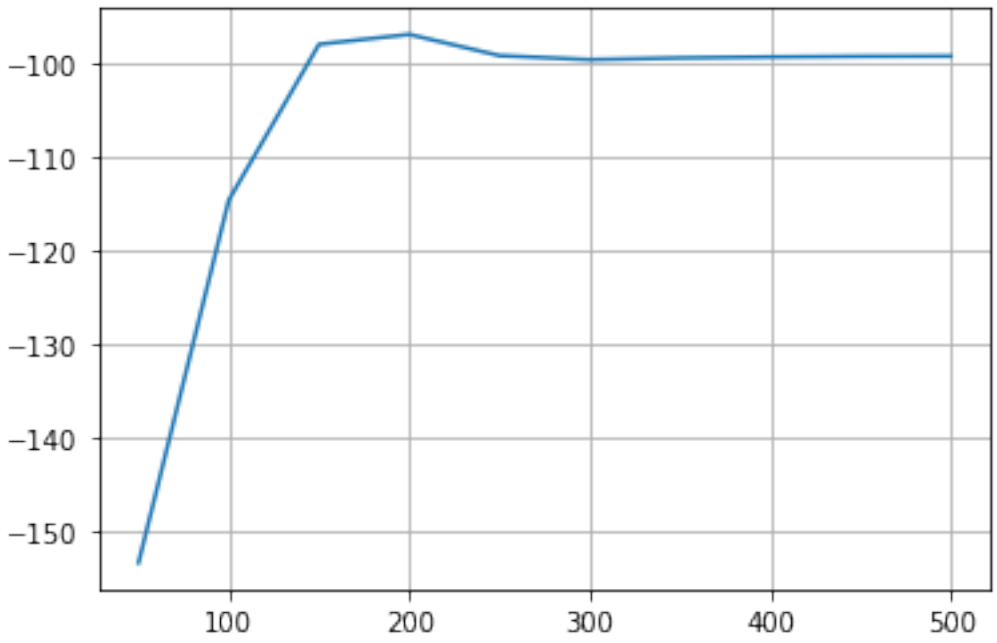
Looking at the POTCAR file, there is now 12 described vectors, so 12 atoms (wich is a lot more than previously!)

4 Question 4

[ ]:
```
from numpy import *
import matplotlib.pyplot as plt

data = loadtxt("results/Q4_energy.txt")

plt.plot(data[:,0], data[:,1],label="Energy")
plt.grid()
plt.show()
```



According to this plot, 300 seems to be a safe value for the cutoff to reach the correct energy.

5 Question 5

By runngin the commands `grep 'time' OUTCAR` and `grep 'Iteration' OUTCAR`, we can see that the job took 340 seconds to run over 50 ionic iteration.

6 Question 6

At the first iteration, the energy is 135.33 eV
The final energy is -105.16 eV

We can notice that at the second iteration, the energy is at -103.68 eV So it quickly converge to the final energy.

7 Question 7

By using the command `grep 'E-fermi' OUTCAR`, we get the fermi energy for this crystal, which is here 3.39 eV

I used the POSCAR file sent by mail by Noah Perreau. With the old one, I got 5.04 eV but all the structures were metallic.

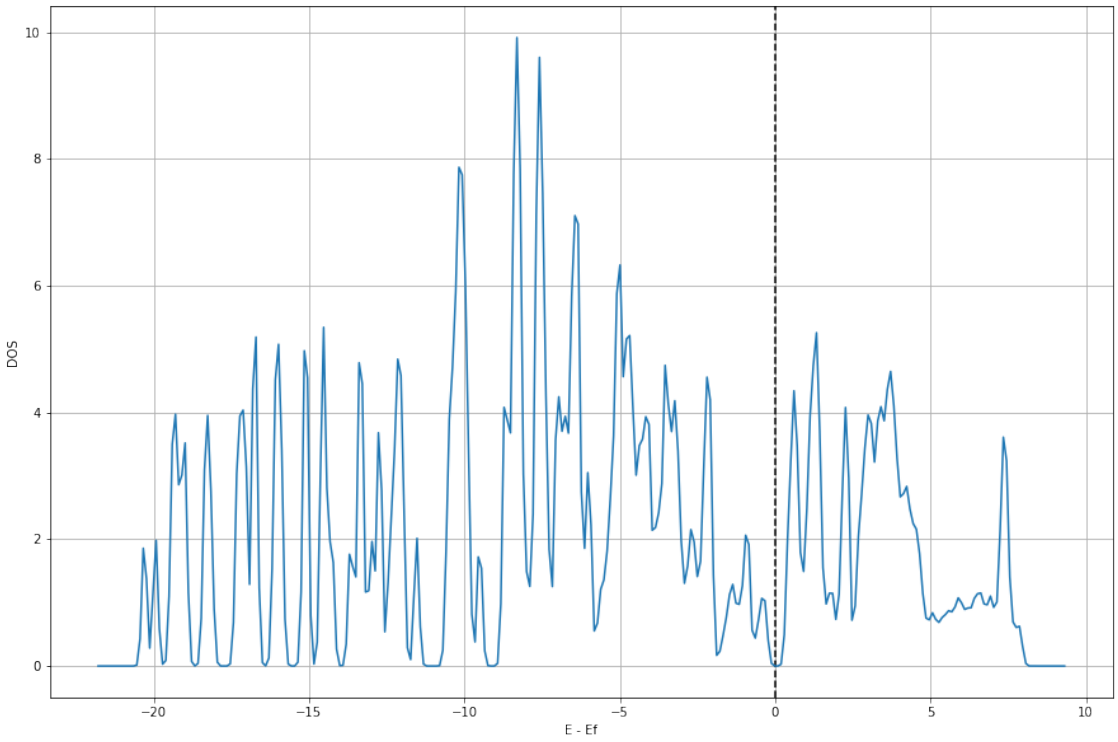
8 Question 8

[ ]:
```
from numpy import *
import matplotlib.pyplot as plt

Ef33 = 3.39

data33 = loadtxt("results/Q8_dos.dat")

plt.figure(figsize=(15,10))
plt.axvline(x=0, color='k',linestyle="--")
plt.plot(data33[:,0] - Ef33, data33[:,1],label="Energy")
plt.xlabel("E - Ef")
plt.ylabel("DOS")
plt.grid()
plt.show()
```



As the density of state is zero at the fermi level, then this is a semiconductor or an insolator.

9 Question 9

In this new POSCAR file, there is 56 vectors, so 56 atoms.

10 Question 10

In the INCAR file, we can read:

`ICHARG = 11`

According to the VASP wiki, this ICHARG parameter determines how VASP constructs the initial charge density.

For a value upper than 10 allow to keep the charge density constant during the electronic minimization. Setting this parameter to 11 allow to obtain the density of states.

11 Question 11

By running the command `grep 'E-fermi' OUTCAR`, we obtain the fermi energy, which is 2.26 eV

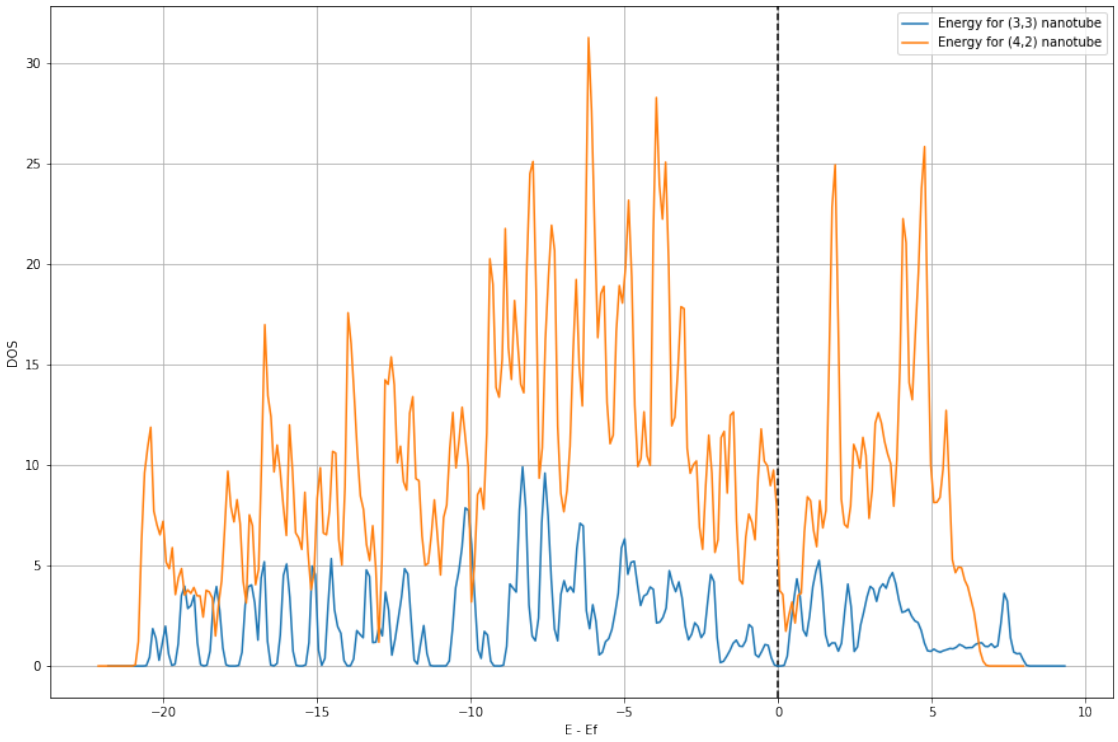
12 Question 12

[ ]:
```
from numpy import *
import matplotlib.pyplot as plt

Ef42 = 2.2647

data42 = loadtxt("results/Q12_dos.dat")

plt.figure(figsize=(15,10))
plt.axvline(x=0, color='k',linestyle="--")
plt.plot(data33[:,0] - Ef33, data33[:,1], label="Energy for (3,3) nanotube")
plt.plot(data42[:,0] - Ef42, data42[:,1],label="Energy for (4,2) nanotube")
plt.xlabel("E - Ef")
plt.ylabel("DOS")
plt.legend()
plt.grid()
plt.show()
```



The DOS for the (4,2) nanotube is no more 0, so this nanotube is metallic.

13 Question 13

One of the most interesting aspect of these results is that it show that the electronic behavior of the same material can be different depending on the mecanic contraints that are applied on it. However, this is strange because these results contradict what we can find on Wikipedia, saying that a (N,M) carbone nanotube is metallic if N=M, quasi-metallic if N-M is a multiple of 3, and semiconductor otherwise. Here, we have the opposite results…