Vu-Linh Nguyen - 2256347
Computational Condensed Matter Physics - Makeup exam

2.1.1 Preliminary steps:

I will work with the system composed by **CdTe.**

- What is the underlying Bravais lattice?

We are using the ibrav=2, which means we are working with the underlying FCC lattice.

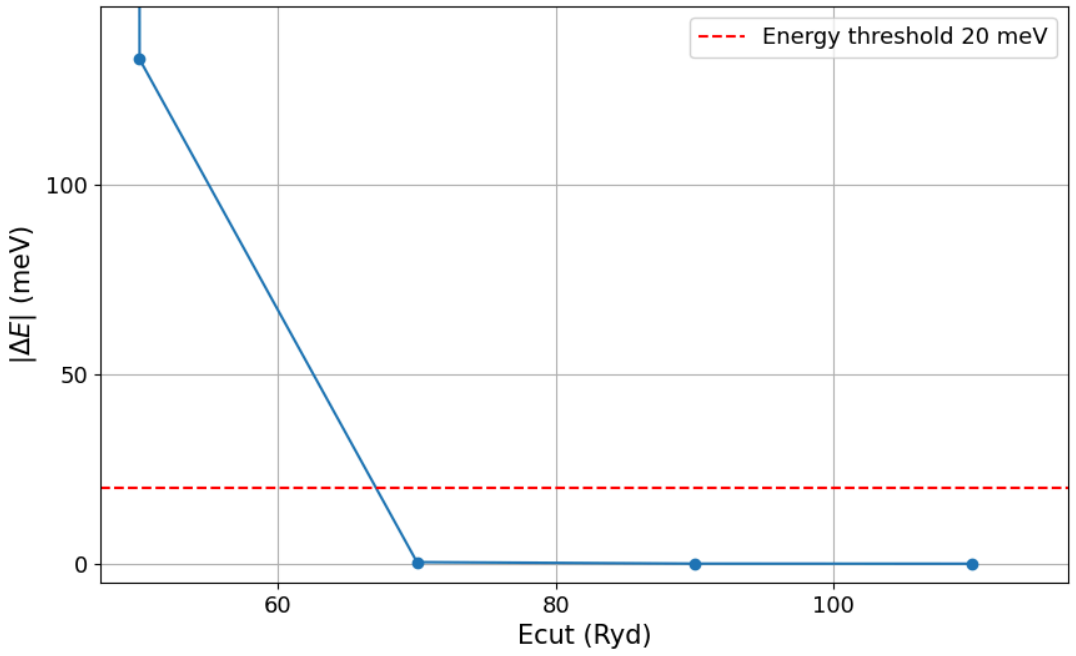
- What are the reciprocal lattice vectors and the basis vectors of atoms A and B (write them down explicitly).

$\vec{b}_1 = \frac{2\pi}{a}(-1, 1, 1)$; $\vec{b}_2 = \frac{2\pi}{a}(1, 1, 1)$; $\vec{b}_3 = \frac{2\pi}{a}(-1, 1, -1)$

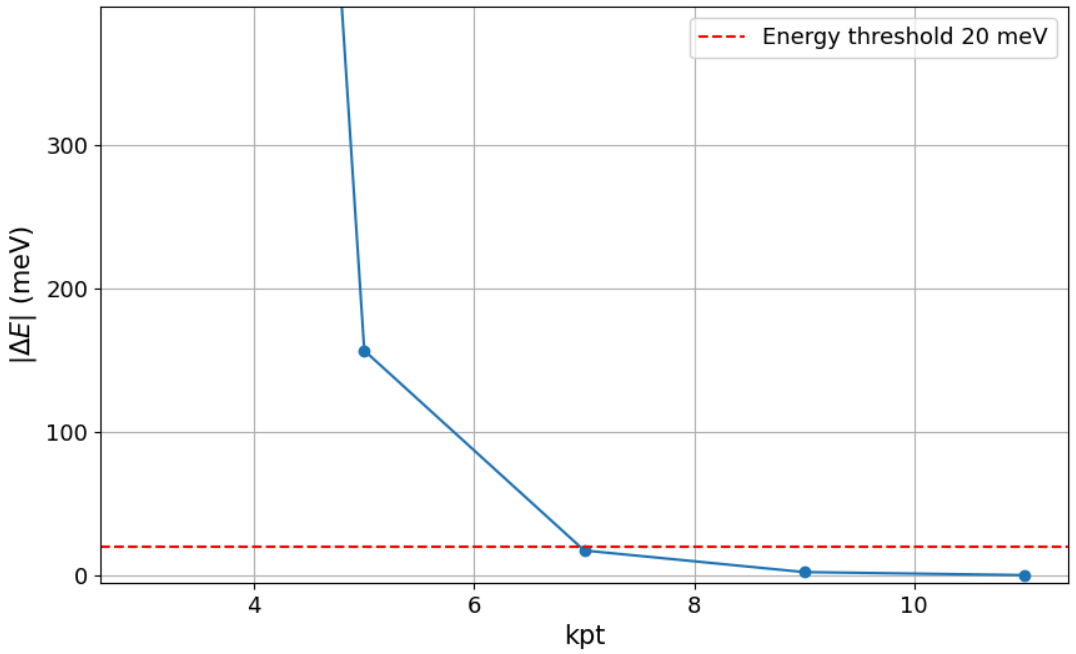
- How many valence electrons does your system contain?
  It depends on the Pseudo potential I choose, I have 2 atoms Cd and Te in my primitive cell. Cd has 20.00 valence electrons. Te has 16.00 valence electrons. In total, I have 36 valence electrons.

2.1.2 Convergence test

Our convergence test threshold is 10meV/atom, for the whole system is 20meV.
First, we find an energy cut-off to control our number of plane waves used to expand the Kohn–Sham states. I found the absolute difference between two nearest energy cut-offs goes below our threshold at Ecut= 70 Ryd.



Second, we find a good number of kmesh for the accuracy of our BZ integral. We found kmesh=7 would make our absolute difference of consecutive kpoint energy below the given threshold.



2.2 Structural Relaxation:

- What is the theoretical pressure calculated by quantum espresso for the structure you set up?
  We start with the pressure P=1192.79 kbar

- If you had to relax the structure by hand, without using quantum espresso relaxation routines, what would you do?
  I can do it by hand by guessing, because our pressure is positive. If we relax, our crystal structure will expand, and I will increase my celldm(1), run scf calculation, check the output file, and do it until I get P=0 kbar.

- Once you are sure that your calculation has reached the theoretical equilibrium volume, write down the final value of the volume and the corresponding lattice constant.
  Do by hand

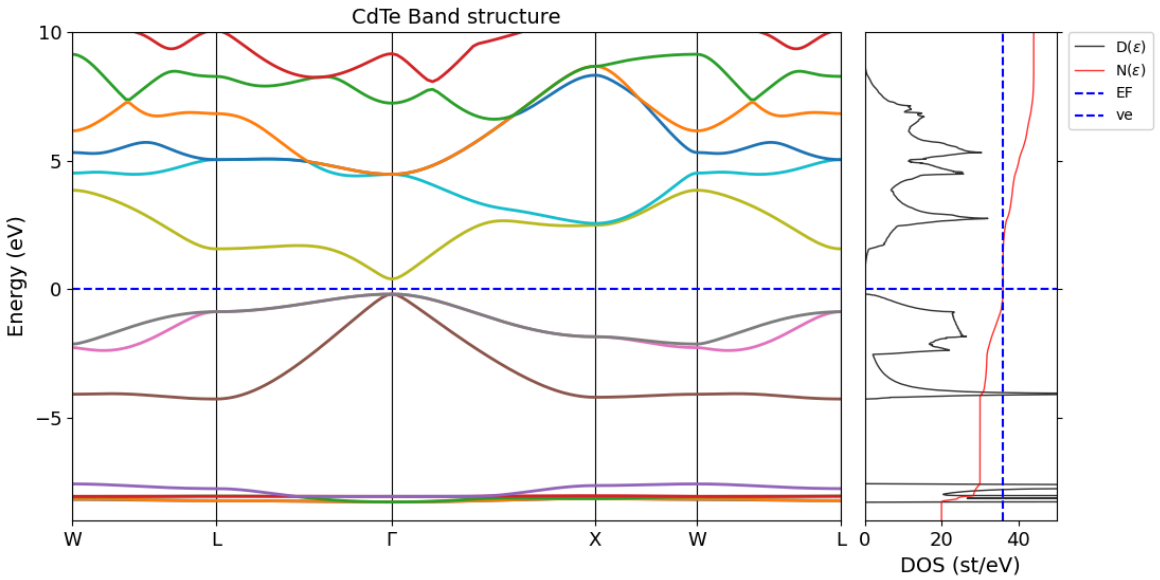
Lattice constant (a.u)	P (kbar)
10	1192.79
15	-52.56

12	59.93
14	-55.38
13	-32.45
12.5	-0.10

I get -0.1 kbar at lattice constant 12.5 a.u, whose volume is 488.2812 (a.u.)^3. The initial volume is 250.0000 (a.u.)^3, we increase up to 95% from initial to get our crystal to relax to P=0.

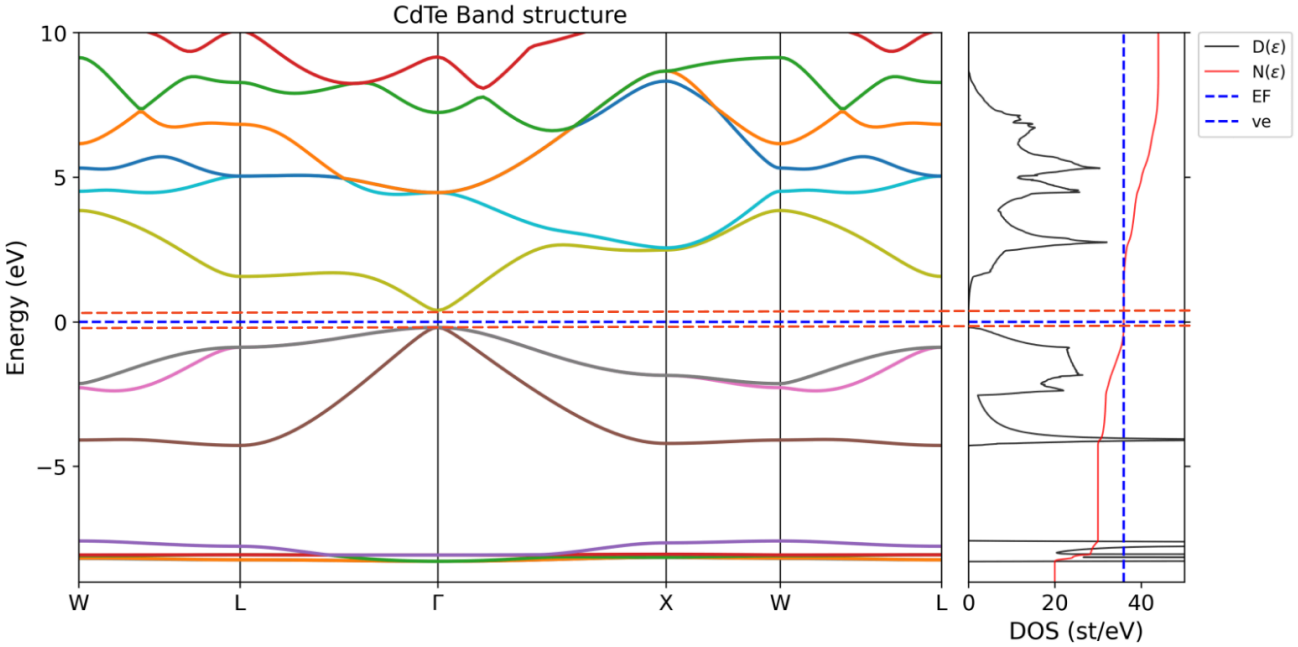
2.3 Band Structure and Density of States:

After the careful calculation, I found out the band structure and density of state. As you can see our fermi level doesn't touch the region where we don't have any density of state anymore, this might be because of the inaccuracy of the number kmesh for BZ integral, I choose 24, I expect the fermi level would touch the dos, where it becomes zero.



Now I plot new two red lines and Bandstructure and density of state plot, from this I predict we have the direct bandgap in here. It means we can emit photons by returning electrons

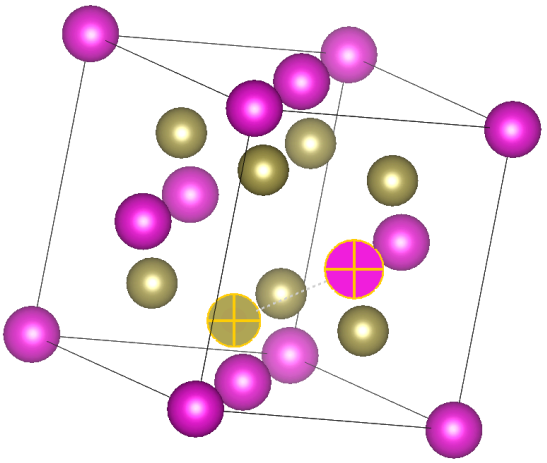
from the conduction to the valence band.



- Do you think the actual experimental band gap will be smaller or larger than the one you computed? Why?
  The bandgap would be larger because PBE is not an accuracy functional to estimate the bandgap, and also DFT is original as a method of ground state energy not excited energy.

2.4 Atomic Displacements and Forces

- How many bonds does each A atom form to B atoms and vice-versa? How long are they? What are the bond directions?
  They have 4 bonds, their distance is 2.86427(0) Å = 5,412685848 a.u. The bond directions are not the same. They can be ¼(1,1,1), ¼(-1,-1,1), ¼(1,-1,-1) and ¼(-1,1,-1)



- Displace the atom in the origin by f 0.05 × sqrt(3) times the lattice constant along the body diagonal. How do you do it?

I need to change the Cd position x y z in the way that have the relation which the direction of the body diagonal. I observe that $\vec{a}_1 + \vec{a}_2 + \vec{a}_3 = a(-1, 1, 1)$ the magnitude is a*sqrt(3), so to change it to 0.05*3 times the lattice constant, I would change the x=y=z=0.05=0.05.

- Compute the resulting forces: what are the magnitude and direction of the force? What will happen when you let the structure relax?
  The force is 0.13929 Ry/au, and their directions are not the same for Cd and Te atoms
  They are (I suppose the direction has the relation with the primitive vectors)
  Cd force = 0.00000000 -0.09849371 0.00000000
  Te force = 0.00000000 0.09849371 0.00000000

- How many steps does it take to converge to the equilibrium structure?
  8 steps

- Produce a plot of the variation of the energy and of the forces during the relaxation, as a function of the displacement. Comment your results (max. 100 words).

The energy and the force get minimized after the relaxation.