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Computational Condensed Matter Physics - DFT Makeup exam

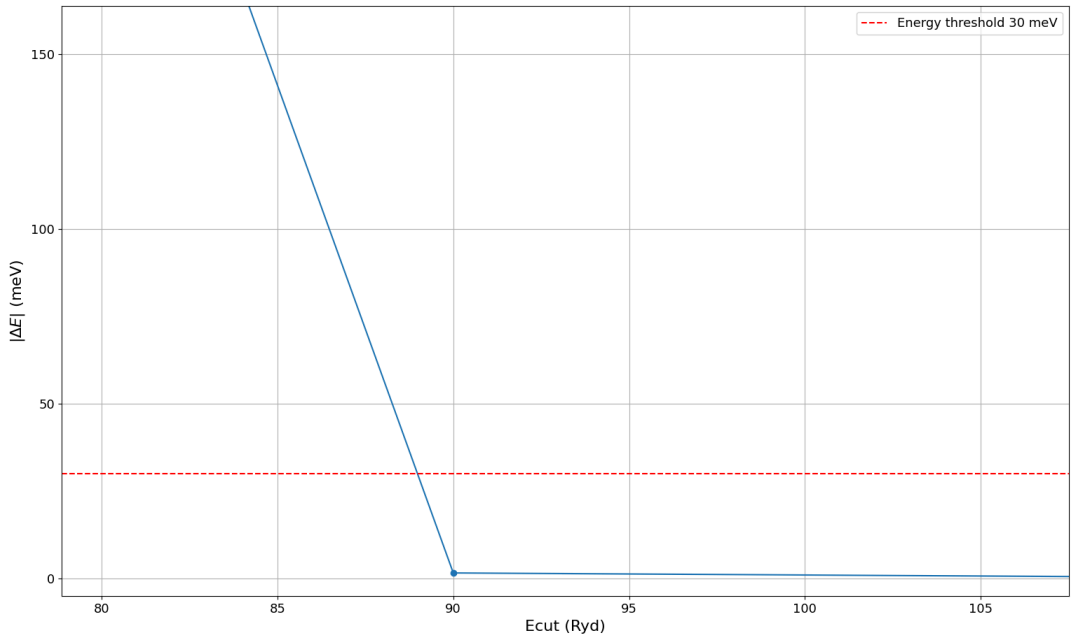
2.A.1

Atoms	Mg	B
Valence electron (Pseudo file)	10	3
Total electron	12	5
Core electron	2	2

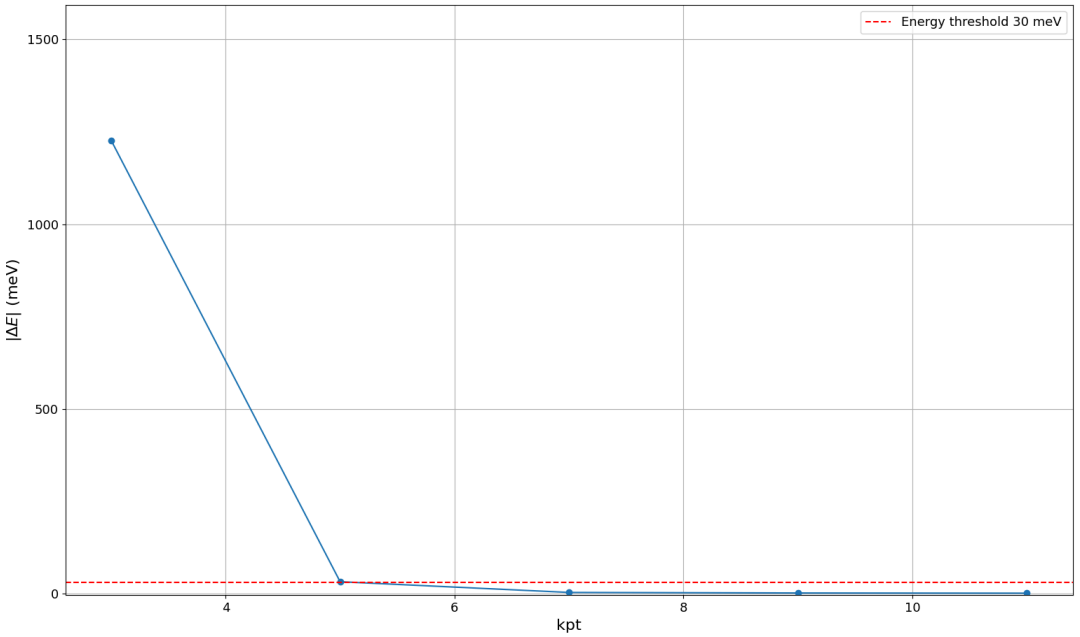
In our system, we work with primitive cell, we have 1 Mg and 2 B atoms in our system. So in total we have 10+3*2 = 16 valence electron, 12+5*2=22 total electron, and 22-16=6 core electron. We suppose Mg would have only 2 valence electron, but I think they take more valence electron for flexibility.

2.A.2

First, I find the energy cut off of for my plane waves



And also to find the dense of my k-point for BZ integral



I found 90Ryd and 6kpoint

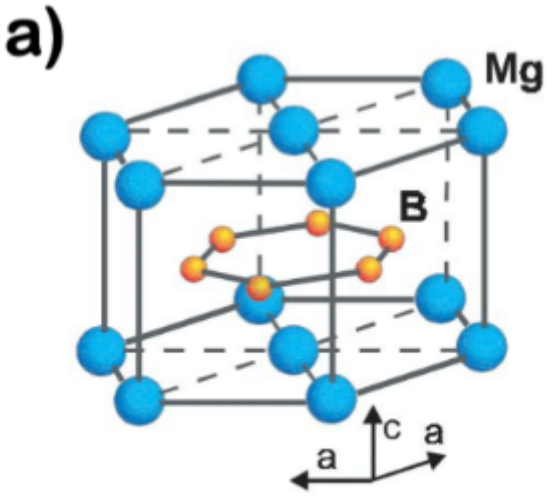
A.3 Force are zero because we are in the high symmetrical point, the force from different sites cancel out each other.

We have stress tensors are anisotropic. They are the same in x and y direction but not in z direction $\sigma_{xx} = \sigma_{yy} = -8.24$ and $\sigma_{zz} = -3.23$. If we perform the relaxation, our system would srhink due to the negative stress.

B.1

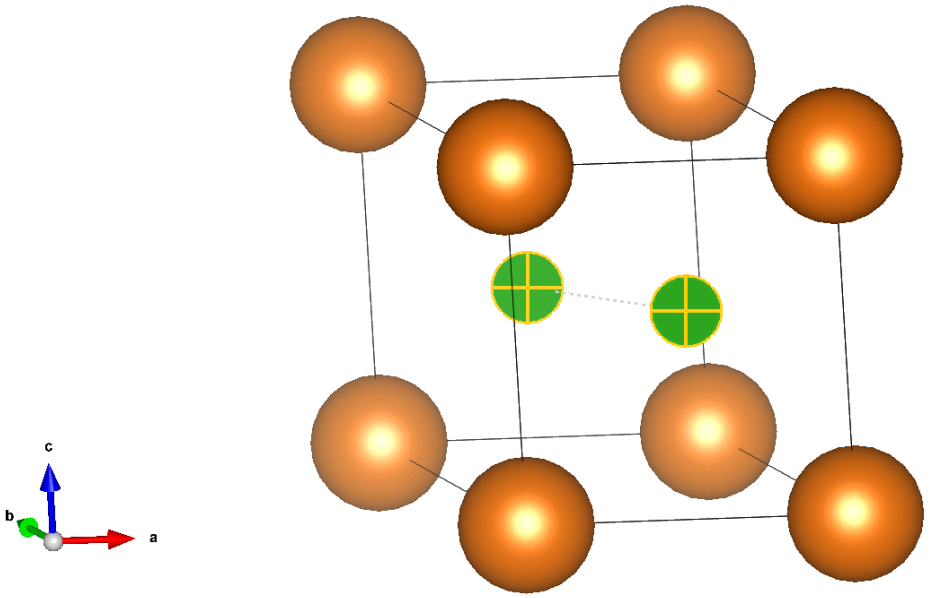
After the relaxation, our volume shrink from 195.5883483 B^3 to the volume 194.87441 a.u.^3 around 0.365%. Our new ration of c/a=6.649737961/5.817144168=1.14312758.

What is the interatomic in-plane B-B distance, I assume this the smallest distance,

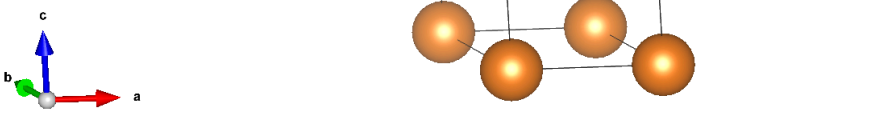


Our primitive vectors are v1 = a(1,0,0), v2 = a(-1/2,sqrt(3)/2,0), v3 = a(0,0,c/a)

So the we have in-plane B-B distance = |-1/3 *v1 + 1/3* v2| = a/3(sqrt((-1-½)^2 +¾) =a/sqrt(3) =5.817144168/sqrt(3) = 3.35852975131 a.u. Compared with Vesta, 1.77726 A = 3.35851695075 a.u

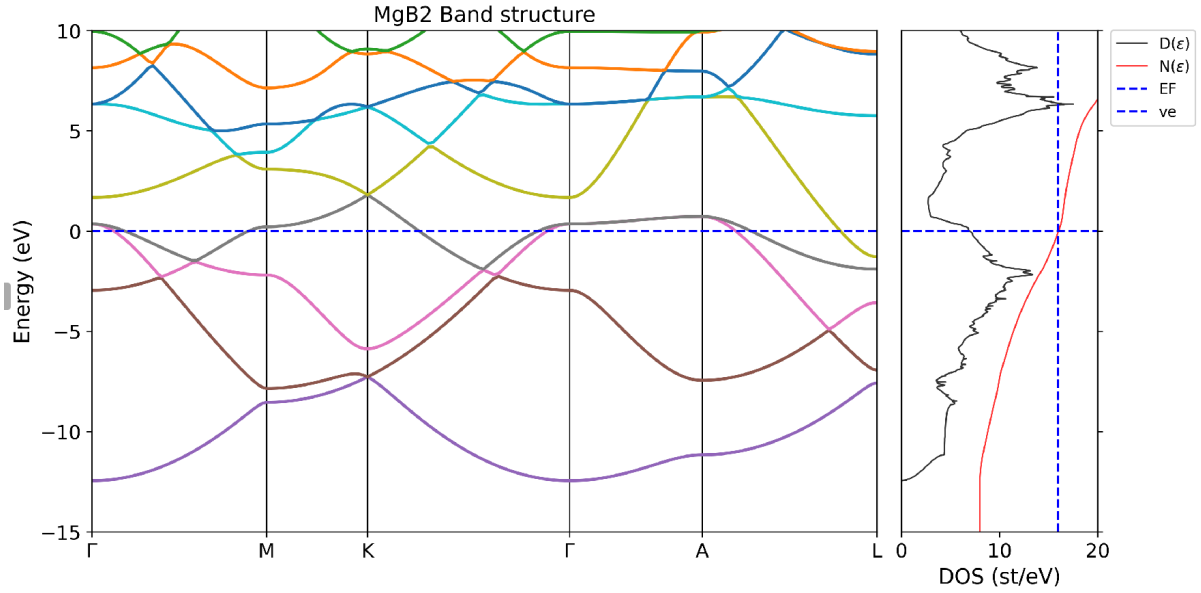


What is the out-of-plane B-B distance? While the distance between neareat B-B distance is c=6.649737961. Which Vesta, I got 3.51889 A = 1.88971616463* 3.51889 a.u= 6.64970331455 a.u



We can check our result with VESTA, but I think we should check by using the primitve vector, or cell_parameter.

B.2 After obtaining the ambient pressure (P=0), we use the new structure to have the bandstructure and density of state calculation. I got



At first, I tried with kmesh=18 for the nscf calculation, and choose emin=-10, and emax=20, however, the number of electron below the fermi level is not 16, and the density of state looks a mess. I increase the BZ integral accuracy of DOS by increasing the kmesh to 24, and emin to - 76, emax is the same. And I got the figure above. As you can compare, I achived the same with the result from the provided bandstructure of the exam

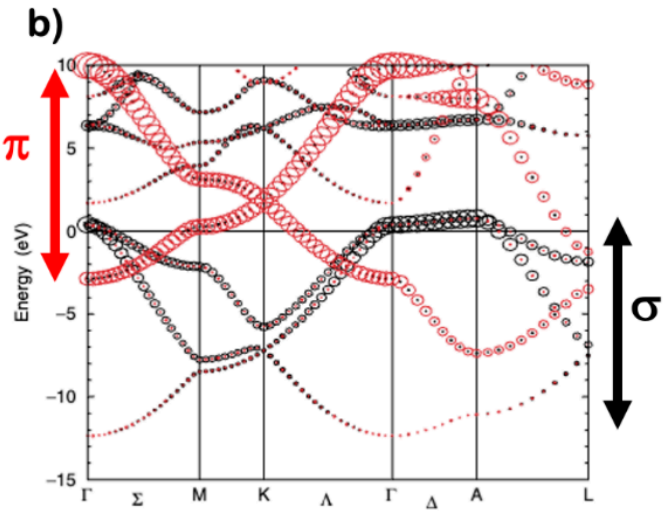
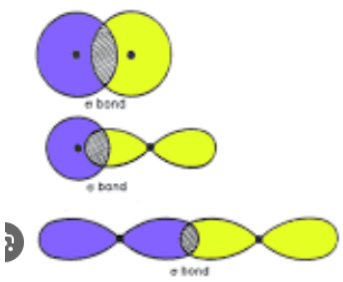


FIG. 1 (color). Band structure of MgB_2 with the B p character. The radii of the red (black) circles are proportional to the B p_z (B $p_{x,y}$) character.

B.3 We need to look at the Brillouin zone path again of the hexagonal, the FA path represents the bond interaction changing in the z direction, the sigma bond would not change much in z direction, but the pi bond does depend on the z direction



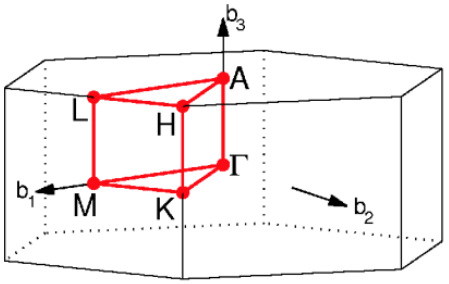
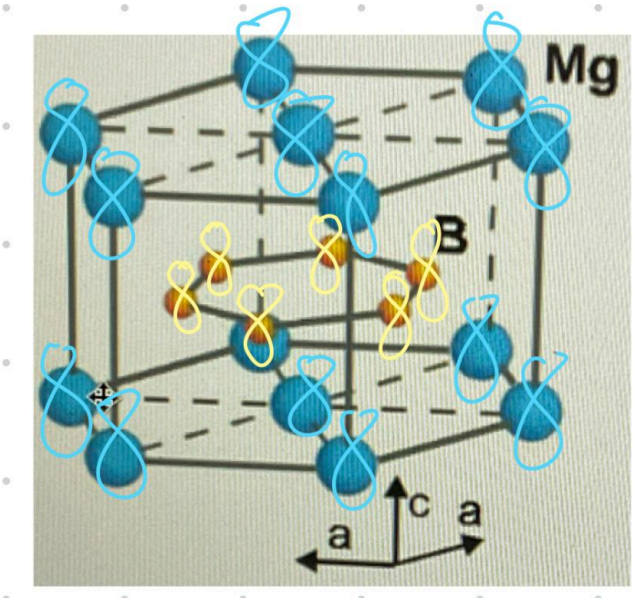
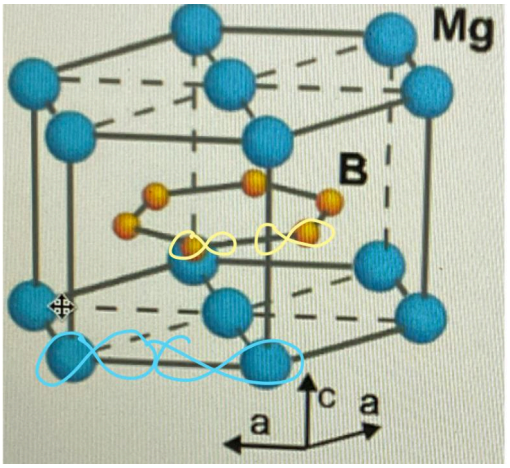


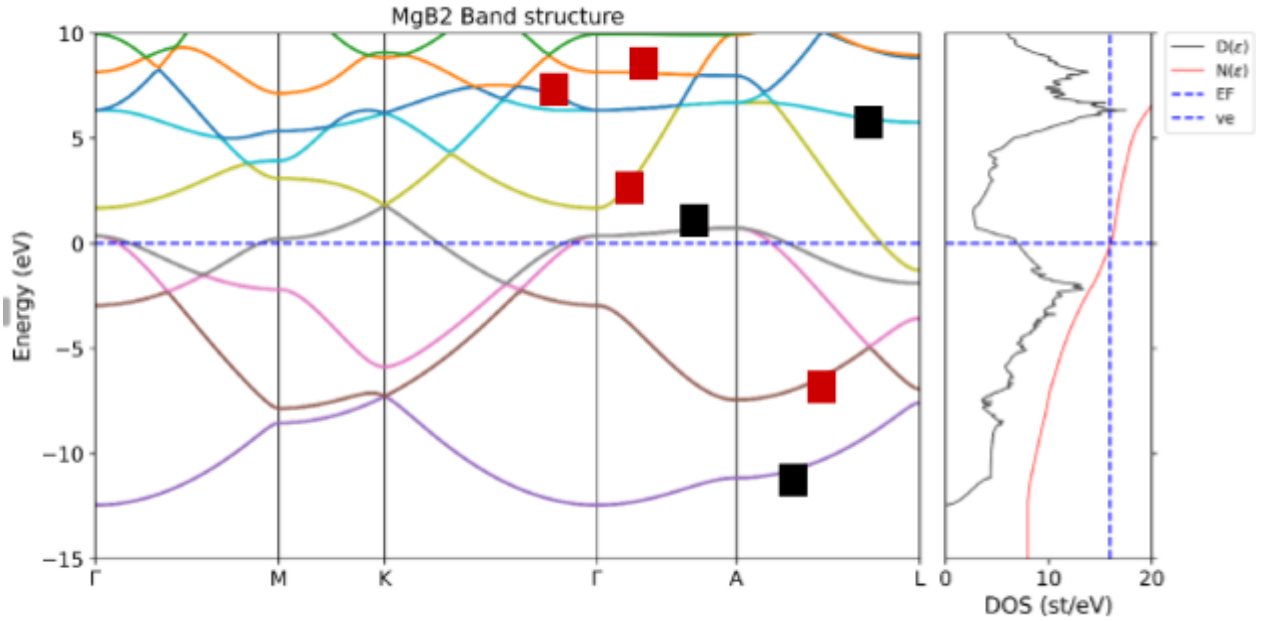
Figure 13: Brillouin zone of HEX lattice. Path: Γ-M-K-Γ-A-L-H-A|L-M|K-H. An example of band structure using this path is given in Figure 38

The figure below described how the sigma and pi bonds are froming inside our crystal

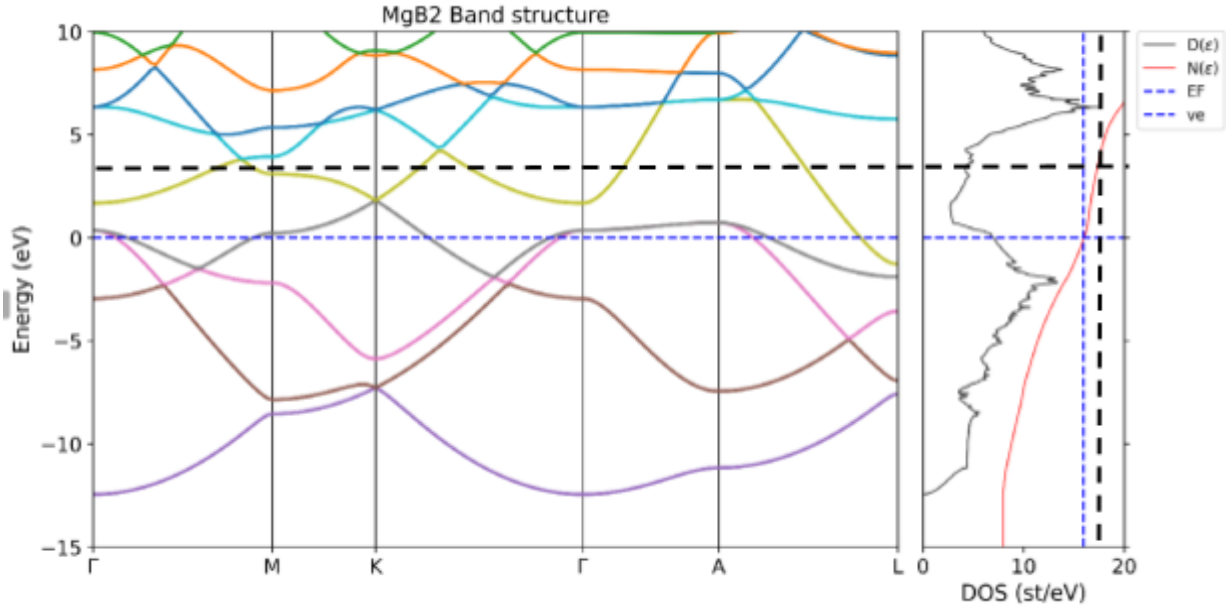




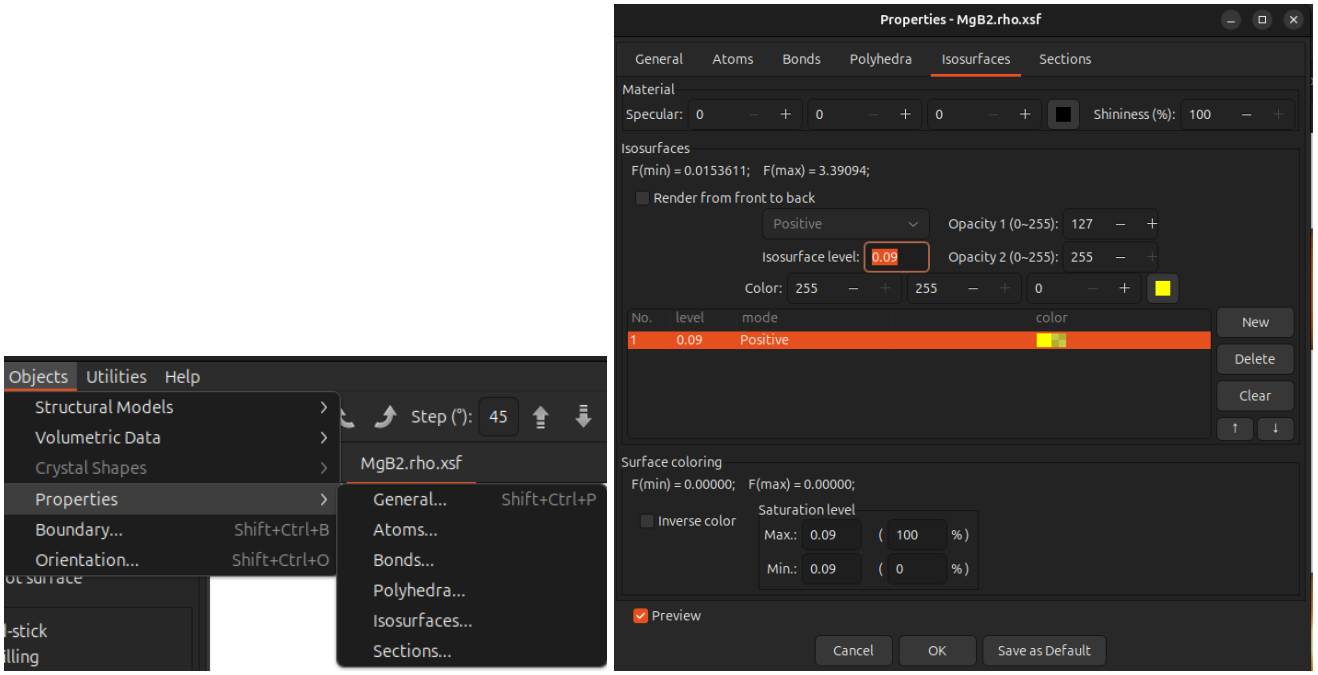
Because of this reason, we can guess where is our pi and sigma bond in our crystal. Because our bands are quite entangled with each other, I use the red and black square to identify pi and sigma bond, where we have their are significant/slight change in the FA direction.



Our electronic states on the Fermi surface would be mainly contributed by the sigma state or px and py orbital as you can see the purple and grey bands go up and down on the Fermi level. My result would depend on the number of valence electrons in our system. Because if we increase or decrease our valence electrons in the system, we can shift up and down our fermi level, that would change our electronic states of the Fermi level. For example, we shift our fermi level by increase our valence electrons to around 18 valence electron (big black line), we would have our electronic states on the Fermi surface from the pz orbital or from the pi bond.



Extra plot:
I also plot the charge density of the MgB2. We change the isosurface level to be small enough to see the charge density



I got the ground density of state of MgB2, it showed that I have the strong sigma bond near the B atoms and slight amount charge density around the Mg atoms