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Computational Condensed Matter Physics - Makeup exam

1. **Preliminary steps**

My number is 4, so I need to work with the system of X= Ca and Y = K

2. **Electronic properties of XB3 C3 in the ground-state structure:**

2.1 Initial Structure Setup:

2.1.1 The structural parameters of the XB3 C3 compound are reported in Table 1. Before setting up the calculations, answer the following:

- • What type of Bravais lattice does this structure belong to?

We work with Cubic structure

- • How many atoms are there in the unit cell and what are their crystallographic positions?
  Our Wyckoff positions are Ca (2a), B (6c), C (6d),
  So where have 2 Ca atoms, 6 B atoms and 6 C atoms, in total we have 14 atoms in the unit cell.
- • How many formula units are contained in each unit cell?
  We have 2 formula unit in the unit cell.

2.1.2

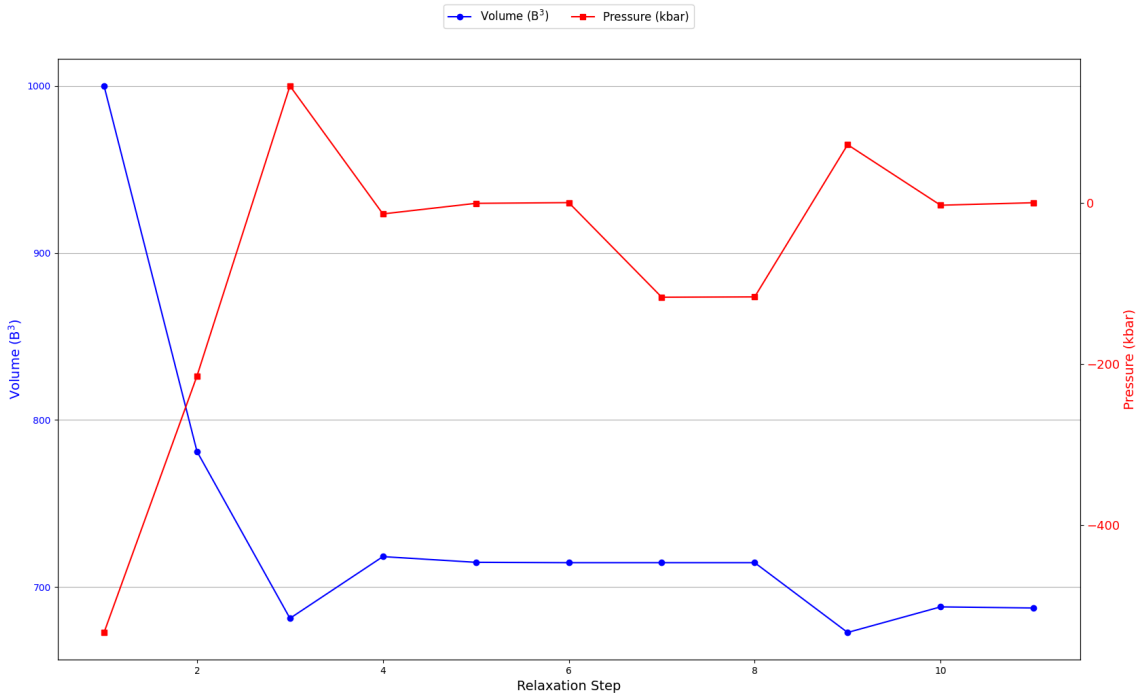
- Report the volume of the unit cell and the corresponding pressure (in kbar) obtained from your SCF calculation.

It takes me 1 hour to find the right crystal structure, force =0
The volume is 1000.0000 (a.u.)^3, with the lattice parameter 10.0000 a.u. Pressure is -533.71 kbar

- Based on the calculated pressure, would you expect the unit cell to shrink or expand if relaxed to zero pressure? Explain your reasoning (max 50 words).
  Because we have negative pressure, our lattice would shrink its volume if we do the relaxation.

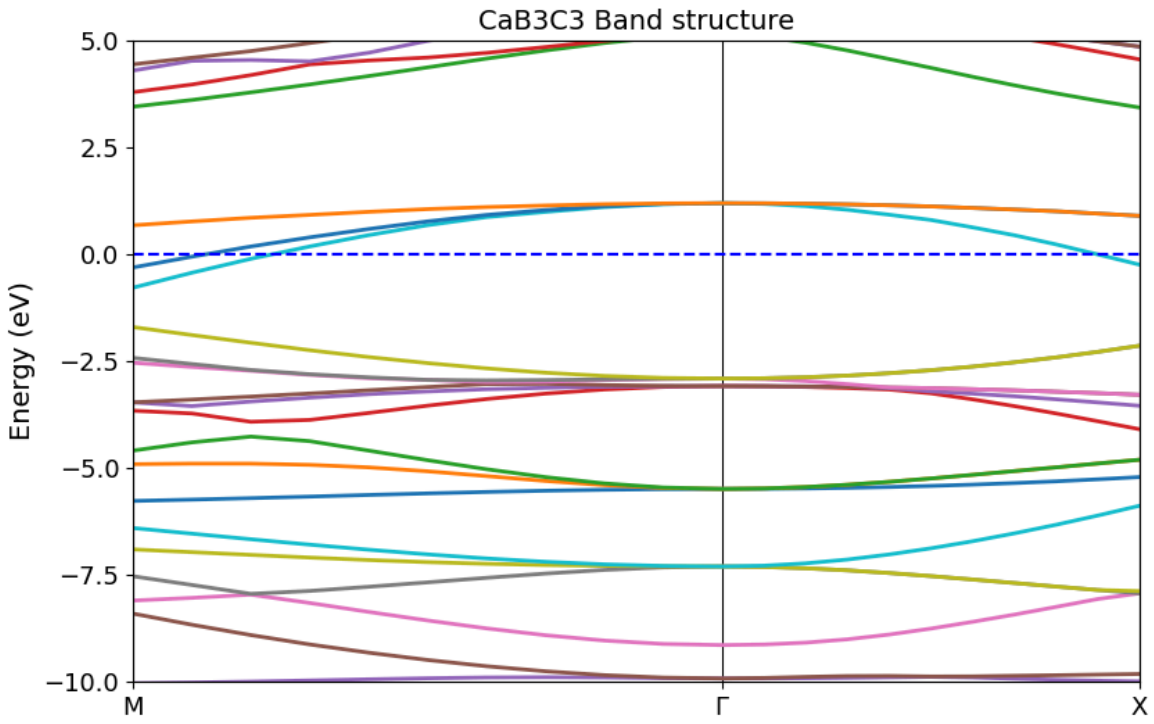
2.2 Relaxation to the ground-state structure

Relax the structure to zero pressure: what are the corresponding volume and pressure? What is the lattice constant? Is the result consistent with your expecations? Why? (100 words).
Volume 687.39050 B^3, we have the lattice parameter=8.82540221891B, and pressure = -0.08kbar. After two relaxation calculation with 11 steps. This is what I expect, because which negative pressure our crystal need to shrink.

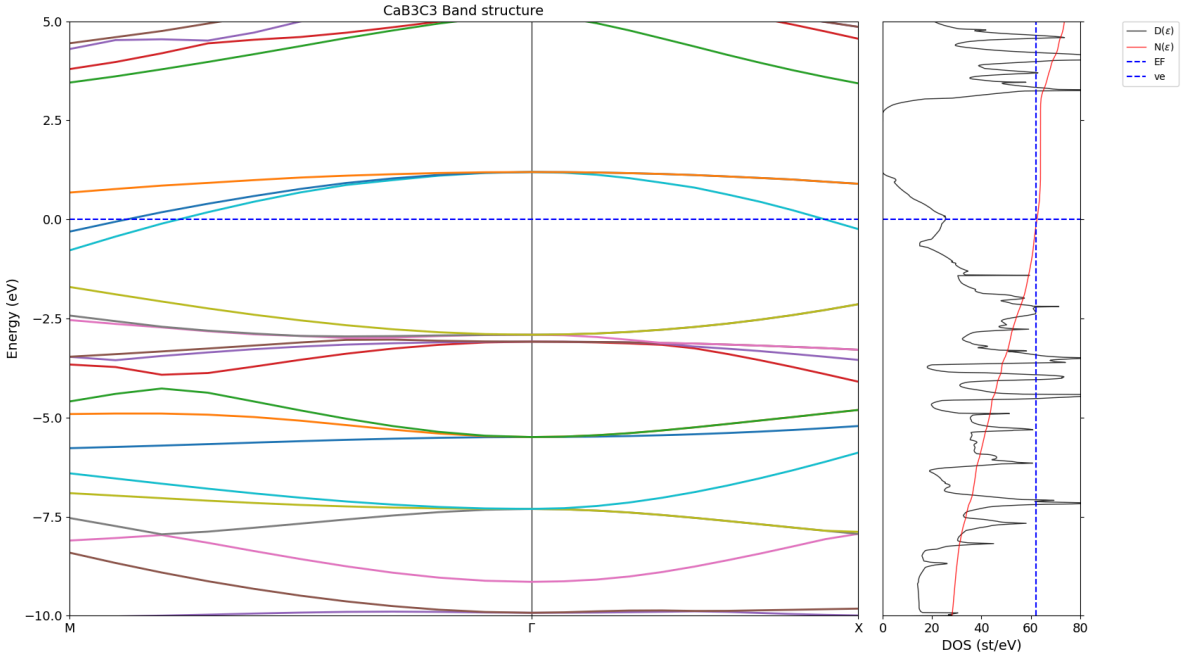


3. Electronic Structure

- 3.1.1 Explain what is meant by an electronic band-structure calculation and describe briefly how Quantum ESPRESSO computes it (max 100 words).
  It means we calculate the corresponding of energy inside the BZ for particular band, and k-point position in the BZ. Quantum expresso would use the ground state charge density from scf calculation, and run the non-scf process on the band calculation along symmetrical lines.
  After doing another scf calculation, I found P=-13.66kbar, I think this is because the unaccurate from the small number of kpoint. However, I assume this is acceptable.
    - Compute and plot the electronic band structure of your XB3 C3 compound along a high-symmetry path in reciprocal space. To reduce the computational load, use the minimal path M − Γ − X. If the calculation is slow, reduce the number of points along each segment (10 points/segment are sufficient). You can find a list of special k-points in table 2.
      I got the bandstructure for kmesh = 2 2 2



3.1.3 Compute the corresponding density of states (DOS) using a 6 × 6 × 6 k-point grid and the tetrahedron method.



The bandstucture on the right and the density of state on the left, as you can see, this crystal structure is a metal

3.1.4 Explain briefly how Quantum ESPRESSO computes the DOS (max 100 words).

They calculation by taking the the integral/sum inside the brillouin zone for spercific energy g(epsilon) = \sum_nk \delta(Enk - epsilon). I think they can estimate this delta as a Gaussian, when they do the DoS calculation, I haven't checked this.

3.1.5 Using your band structure and DOS, answer the following (max 200 words total): (i) What is the Fermi level of your system and how did you determine it? (ii) Is the system metallic or insulating? Justify your answer. (iii) If metallic, report N (EF) (DOS at the Fermi level). If insulating, report the band gap.

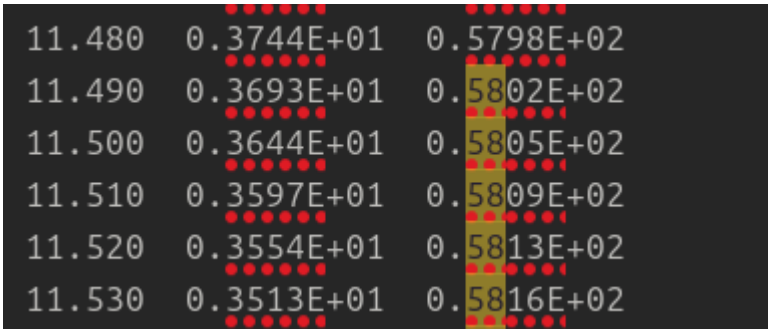
Our fermi level is 13.013 eV, I find the fermi level inside the file CaB3C3.dos file, this is the place where the integral of density up to this energy = number of valence electron inside your system

N = \int_{-\infty}^{E_f} g(\epsilon) d\epsilon), and N(eF) = 62.

3.2 Rigid-Band Doping:

3.2.1 Where would the Fermi level fall if you added/subtracted one or two electrons per formula unit (f.u.)?

If I remove two electrons per formula unit, I lost 4 electron, it would be around, the fermi level is 11.49 ev



11.480	0.3744E+01	0.5798E+02
11.490	0.3693E+01	0.5802E+02
11.500	0.3644E+01	0.5805E+02
11.510	0.3597E+01	0.5809E+02
11.520	0.3554E+01	0.5813E+02
11.530	0.3513E+01	0.5816E+02

If add 4 electrons, Ef=16.66

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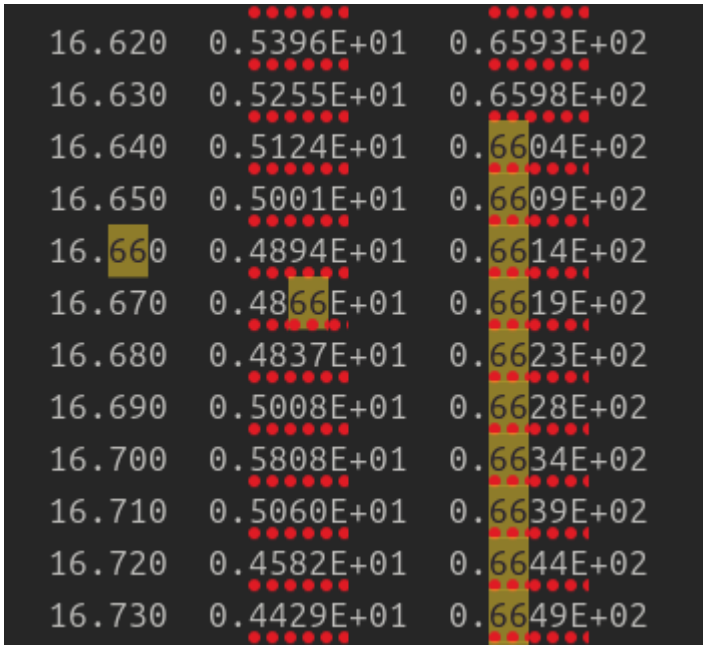

16.620	0.5396E+01	0.6593E+02
16.630	0.5255E+01	0.6598E+02
16.640	0.5124E+01	0.6604E+02
16.650	0.5001E+01	0.6609E+02
16.660	0.4894E+01	0.6614E+02
16.670	0.4866E+01	0.6619E+02
16.680	0.4837E+01	0.6623E+02
16.690	0.5008E+01	0.6628E+02
16.700	0.5808E+01	0.6634E+02
16.710	0.5060E+01	0.6639E+02
16.720	0.4582E+01	0.6644E+02
16.730	0.4429E+01	0.6649E+02

3.2.2 Which physical properties would be affected by this change, and why?

If we remove 4 atoms, our system still is a metal, but if you increase I think I need to make the detail calculation, but we can have a gap near the fermi level, so it can become insulator or semiconductor.

3.3 Physical Doping:
Now, i change Ca -> K, our system has the dopping of 4 valence electron in the system