Weekly Report

Siyu Liao

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1 Introduction

This week I mainly focus on analyzing the COHP of the results of last week and visualizing fermi surfaces. Besides, I have also found something interesting when reading some papers.

2 Progress

2.1 COHP analysis

COHP analysis is of great importance to uncover the specific orbital couplings and I expect to acquire some clues about which couplings dominate the band structure changes. However, I face some data processing problems when during with the results of Lobster. I found that neither Pymatgen.io package or Wxdragon(A package that Lobster recommends) have some problems that I cannot fix, so I tried to write some scripts with gnuplot to visualize the results of Lobster. What's more, Lobster could calculate the couplings between specific orbital but it lacks of interpretations about the results in Documentation, so I have to guess which column refers to which coupling. Therefore I suppose I'd better do the furthur analysis after I totally handle and verify it.

In the following I will give an example of COHP analysis using the result of last week—GaP(lattice constant = 5.15Å).

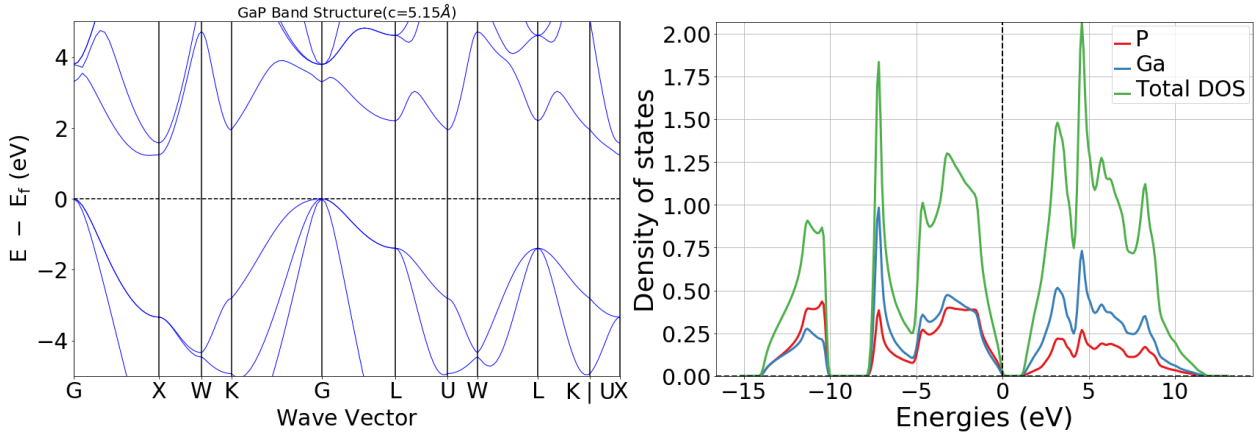

Figure 1: GaP's band structure(left) and DOS(right)

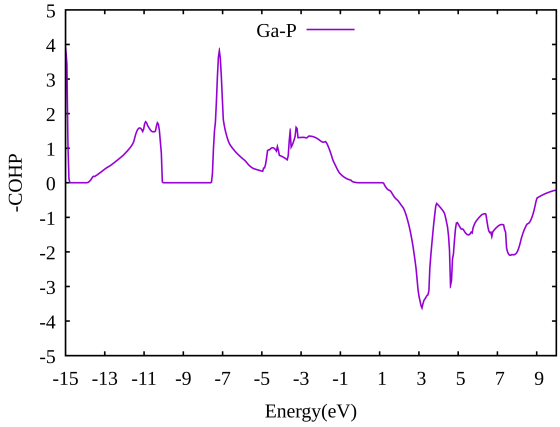

Figure 2: GaP's COHP. Y value bigger than zero means anti-bonding and vice versa

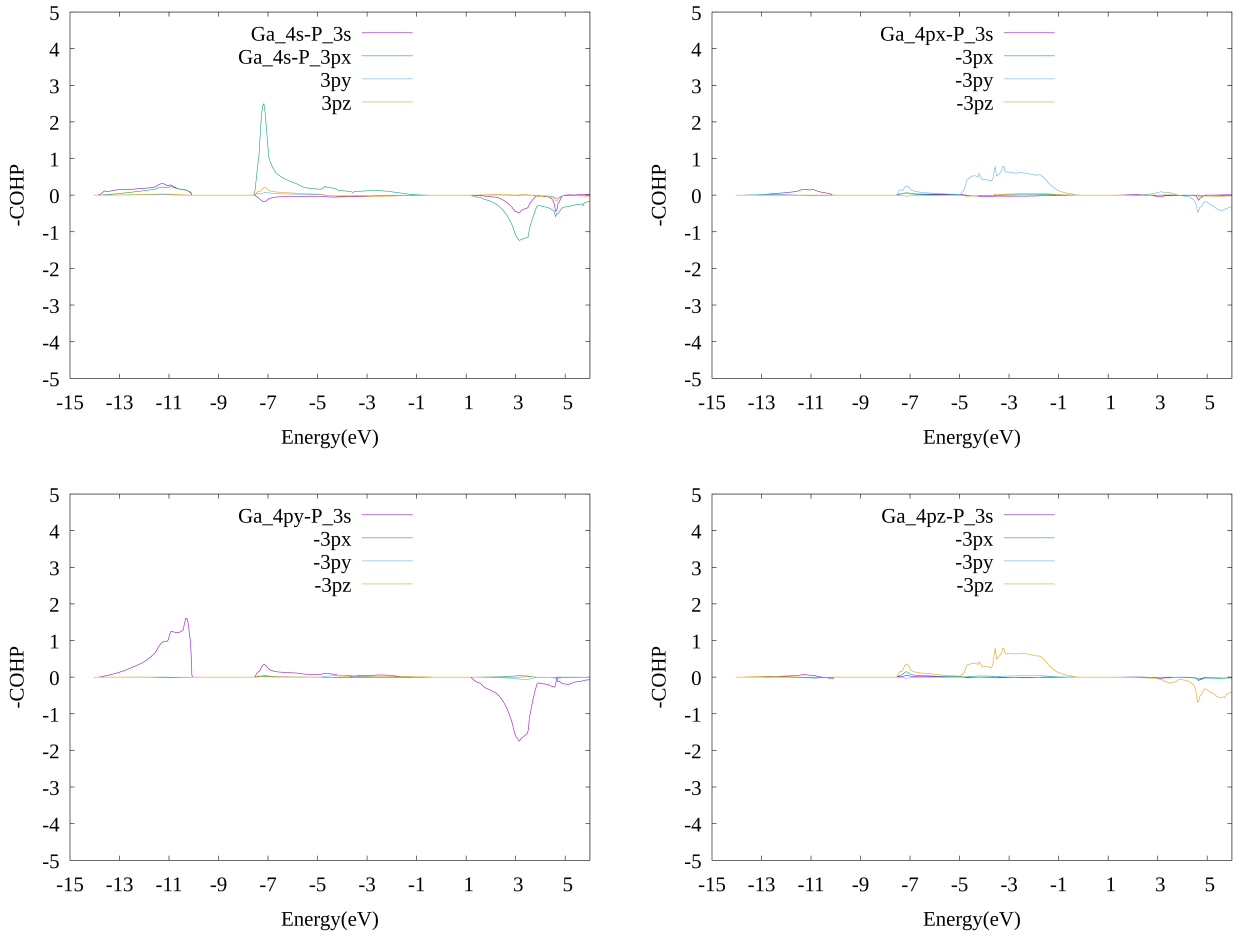

Figure 3: GaP's COHP between specific orbitals. Here I draw the picture by different Ga atomic orbitals coupling with P s,px,py,pz orbitals

A question is that when I try to generate Ga d orbitals with P orbitals, I got nothing. I'm not sure if it is because Ga d orbitals have much lower energy thus hardly coupling with P orbitals or I make some mistakes about the results of Lobster.

Combining COHP analysis with DOS and orbital contribution, we can find which orbitals and their couplings dominate the energy in certain k-path that we are interested in. So generally speaking, I assume I have handled how to analyze the reasons of indirect or direct band gap in specific materials.

2.2 Fermi surface

To see the ferimi surface of semiconductors, we have to artificially increase or decrease the fermi energy to make it cross some bands. Thanks to Vaspkit and Xcrysden, I visualize the fermi surface of GaP. By lowering or lifting the fermi energy by 2 eV(The black dashed line in Figure 4), we can see the highest valence bands(band 8 and 9) and lowest conduction bands(band 10) in Figure 5.

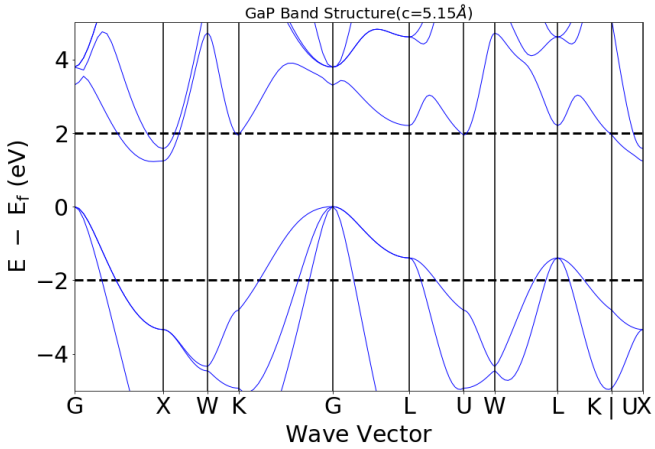

Figure 4: GaP's COHP. Y value bigger than zero means anti-bonding and vice versa

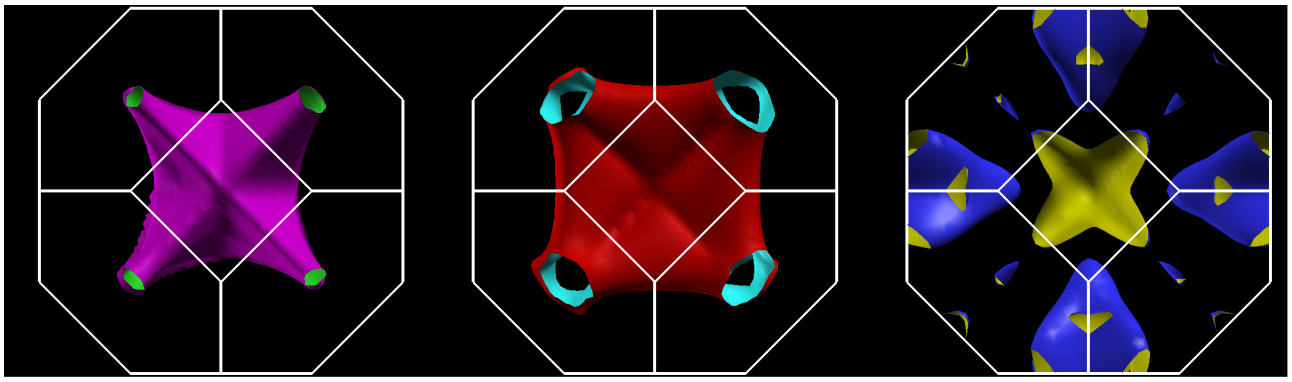

Figure 5: GaP(5.15Å)'s fermi surface, from left to right is band 8, 9 and 10

In order to get the trend of fermi surface during the modulation of lattice constant, I make an animation of these three bands when GaP's lattice constant gradually change from 5.15Åto 5.75Åwhich is in the attached file. There are two

questions that disconcerts me. First, 2eV is set for convenience. I don't know what value is suitable and if it is proper to set it unchanged when the lattice constant changes. Second, in this way I think we just get the 3D version of band structure. Up to now I cannot find more physics in them than 2D band structure.

2.3 Others

This week I happen to read a paper about In2Se3 and it really catched my eyes. According to their results, single layer In2Se3 without SOC holds indirect band gap, but when taking SOC into account In2Se3 turns to direct band gap(Figure 6). In our previous study I always thought that SOC is so small that we can neglect in any indirect or direct band structure analysis. And I haven't find any papers discussing the tight binding model of 2D In2Se3 with or without SOC, so I'm wondering maybe this could be a topic for furthur study.

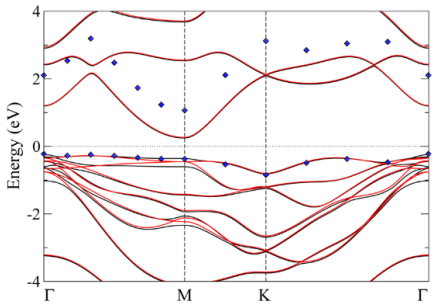

Figure 7. Calculated bandstructure of a β-In_2Se_3 single layer with (black line) and without (red line) including of the spin−orbit interaction, with the filled diamonds showing the GW with spin−orbit calculation. Fermi level is set to 0 eV.

Figure 6: Band structure of In2Se3(from Ref 1)

Besides, I'm thinking about how to bridge the tight binding model and VASP band structure and I find maybe Maximally localized Wannier functions(MLWF) theory could do this job. By MLWF, we can using tight binding model to describe bands in some range. Once we get the tight binding model, we can use lowdin perturbation to expand the high symmetry points to get a smaller model between the bands we care about. This theory is kind of complex and I'm still learning it. Perhaps it would be helpful.

3 Reference

1. L. Debbichi, O. Eriksson, and S. Lebègue, Two-Dimensional Indium Selenides Compounds: An Ab Initio Study, DOI:10.1021/acs.jpclett.5b01356