Weekly Report

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1 Introduction

Before we start to do a series of calculation about GaN/GaP/GaAs or something, I think there are still something required to be solved to make sure that our calculation are correct and reliable. Besides, I will try to answer some of the questions remained in the last discussion.

2 Progress

2.1 Where does band gap appear

In the last report, I don't give the specific lattice constant where GaP's band gap appears. So here I narrow the interval between 6Åand 5.5Å. It turns out that band gap form when the lattice constant is around 5.85Å.

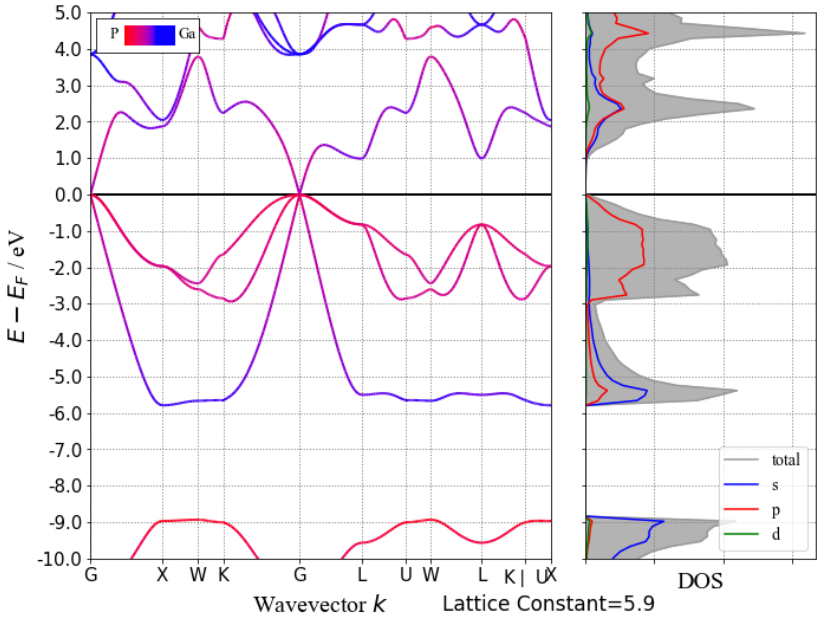

Figure 1: Lattice constant = 5.9Å

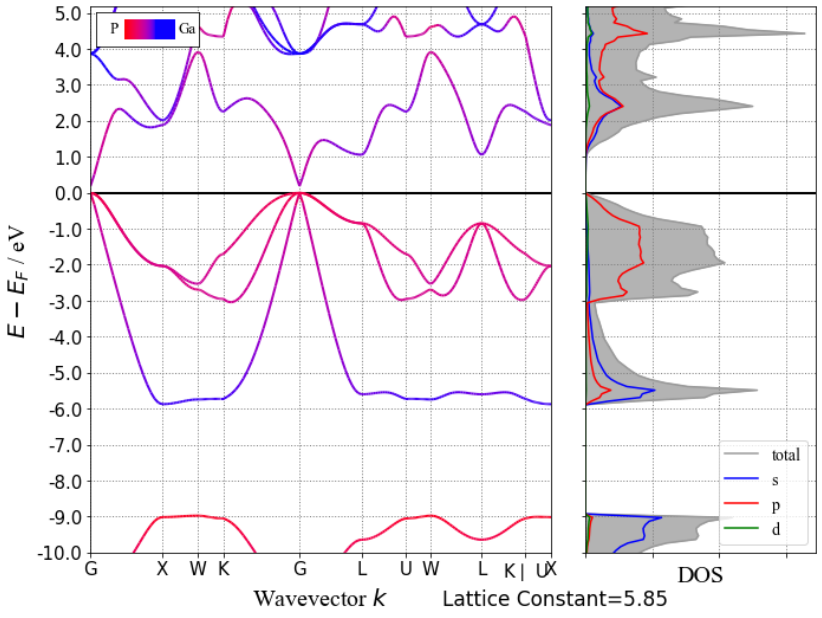

Figure 2: Lattice constant = 5.85Å

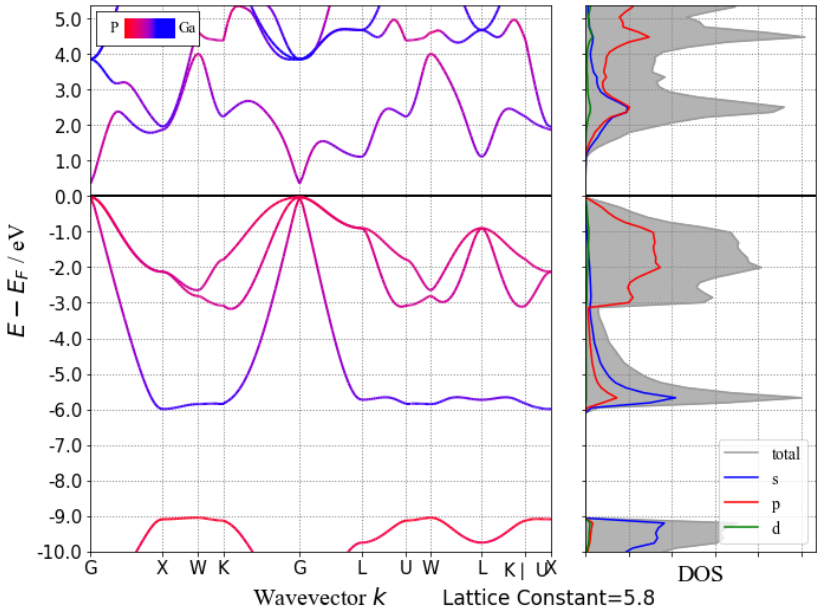

Figure 3: Lattice constant = 5.8Å

I assume that if there is anything interesting, it should be related to topology. To be specific, if the band structure is symmetry protected at Γ Points in some range like graphene? After combining the band structure trend with some back ground theory, I think the band gap of Group 3-5 compounds is trivial situation in topology so it would be described by a continous model by LCAO and no need for special care on performing calculation in other system of Group 3-5 compounds.

2.2 COHP and d bands occupation

Figure 4-8 show band structure, DOS and Ga s,p,d COHP with P repectively when GaP's lattice constant gradually change from 5.9Åto 5.15Å. d band COHP is about 10 times weaker than s or p COHP. To make it visible I enlarge x ticks in d band COHP.

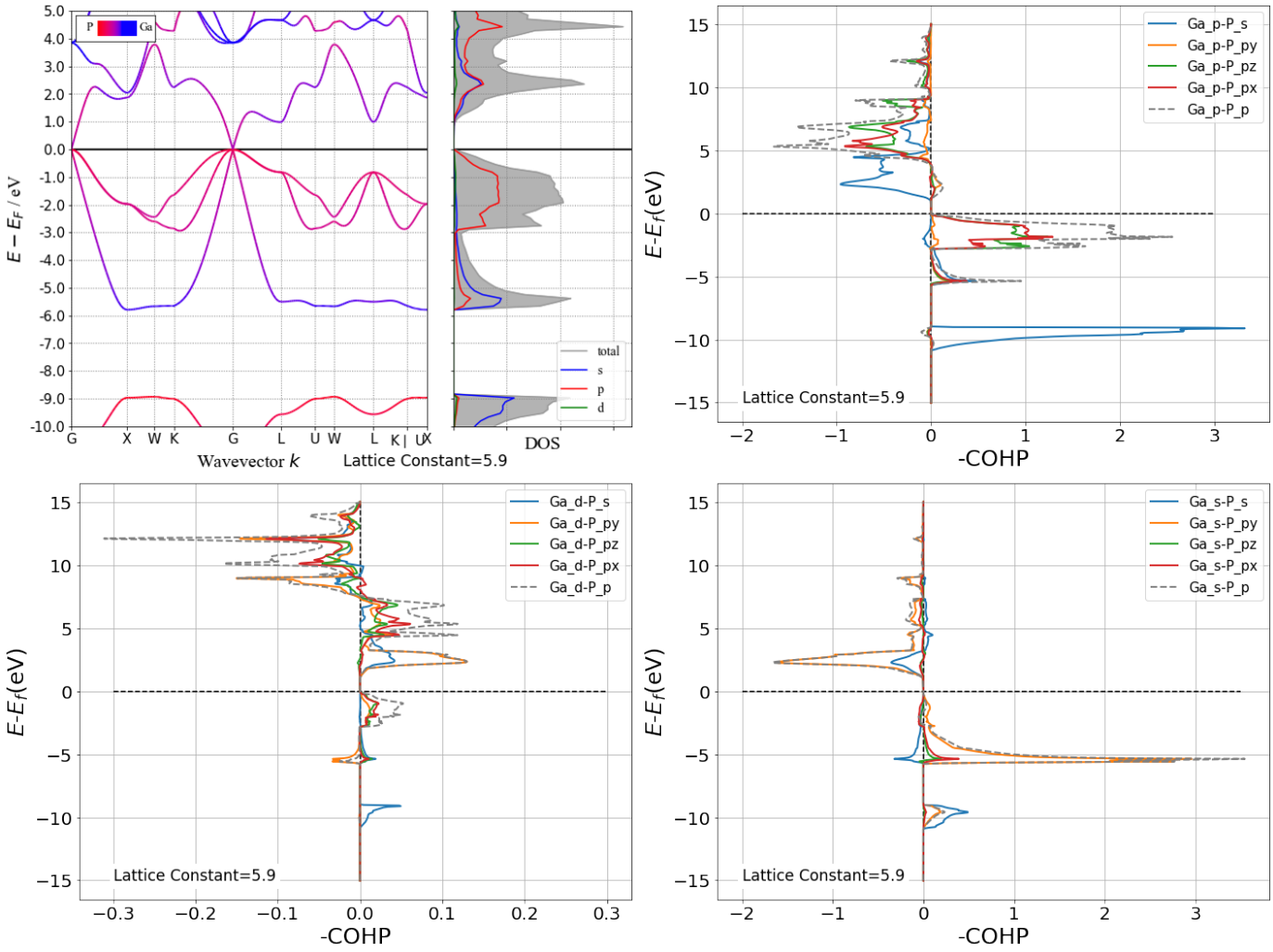

Figure 4: Lattice constant = 5.9Å

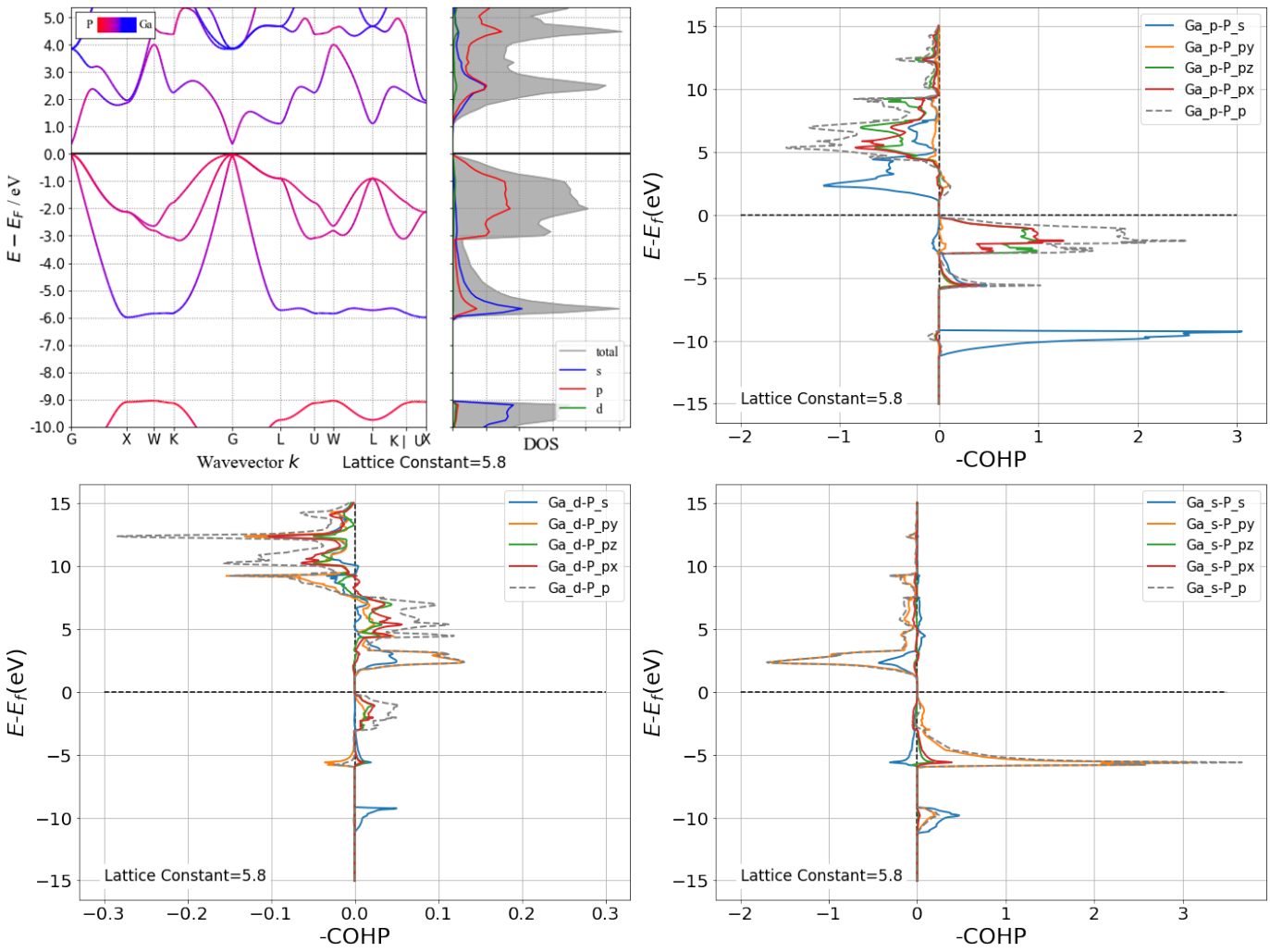

Figure 5: Lattice constant = 5.8Å

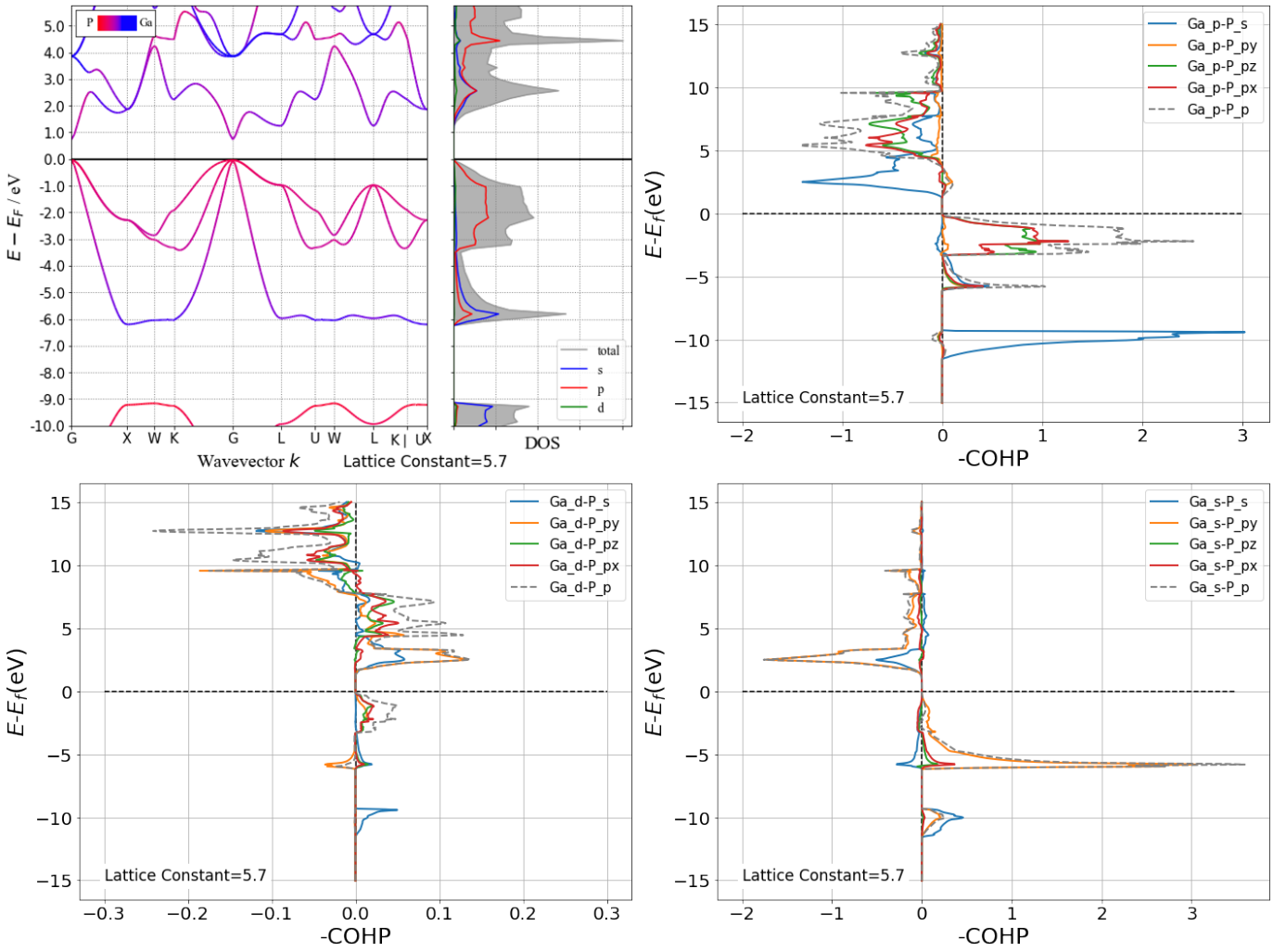

Figure 6: Lattice constant = 5.7Å

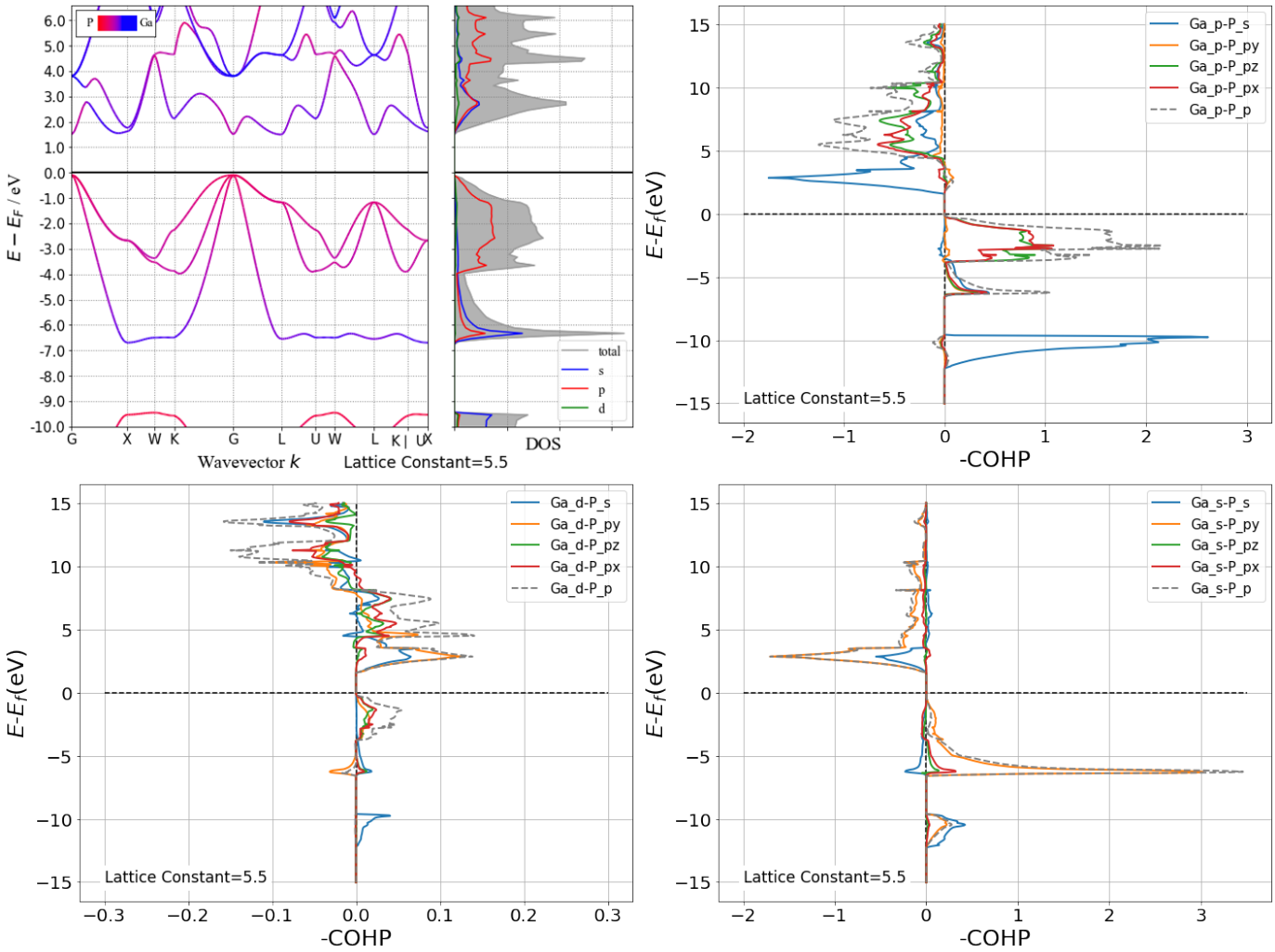

Figure 7: Lattice constant = 5.6Å

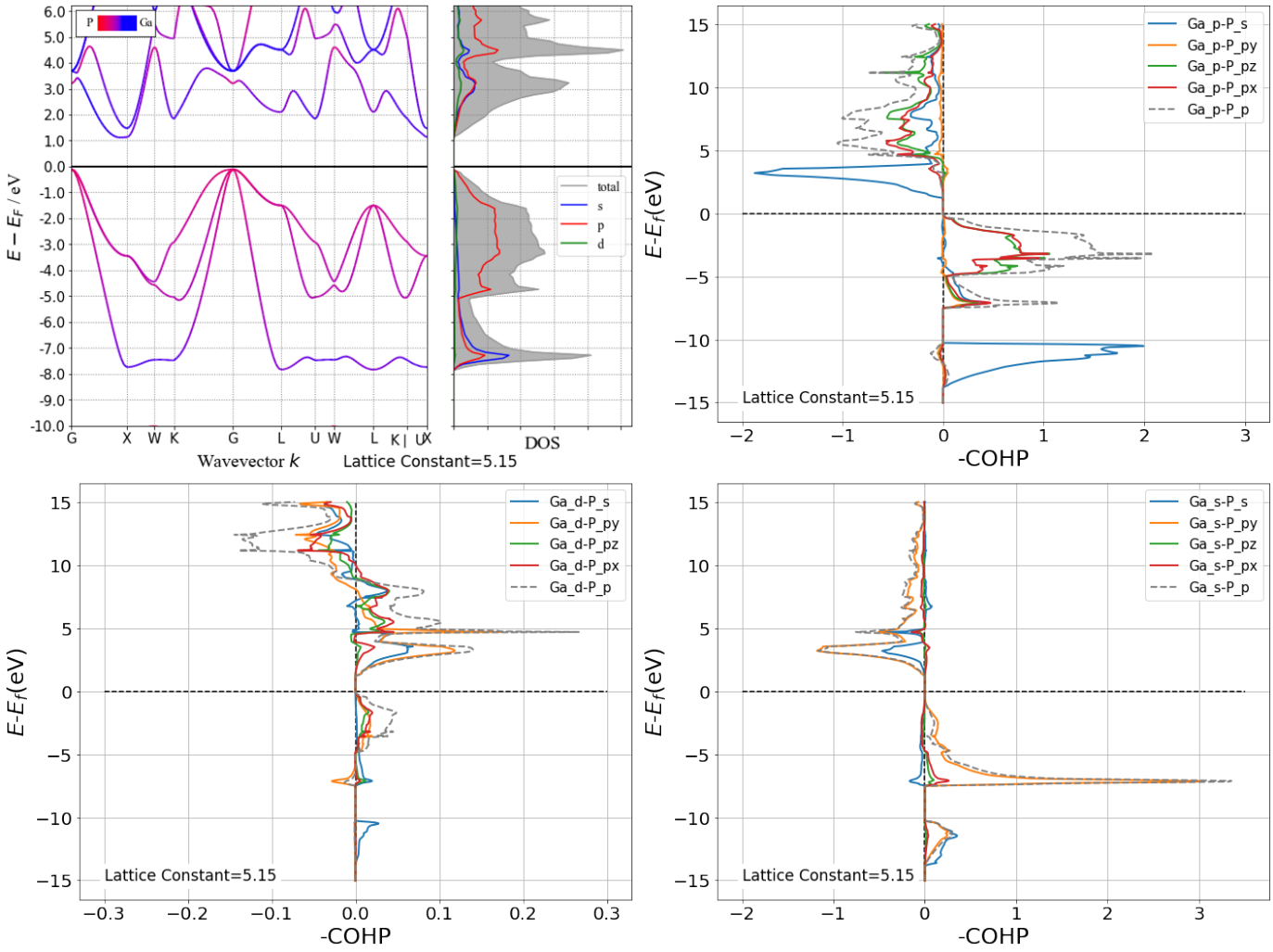

Figure 8: Lattice constant = 5.5Å

To see d band influence, let's put d band together in figure 9.

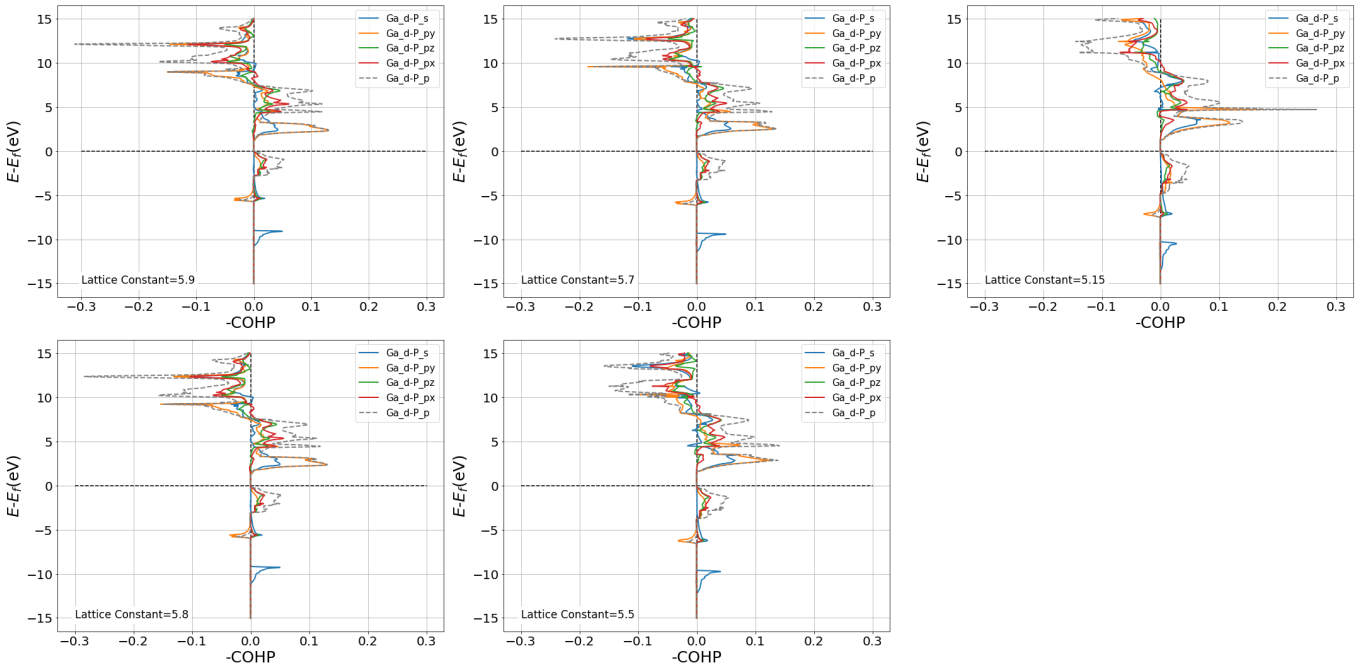

Figure 9: Ga d band COHPÅ

There are two interesting things:

1. The bonding increses near the fermi level and anti-bonding decreases a little bit during the reducement of lattice constant.

2. The strongest COHP of d band is with P py orbital. To be specific, is d_{xz} and $d_{x^2-y^2}$. I suppose that could be explained by the principle of symmetry matching in chemical language. In group theory lanuage, at the Γ point, the atomic d orbitals belong to Γ_{15} and Γ_{12}, respectively, and thus have the same Γ_{15} irreducible representation as the p-like VB edge state; the coupling between p and d orbitals at the Γ point could be quite significant. However, the s-d coupling is forbidden because the atomic d orbitals have no common irreducible representations with the s-like CB Γ-valley state. Therefore, the existence of the occupied d orbitals will have a significant influence on the formation of the band gap by pushing the VBM up and leaving the CB Γ-valley intact. At the X point, five d orbitals belong to the X_1, X_2, X_3, and X_5 irreducible representations, respectively, and, therefore, can couple to the CB X valley. At the L point, five d orbitals belong to L_1 and two L_3, respectively, and same as the X point, the d orbital state can couple to the CB L valley. (Extract from reference 1)

Of course there are a lot of things to explore about COHP, I will try to find out

more information next week.

What' more, I came across a very strange thing when doing COHPs. Theoretically, POTCAR files with Ga_d would be better for COHP analysis since it treat d bands as valence bands. But the result of using Ga_d is abnormal like Figure 10 shows.

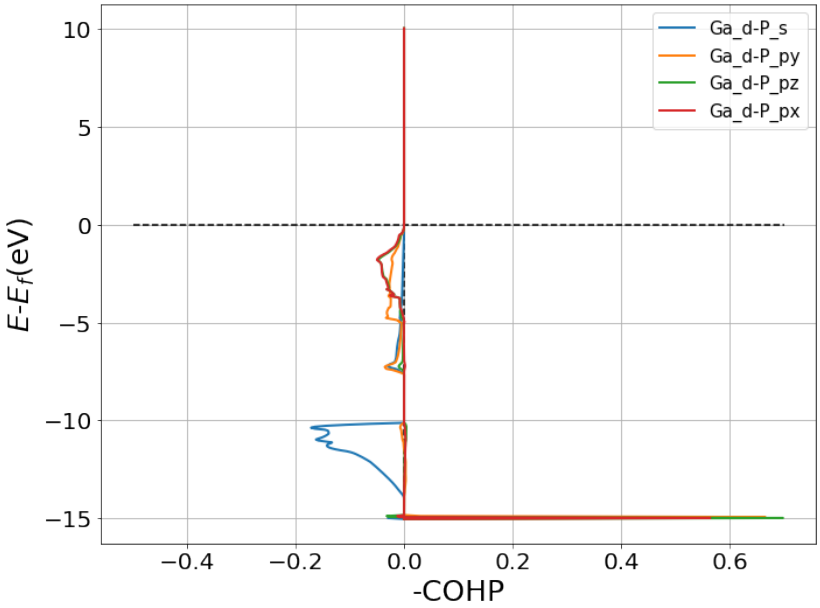

Figure 10: POTCAR Ga_d COHP when Lattice constant = 5.15Å

The above various COHPs is calculated by POTCAR Ga. I didn't find any instructions of which POTCAR file to use when doing COHPs and I'm not sure if the above results is correct. That's a big question for me.

2.3 s-p coupling

The question about s-p coupling hybridization is relatively easy to explain. I suppose there is s-p coupling hybridization as long as there are s and p orbital contribution in the same place in DOS picture. Meanwhile, sp hybridization orbital is just a unitary transformation of regular sp orbitals, just as in Wannier90 we can both set the basis functions to be s,px,py,pz or sp2,sp3 or sp3d2.

2.4 LCAO and Wannier functions

Wannier analysis is crucial. We can directly get the corelation integral in tight binding model from Wannier90 and combine it with our PythTB model. However, this week I face some problems with the usage of Wannier90. In my

university's supercomputer there is no VASP version that contain Wannier90. For the past few days I've been try to contact with administrators to install one but haven't got a reply. So I tried to compile a VASP with Wannier90 in my PC. The problem is I find that VASP cannot engender .mmn and .amn file as tutorial book says. I haven't figured out if is because I fail to compile Wannier90 or I set some parameter wrong in wannier.win file.

3 Summary

In summary, this week I left two questions:

1. The difference of POTCAR file *Ga* and *Ga_d* when doing COHPs.
2. The usage of Wannier90.

They are eleborated in the above sections.

4 Reference

1. Lin-Ding Yuan, Hui-Xiong Deng, Shu-Shen Li, Su-Huai Wei, and Jun-Wei Luo, Unified theory of direct or indirect band-gap nature of conventional semiconductors, PHYSICAL REVIEW B 98, 245203 (2018) DOI: 10.1103/PhysRevB.98.245203 I.