

Weekly Report

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1 Introduction

The goal of this week is finding a question about indirect band gap and giving an explanation it. I try to extract some data from Material Project. Up tp now the result is not desirable and lots of questions come up in the way, but I think I have found something interesting.

2 Progress

2.1 Part I

Considering the question's complexity, I started with narrowing the range, which means set some variables that would affect band gaps fixed. Then generalize them gradually. So after hanging around with the Material Project, I focus on Group V, VI, VII components with AB compositions and zinc-blende structures (this structure has relatively simple bandstructure). By Material Project API, 9 components are extracted and I make a picture of Bandgap VS Lattice constant, which are showed in Figure 1.

The most ad hoc thing happens in Ga-Group VII components. You can see the direct-indirect-direct trend with the growing atom number of Group VII elements. There are already some paper(1) discussing it. The occupied cation d bands is a prime element in determining the directness through the s-d and p-d couplings and the extreme large electronegativity of N will make the band gap direct.

Al-Group VII components appear to have regular trends with the increasing atom number of Group VII element. The bandgap decreases as the lattice constant increases. However, if we have a look at the bandstructures of them, there are still some interesting properties, Figure 2 shows the bandstructure acquired from Material Project.

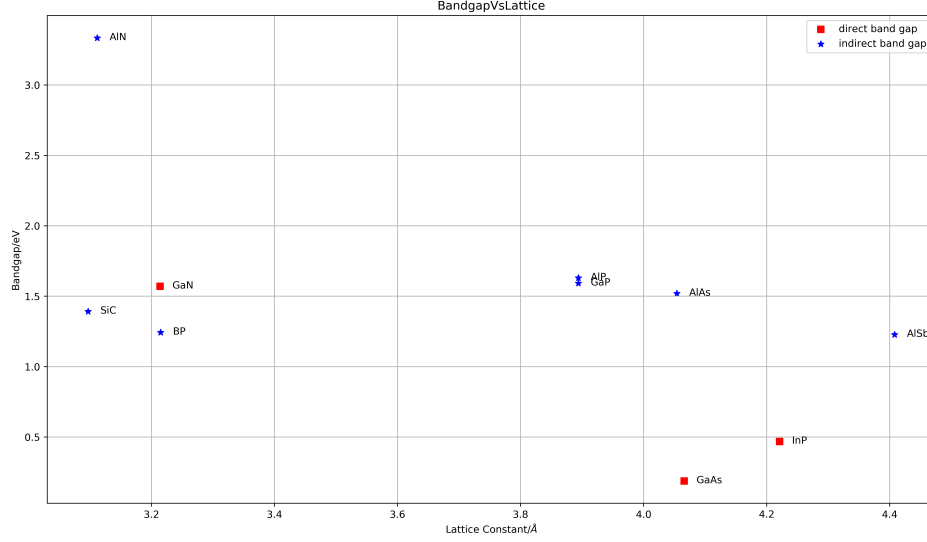


Figure 1: Bandgap Vs Lattice constant

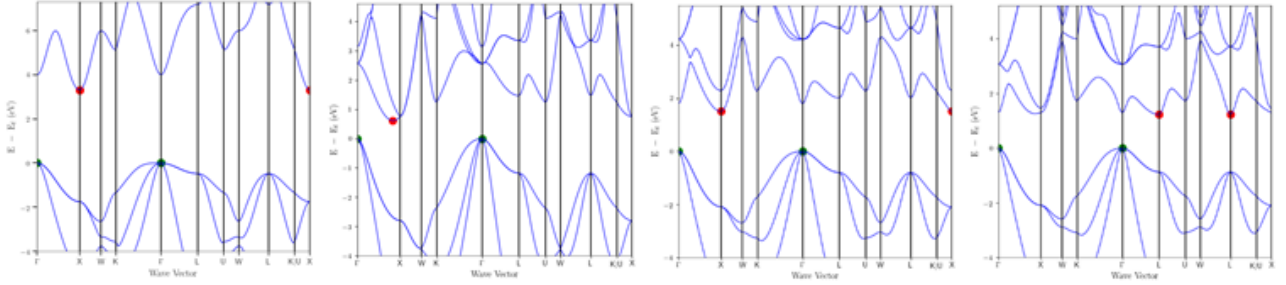


Figure 2: Band Structure of Al-group VII components, from left to right is *AlN*, *AlP*, *AlAs* and *AlSb*

We can see that the CBM (conduction band minima) of *AlSb* appear at *L* while others appear at *X*. The CB of *L* valley gradually goes down with the trend. I assume maybe it is result of increasing cation d bands coupling with s or p bands. I haven't seen any paper talk about it, so maybe that's a point for further study. Besides, when I check the bandstructure of *AlSb* at Material Project, another phenomenon catches my eyes. I will talk about it in Part II.

2.2 Part II

There are two stable structure of *AlSb*, which point groups belong to $\bar{4}3m$ and $6mm$ separately. The former one holds indirect bandgap while the latter one holds direct bandgap. I'd like to present them here.

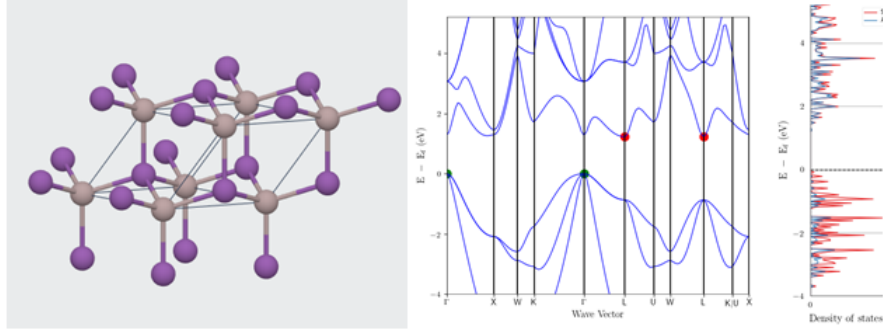


Figure 3: AlSb with $\bar{4}3m$ point group

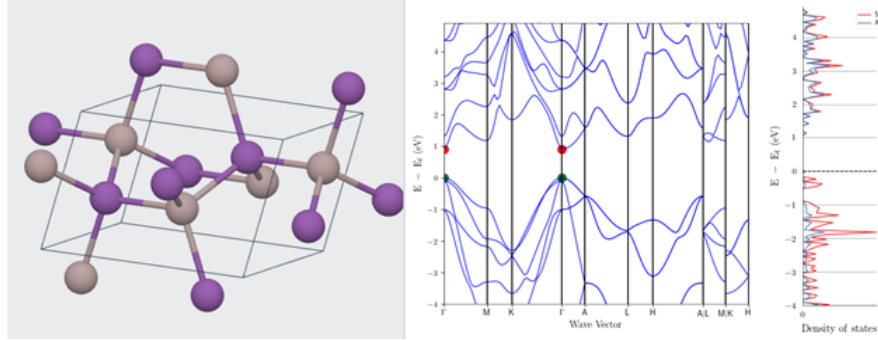


Figure 4: AlSb with $6mm$ point group

From the bandstructure picture, we can see that compared with $\bar{4}3m$ *AlSb*, the L valley of $6mm$ *AlSb* stay the same place and the Γ valley suffer an apparent reduction which results in CBM taking place at Γ point. How does it happen? we can see a slightly different bond length within two structures. From DOS picture we can see that $6mm$ *AlSb* has a wider p bands at $-1 \sim -3$ eV and narrower near the fermi surface. Is it results in stronger or weaker s-p bonding with CB Γ points? That's all I can think of from these pictures. So the recent days I was working on drawing the bandstructure picture with an apprehensible way.

Perhaps it can shine light on how structures moderate the type of bandgap. First, I try to simulate the bandstructure with PythTB, but it seems a little bit difficult for me to paint such a delicate structure. I haven't figured out how to represent complex orbital couplings through *set_hop* function in PythTB. Both theoretical and technical study are needed to accomplish this goal. Meanwhile, I'm worried that whether the PythTB package is accurate enough to express this small difference, for some models always get direct bandgap as I suggest in the previous report. Another way I can think of is through precise tight bonding basic functions. I have just found some papers about it and I will try to handle them in the following week.

3 Summary

Generally speaking, This week I only raises two questions:

1. What affects the bandstructure trend of Al-Group VII components
2. How does the structure of *AlSb* affect the type of bandgap

I'm not sure whether they can be called questions or whether they are valuable, but at least I believe I have taken a step towards the question.

4 Future work

PythTB package should be given first priority. Besides I list some papers I think it meaningful to read in the following weeks. They are about tight bonding model.

1. Su-Huai Wei and Alex Zunger, Predicted band-gap pressure coefficients of all diamond and zinc-blende semiconductors: Chemical trends,
DOI:10.1103/PhysRevB.60.5404
2. Yaohua Tan, Michael Povolotskyi, Tillmann Kubis, Timothy B. Boykin, and Gerhard Klimeck, Transferable tight-binding model for strained group IV and III-V materials and heterostructures,
DOI: 10.1103/PhysRevB.94.045311
3. Jean-Marc Jancu, Reinhard Scholz,* Fabio Beltram, and Franco Bassani, Empirical sp³s* tight-binding calculation for cubic semiconductors: General method and material parameters,
DOI: 10.1103/PhysRevB.57.6493

5 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)