

Weekly Report

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1 Introduction

This week I've been focusing on the article *How Chemistry and Physics Meet in the Solid State*. Out of question it is really a beautiful paper. I think what inspires me most is that Prof. Hoffmann teaches us how to analyze solid state questions with 'Chemists' intuition' but without loss of Physicists' preciseness. So here I will try to use my own words to trace the footprint of this paper to answer the following questions:

- How do real space and k-space relate to each other?
- How do band structure, Fermi surface and Brillouin zone interact with each other?
- What role does Chemistry play in those process?

Besides, I will also mention the question unsolved in the email.

2 Progress

2.1 How Chemistry and Physics meet in Solid states

First let me list all the possible concept that will be mentioned.

Real space	k-space
Structure	Brillouin zone
Bonding	Band structure
Potential	Fermi level
DOS	

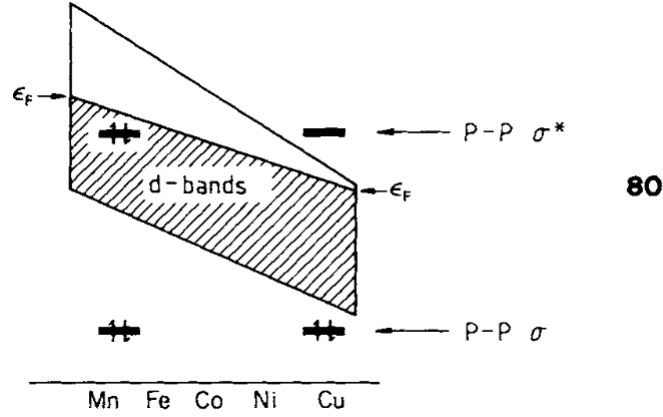
Let's begin with a few atoms getting together to form an aggregation. They will generate specific structures and covalent or ionic bonds. Once the structure is fixed, we can turn our eyes to reciprocal space. It is proposed to simplify the periodic potential situations according to Bloch theorem. K-space, built on reciprocal space, is a discrete lattice space based on reciprocal vector. In reciprocal lattice, we can divide them into different regions under some criterion, which are called Brillouin zones. Thanks to symmetry, all the Brillouin zone have the same volume and translate them into a same region for convenience, so all we need to care about is the First Brillouin zone.

Now all the preliminary work has done. It's time to think of the key point of solid state—energy. Perturbation theory tells us that in k-space energy will split into several separated energy bands, which is called band structure. In chemistry we often refer to as s,p,d,f orbitals. Different atoms usually have different energy levels, which could result in hybridizations between orbitals. Those interactions are exactly bonds in real space.

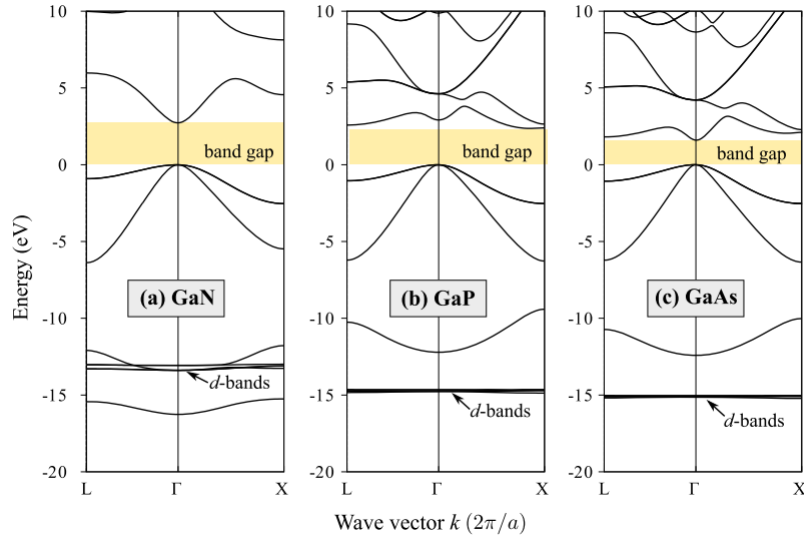
Finally it's the stage of electrons. Usually we only concern about outer electrons which are active. they would take up the bands from low bands to high bands. The highest occupied molecular orbital is called Fermi level. The process of the enlargement of Fermi level with the increasing number of electrons is like an expanding balloon. When Fermi level is near the edge of Brillouin zone, its shape will suffer a distortion, and we can trace this process to draw the band structure. I cannot emphasize the importance of Fermi level too much. Nearly all the chemical action happens near the Fermi level.

So what does the electrons and Fermi level act in real space? That's when Density of State (DOS) plays its role. It reflects the number of electrons on different energy. I tend to regard DOS as a bridge between k-space and real space. It provides an intuitive understanding of occupied states and Fermi level in k-space while also stands for a powerful tool about converting real space information into k-space, just as Prof. Hoffmann shows in the paper, 'localization in energy space (such as we see for the P pz projection) implies localization in real space.'

How does chemistry affect this process? First, the elements' properties such as mass, electronegativity and outer electrons determine the types of bondings, thus the structures. Then comes the whole story which is mentioned above. I think what is interesting is that a slight transformation of chemistry may induce huge property moderation. For example, the AB_2P_2 structure mentioned in this paper. The picture tells us how the $P-P \sigma^*$ bonds change from occupied to unoccupied with the trend in transition metals.



Similar example can also be found about direct or indirect band gap. The following picture shows that more electronegativity in the anions will gradually make the band gap of the semiconductors more direct, which is presented in Reference2.



In addition, I'd like to share some of the ideas in this paper that touch me a lot.

1. Crystal orbital overlap population(COOP): To be honest, it's the first time that I get to understand how this concept refer to. We can see clearly the bonding or antibonding in COOP picture, which is extremely useful to predict or analyze DOS.

2. Folding bands: It reminds us that for a given complex structure, we can always try to simplify it into basic model that will give an intuitive understanding of band structures.
3. The Peierls Distortion: It plays a crucial role in determining the structure of solids in general. I assume the Peierls Distortion describe how atoms move spontaneously away from the prefect structure. I can't help relating it with the strain-induced effect when it comes to indirect band gap. I will try to explore them in details in the next few weeks.

2.2 Unsolved questions

Last week Prof. Sun mentioned that there are two papers(Reference 3 and 4) we should not appreciate. I think it's because those two papers emphasize too much on the algorithms and lack of further analysis, which makes them more like an application of algorithms with physical datasets. They remind me that always keep it in mind that machine learning is just a small step of data driven research. We should always give priority to data collection and post analysis.

3 Summary

Actually I'm discontented with this report. Though I thought I have learned a lot from the article, I found it's hard for me to extract essential viewpoint and raise my own new ideas. So this report is more like a summary of Solid State Physics. Perhaps I should have manipulated some examples by myself to get a better understanding. I hope it can be improved in the following report.

4 Questions

This week I also keep learning Prof. Sun's blog and I found something interesting. The last slide offers 16 papers for students to reproduce. I'm wondering usually how much time does it take for a graduate student to accomplish and if it would be helpful for me to try to reproduce some of them?

5 Reference

1. Roald Hoffmann, How Chemistry and Physics Meet in the Solid State
2. 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)
3. In-Ho Lee, Jooyoung Lee, Young Jun Oh, Sunghyun Kim, and K. J. Chang, Computational search for direct band gap silicon crystals, PHYSICAL REVIEW B 90, 115209 (2014)

4. Mayeul d'Avezac, Jun-Wei Luo, Thomas Chanier, and Alex Zunger, Genetic-Algorithm Discovery of a Direct-Gap and Optically Allowed Superstructure from Indirect-Gap Si and Ge Semiconductors, *Phys. Rev. Lett.* 108, 027401 (2012)