Weekly Report

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1 Introduction

This week I've been trying to make up the shortage of the theorectical background about band gap and to get some inspirations from somr papers about indirect bandgap. Besides, two unsolved questions will also be mentioned here.

2 Aforementioned questions

2.1 Pymatgen.io

Last week I haven't finished using Pymatgen.io to draw a bandstructure. The following pictures are the bandstructure of Si through Pymatgen.io with my own vasp running and through Pymatgen library.

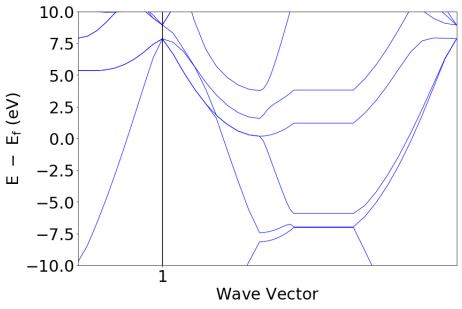

Figure 1: Pymatgen.io with my own vasp running

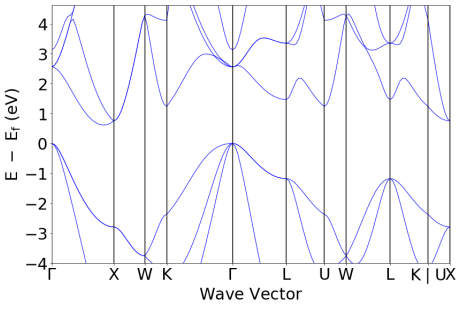

Figure 2: True Si bandstructure

You can clearly see that the left picture is awful. I guess it is because Pymatgen.io require the input file KPOINTS contains dense points in the symmetry line with special notations in the high-symmetry points. Anyway I assume if a bandstructure plot is needed through pymatgen.io, I can quickly pick it up.

2.2 Hubbard model

In last report, I mentioned that "None of NFE model, Hubbard model, t-J model or simple TB model could explain indirect band gap." Actucally I saw it by chance on Quora. After furthur inquiry, here is my perspective about this statements: the Bose-Hubbard Model is expressed in the following form:

$$H = \sum_{i,j} \sum_{\sigma} t_{i,j} c^{\dagger}_{i,\sigma} c_{j,\sigma} + U \sum_{i} n_{i,\uparrow} n_{i,\downarrow} = H_t + H_U \tag{2.1}$$

where$t_{i,j}$ denotes nonvanishing matrix elements of the Hamiltonian between the orbitals centered on these sites, $c^{\dagger}_{i,\sigma}$ denotes the creation operator for an electron of spin σ in the orbital at lattice and $n_{i,\sigma} = c^{\dagger}_{i,\sigma} c_{i,\sigma}$ denotes the number of particles on site i.

It is proposed to describe electrons in 3d transition metals, which conduction electrons suffered strong Coulomb repulsion. I think the reason why it fails to explain indirect band gap is that the Coulomb interaction between electrons in orbitals on different sites is neglected and the onsite Coulomb interactions U have no dependence on momentum transfer while the couplings is exactly the key to indirect band gap as some papers suggested. Therefore, Hubbard model doesn't have much difference compared with Nearly-free-electron model about the questions we care for.

To sum up, based on my understanding, Hubbard model uses the form just like second quantization to modify a group of transition metals and has been widely used in Mott insulators and superfuild, but not quite into direct or indirect band gap. We should focus on the theory that takes the couplings between different orbitals(like s-d or p-d couplings) into account.

3 Progress

Here I want to share a few meaningful papers I read last week.

3.1 Unified theory of direct or indirect band-gap nature of conventional semiconductors

In the article, the author proposes that since valence band(VB) and conduction band(CB) have different irreducible representation, the occupied cation d bands would have different levels of couplings with VB and CB, which prehaps repels the CB X valley and L valley up. Besides, the effect of the bond length and electronegativity are also discussed. A larger lattice and more electronegativity in the anions will make the band gap of the semiconductors more direct.

Meanwhile, in Reference(2), similar theory was proposed to explain band structure of indium oxide. The author verified the energetic position of the In 4d–derived orbitals affects the hybridization of In 4d levels with O 2s and O 2p

levels. If a splitting of this magnitude occurred near the top of the valence band an indirect band gap could result.

I think this work is really inspiring as it not only raise a promising theory but also provide some features that we should consider in our data mining and filtering proceduce.

3.2 Computational search for direct band gap silicon crystals

The author proposes a computational method for predicting and filtering direct band gap silicon crystals. I would like to conclude it as an annealing algorithm to generate new structures and a genetic algorithm for optimazation, then use delicate vasp calculation to screening out direct band gap structure.

I think it provides a possible method about the second step(machine learning) of our research. However, no theorectical explanation was given in this article. In my view maybe the different point groups of structures would affect the hybridization of orbitals in some way.

4 Summary

This week is still about studying some background knowledge. I suppose I have got a grasp of the indirect band gap and what aspects we should take into consideration, but more reading is needed in the next few weeks for me to get a clearer physical picture of the questions.

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)

2. Paul Erhart, Andreas Klein, Russell G. Egdell, and Karsten Albe1, Band structure of indium oxide: Indirect versus direct band gap, PHYSICAL REVIEW B 75, 153205 (2007)

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)