Weekly Report

Siyu Liao

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1 Introduction

These weeks my work can be seperated into two parts: the workflow and machine learning about indirect band gap.

2 Progress

2.1 Workflow

First, I make some animations about fermi surface versus bandstructures which I will attach in email. From the animations we can get an intuitional feeling of how bands look like in real 3D reciprocal spaces. These animations are made by fixing the lattice constant and letting 'fermi energy' vary, so next I make some pictures about bandstures versus COHPs when lattice constant changes.

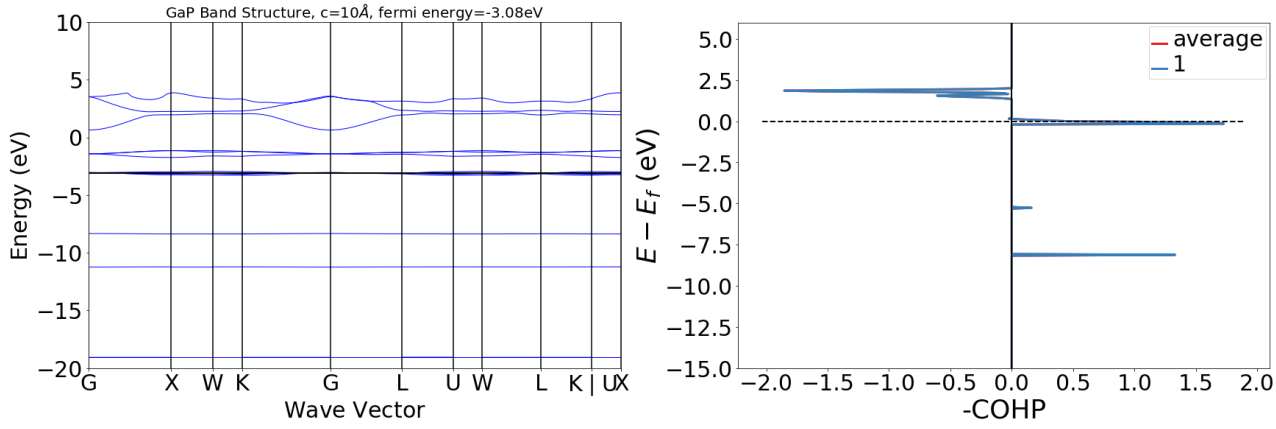

Figure 1: GaP's band structure versus COHPs when lattice constant equals to 10Å

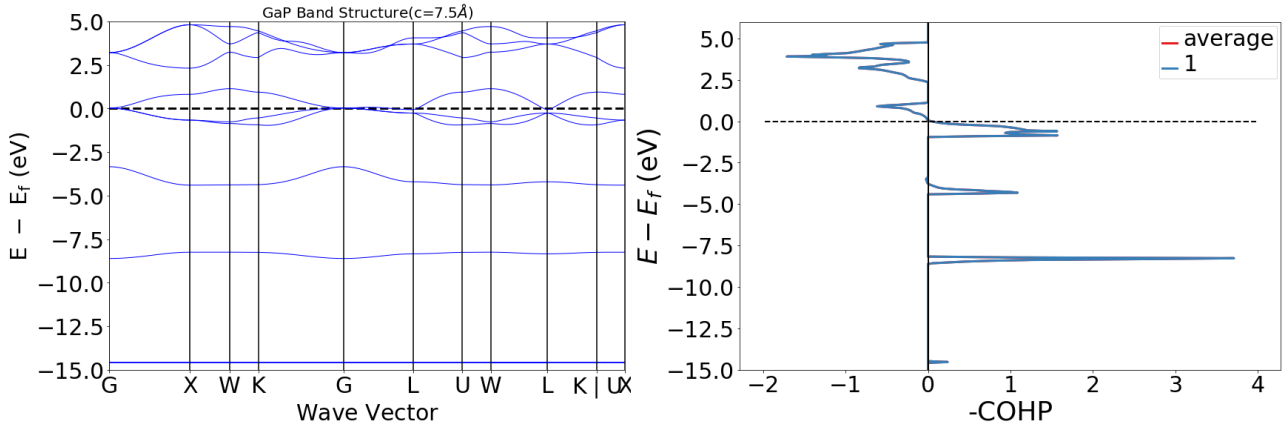

Figure 2: GaP's band structure versus COHPs when lattice constant equals to 7.5Å

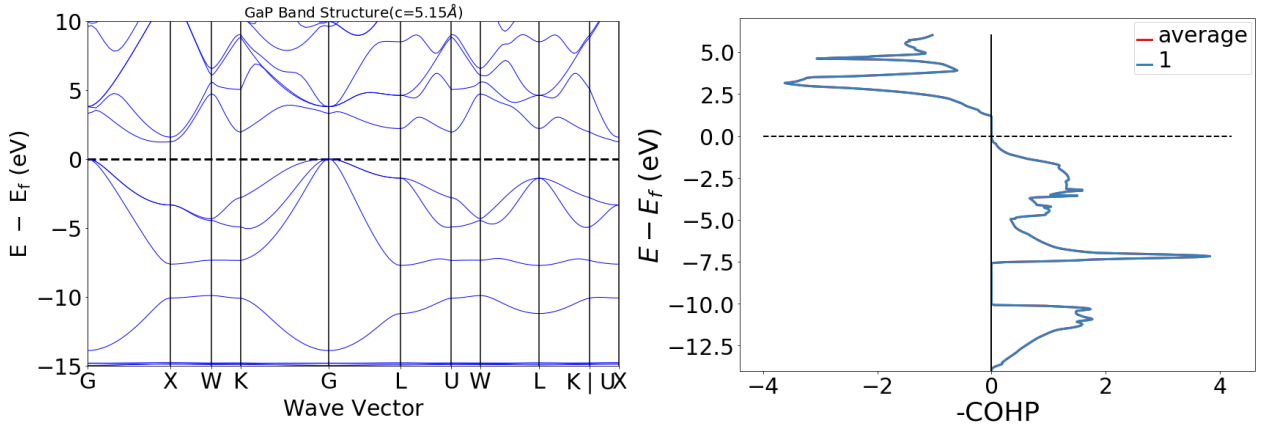

Figure 3: GaP's band structure versus COHPs when lattice constant equals to 5.15Å

From the above pictures we can find that when two atoms get closer, the atomic orbitals start to couple. First it's the outer orbitals(in GaP is Ga 4s 4p and P 3s 3p). Then Ga 3d orbitals take part in coupling. Finally when GaP forms its stable sturcture, the gap between s and p orbitals in COHPs would disappear and become kind of sp hybridizations. When it comes to the valleys or peaks in bandstures or COHPS, I think we should turn to tight binding model and symmetry analysis.

About the workflow, my idea is that since roughly speaking we have two kinds of trends that is valuable to show(changing lattice constant to see band-structure modulation and changing fermi energy to see fermi surface modula-

tion), we can use to some GUI tools to realize them. For example, set one place for entering the material, one button for changing the lattice constant and one button for changing the fermi energy. Then present all the pictures we got with respect to aboved parameters. Perhaps add a tight binding simulation module which corresponds to the parameters. I assume it is realizable but will be very time consuming. Now I'm learning GUI and it's a little bit difficult for me.

2.2 Machine learning

Finally with Prof. Sun's help I know how to extract indirect band gap information from MP. The hardest part is how to find a suitable descrtiptor. I made some experiments but the results are not desirable. I tried atomic volume, band gap, electronegativity, space group and outer electrons for features. The dataset contains 1750 materials and after data cleansing its form is showed in Firgure 4.

	formula	atomic_volume	band_gap	outer_electron	diff_electroneg	spacegroup	band_gap.is_direct
0	BaTe	44.545542	1.5930	16	1.21	m-3m	0
1	CCl4	30.166800	4.5130	11	0.61	2/m	0
2	BaO	21.478261	2.3711	8	2.55	6/mmm	0
3	Ba5Sb4	42.160101	0.2616	15	1.16	mmm	0
4	Ca2Sn	36.168984	0.6909	14	0.96	m-3m	0
5	Ca2Si	30.701680	0.5848	6	0.90	m-3m	0
6	Ca2Ge	31.355789	0.6088	14	1.01	m-3m	0
7	Ca2Pb	37.144004	0.6818	14	1.33	m-3m	0
8	AlSb	30.271563	0.9179	24	0.44	6mm	1
9	BaF2	20.669812	6.6232	9	3.09	m-3m	0

Figure 4: Indirect band gap dataset

Then I train simple tensorflow model. Figure 5 and 6 shows the results.

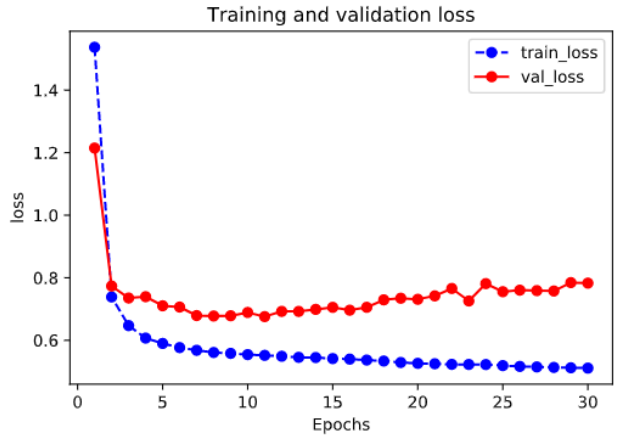

Figure 5: Training and validation loss during epochs

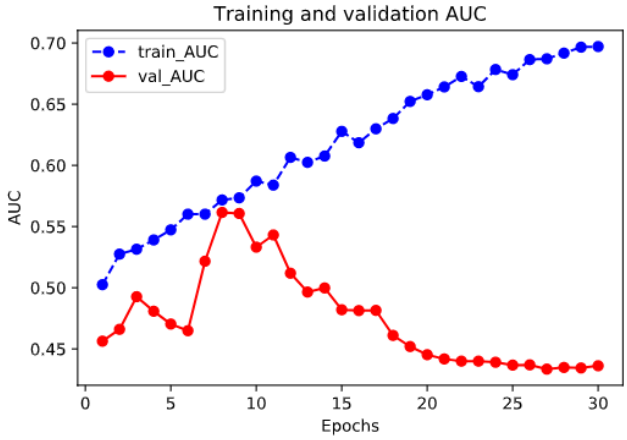

Figure 6: Accuracy during epochs

From the validation accuracy curve we can see that the model is seriously overfitting and the extrme low validation accuract suggests that these feature cannot reflect indirect band gap. I think the reason is that those features fail to show important structual information and it's the hot topic of nowadays machine learning application in material science. Therefore I search some relative papers and find that maybe the Crystal Graph Convolutional Neural Networks(CGCNN) proposed by Tian Xie and Prof. Grossman is helpful. It uses one-hot encoding and other skills to represent the atomic environment, as showed in Figure 7.

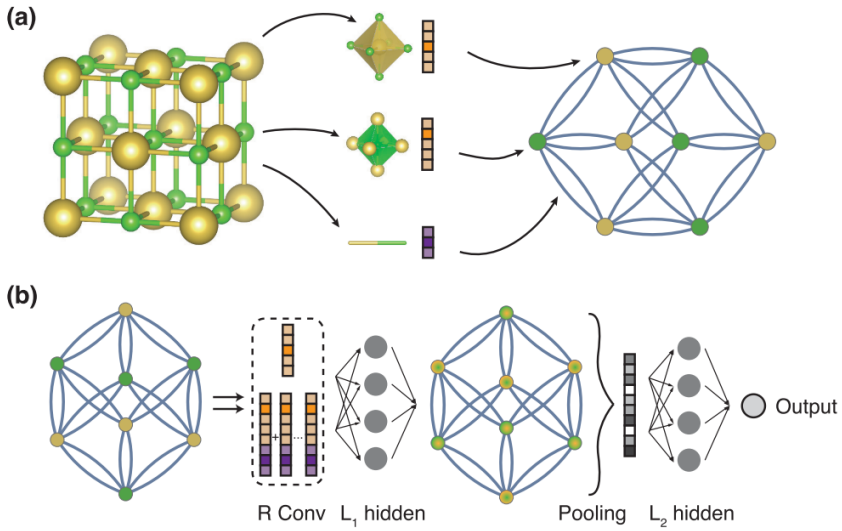

Figure 7: Illustration of the crystal graph convolutional neural network (CGCNN) (from Reference 1)

I'm think about utilizing this model and add some unique descriptors of indirect band gap information to see if we can train a viable model. CGCNN is a litte bit complex(It bases on Pytorch) and now I'm tring to understand the details of how it works.

3 Reference

1. Tian Xie and Jeffrey C. Grossman, Crystal Graph Convolutional Neural Networks for an Accurate and Interpretable Prediction of Material Properties, DOI:10.1103/PhysRevLett.120.145301