Weekly Report

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1 Introduction

The goal of this week is getting familiar with workflow of Data-Driven Material Research and do some theoratical survey about the indirect-band-gap problem. Up to now I have done some practice with MaterialProject(MP) API and Pymatgen package and try to get a smattering of indirect band gap from solid-state physics perspective.

2 Progress

2.1 MaterialProject-API

MP is a data-rich ecosystem that leverages the power of high-throughout computation to generate properties of compounds for accelerated materials design. MP-API provides a convenient and effective way for users to extract and furthur analyze the valuable information. I suppose there are two key points of MP-API:

- Criteria: from which we can readily screen out which propeties we want.
- Properties: results reserved after this query.

Here I follow the guidance of Prof Sun to do some practice with MP-API. Figure1 is Bandgap VS Density of Si compounds using MP-API along with Pymatgen, Pandas and Plotly package,which is immitating the example of BandgapvsDensity.

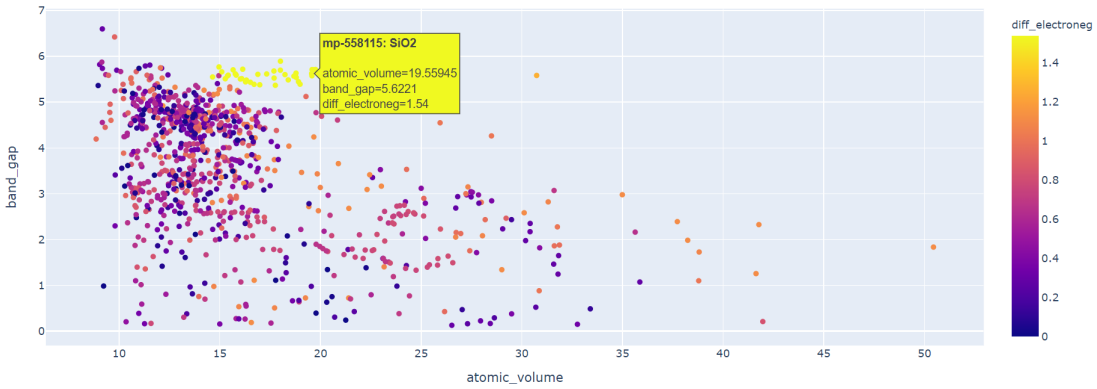

Figure 1: Bandgap VS Density of Si

You can see the interaction verison through: Sicompounds (It seems that a large html file is invisible on github and I haven't figured out how to deal with it.Perhaps I should create a personal homepage next time)

2.2 Pymatgen

Pymatgen stands for Python Material Genomics, which is a robust Python library for materials analysis. Using Pymatgen along with MP-API, we can easily obtain the bandstructure of materials.Up to my knowledge, Pymatgen provides two ways for getting bandstructure:

- Getting bandstructure from the library in Pymatgen. Figure2 is the bandstructure of typical direct-band-gap materials CdTe extracting from Pymatgen.

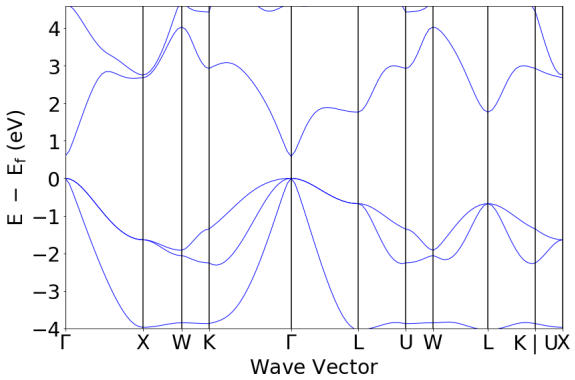

Figure 2: bandstructure of CdTe

- Using pymatgen.io to getting bandstructure from the result of Vasprun.xml. I tend to perform a practice this way, but the work is still in squence on our college's supercomputer centor. Maybe I can present the result in next weekly report.

2.3 Indirect band gap

The type of bandgap is defined by whether the minimal-energy state in the conduction band and the maximal-energy state in the valence band are characterized by the same crystal momentum (k-vector) in the Brillouin zone. However,there is not a unified theory that could explain the phenomenon till now. The following is the limited information I acquire after a week's learning.

1. None of NFE model, Hubbard model, t-J model or simple TB model could explain it. We should consider complex atomic orbitals coupling into each other in the bulk materials which form mini-bands.

2. Perhaps atomic number of constituting elements would influence. The higher atom number a element perserve, the stronger nuclear field it has, which causes the energy bands to align.

3. The existence of the occupied cation d bands is a prime element in determining the directness of the band gap of some semiconductors through the s-d and p-d couplings.(Reference3)

4. The book *Electronic Structure and the Properties of Solids* has a brief explanation using perturbation theory, but I apologize that I still need some time to handle it.

3 Future work

Up to now I think I have a vague frame of this project:

- First we could screen out a database from MP, which should perserve some properties that could affect the type of bandgap, such as such as bond length, electronegetivity, hybridzation between bands, non-trivial topological properties and so on.

- Second we could build a machine learning model that could classify whether a material has direct or indirect band gaps.

- Finally we could figure out how specific properties affect direct or indirect bandgap through the model. and try to find a theoratical explanation for furthur material classification or prediction.

4 Summary

This week is about some preliminary work. Roughly speaking, I assume I have basically handled the use of MaterialProject and Pymatgen and did some survey to clear the aim of this project. Meanwhile, more background knowledge still needs to be learned. Beside, all examples mentioned in the report are submitted to my github https://github.com/Forerain/Summer-Intern-with-Prof-Sun .

5 Reference

1. Anubhav Jain, Shyue Ping Ong, Geoffroy Hautier, Wei Chen, William Davidson Richards, Stephen Dacek, Shreyas,Shreyas Cholia, Dan Gunter, David Skinner, Gerbrand Ceder, and Kristin A. Persson Commentary: The Materials Project: A materials genome approach to accelerating materials innovation. The Journal of Chemical Physics 134, 074106 (2011)

2. Citation As Published Publisher Version Citable link Terms of Use Detailed Terms Ong, Shyue Ping, William Davidson Richards, Anubhav Jain, Geoffroy Hautier, Michael Kocher, Shreyas Cholia, Dan Gunter, Vincent L. Chevrier, Kristin A. Persson, and Gerbrand Ceder. "Python Materials Genomics (pymatgen): A Robust, Open-Source Python Library for Materials Analysis." Computational Materials Science 68 (February 2013): 314–319

3. 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)

4. Walter A. Harrison, *Electronic Structure and the Properties of Solids*