Weekly Report

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1 Introduction

This week I should have done some VASP calculations and relative analysis, but I face some technical problems which I have mentioned in former email. Apart from dealing with those technical problems, I also tried to grasp some VASP postrocessing tools and think about what specific questions we can focus on.

2 Progress

2.1 VASP postrocessing tools

Dealing with VASP results is really a hassle for me. As this week I only got limited results, I think it is time to make it clear. Here I tried Pymatgen, Lobster and some other scripts.

For Pymatgen, I mainly tried to understand the pymatgen.io.vasp.outputs module and use it draw the band structure and DOS of Si as Figure 1 shows. Different color and different rgb proportion are used to represent the orbital contribution.

For Lobster, I install it in WSL2 and run the examples that they offer, but I got a 'Segement fault' error. I assume that it is because WSL2 has some compatible problems with Fortran compiler. Next week I will try it in Linux system to see how good it is.

Besides, I think band structure contribution will be very important to our analysis. Yet I havn't found any scripts that express results as Figure 2 shows. Maybe I could write a script with Pymatgen if necessary.

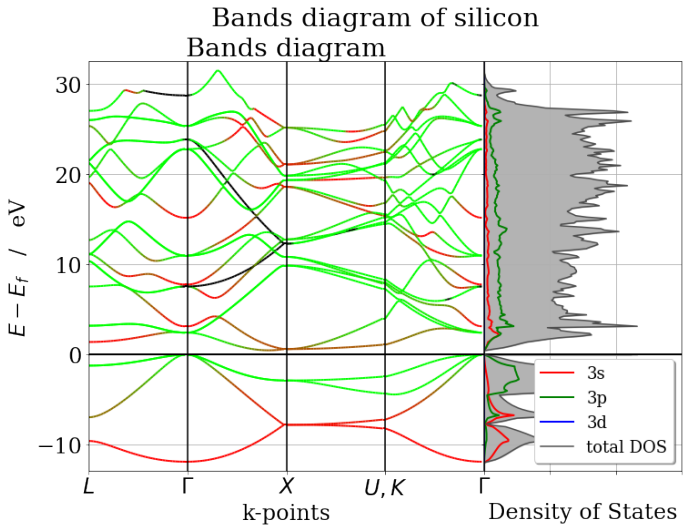

Figure 1: Band structure and DOS of zinc-blende Si

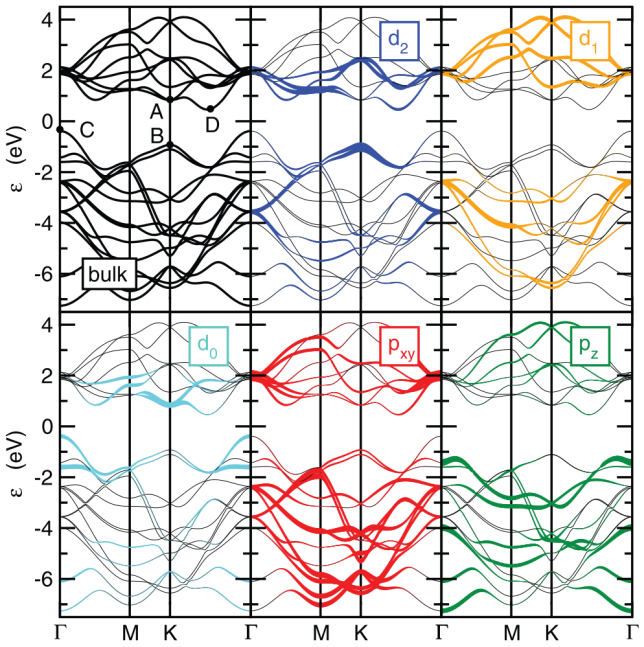

Figure 2: Band structure and orbital character for bulk 2H-MoS2(via Ref 1)

2.2 Thoughts of specific topics

Up to this stage what really worries me is that what specific questions we can start with in order to get a general explanation. This week I think of three possible way for future study.

1. I find that similar direct to indirect band gap changes would also happen in Group oxide. Maybe we can use VASP to analyze band structure contribution to see which orbitals dominate the band structure change.

2. We can choose some ternary or multicomponent compounds and build tight binding model for them. Then changing the proportion or the type of elements to see how band structure changes accordingly.

3. Since hybridization of three dimensions crystals are too complex, how about starting with two dimensions crystals. I think it's more practical to get a general explanation of the indirect band gap of two dimension crystals, and it will also be helpful to genralize it to three dimensions situation.

3 Future work

Now the Primitive task for me is getting VASP correctly installed. Those problems is really grueling but I also learn something during the process. Once it's done, it would extremely improve my efficiency.

4 Reference

1. E. Cappelluti, R. Rold´an, J. A. Silva-Guill´en, P. Ordej´on, and F. Guinea1, Tight-binding model and direct-gap/indirect-gap transition in single-layer and multilayer MoS2, DOI:10.1103/PhysRevB.88.075409