Proposal for the 121B Project

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1 Introduction

Recently, there has been a study of many materials using DFT@B3PW91, one-shot G0W0, and a post-G0W0 method. [1] I will use a similar three methods to compute band structures of gallium nitride. The DFT@B3PW91 has already been done by Dr. Kwon at Caltech, so I will just corroborate the results to get things up and running with the new PySCF computational framework that I am using.

2 Methods

I will be using the wurtzite structure of gallium nitride from the Materials Project. [3] The DFT@B3PW91 and one-shot G0W0 have been in PySCF for quite a while now, but only more recently have there been developments in self-consistent, or post-G0W0, flavors. [2] I am interested in comparing with the two other methods in terms of accuracy and computational expense.

3 What I plan next

I don't imagine that studying this material with these methods will take me the entire quarter. I am interested in photovoltaics and my understanding is that GW, which I plan to study closely this year, lends itself to computing photoemission spectra. Once I get acquainted with computing band structures using PySCF for gallium nitride, I hope to do this for photovoltaic materials, which I will discuss with Professor Goddard throughout the quarter.

References

[1] Jason M. Crowley, Jamil Tahir-Kheli, and William A. III Goddard. "Resolution of the Band Gap Prediction Problem for Materials Design". In: *The Journal of Physical Chemistry Letters* 7.7 (Apr. 2016). Publisher: American Chemical Society, pp. 1198–1203. DOI: 10.1021/acs.jpclett.5b02870. URL: https://doi.org/10.1021/acs.jpclett.5b02870 (visited on 10/08/2023).

[2] Jincheng Lei and Tianyu Zhu. "Gaussian-based quasiparticle self-consistent GW for periodic systems". In: *The Journal of Chemical Physics* 157.21 (Dec. 2022), p. 214114. ISSN: 0021-9606. DOI: 10.1063/5.0125756. URL: https://doi.org/10.1063/5.0125756 (visited on 10/08/2023).

[3] *mp-804: GaN (Hexagonal, P6_3mc, 186)*. URL: https://next-gen.materialsproject.org/materials/mp-804 (visited on 10/08/2023).