**Electronic Band Structure**

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**1.** **Summary**

Our research project centers around furthering the next generation of physicist’s understanding of 2D compounds and their relevance in advancements of technology and industry. We will utilize quantum espresso and jupyter notebook to dive into differences in electronic band structure for diamond (a 3D carbon-based compound), graphene (a 2D carbon-based compound), and graphene under stress.

**2.** **Scientific Background**

Graphene has gotten a lot of attention over the years, as it is a material that, at the correct temperatures, could become a superconductor. However, part of what makes it unique is its electronic band structure, which determines its electrical conductivity. Graphene, at its valence band(shell?), normally has a band gap of zero, which makes it a supremely great electrical conductor, as the electrons can easily move through the hexagonal crystal lattice. Graphene also has a few more unique electrical properties such as: Quantum Hall Effect, Linear Energy-Momentum Dispersion, and Dirac Fermions. The problem with graphene’s lack of a band gap is that it’s not a suitable transistor, which requires a band gap to serve as an on-off switch for electrical current. What makes graphene is such an ideal material of study and excitement is that if we were to reduce the temperature to about 1.7° above absolute zero, and twist it by about 1.05°, with respect to a layer of itself above it, the crystal lattice would have an electrical resistance of zero, thereby making it a superconductor. This angle is referred to as the “magic angle”. A lot of research still needs to be done, however, if we can find a way to achieve the superconductive state of graphene, it will revolutionize the planet and change our society forever.

**3.** **Proposed Research**

For our research, we plan to observe the difference between 2D structures and their 3D counterparts. Expanding upon these observations, the research would then look at the changes in these band structures as they undergo various changes. The research would require the creation or use of a pre-existing compound to be able to obtain a base set of data for the band structure to be used for comparison. Later, various variables of the band structure would be altered to view the effects the changes made and the results would then be transferred to a table and graph for easier visualization. While there are various variables that can be altered, the research’s focus would be the effects of pressure on the band gaps of the structures. With pre-existing research showing that the band gap should decrease as the stress increases, our research should also reflect these results which brings us to the hypothesis: the band gap should be smaller in a 2D structure than a 3D structure, and with added stress, will cause the band gap to decrease.

**4.** **Methods**

For our research project, we will need to utilize the pw.x, bands.x, and possibly the plotband.x command or jupyter notebook to generate graphs for at least 3 different band structures: Diamond, graphene, and graphene-under-stress. We will need to run both an SCF and bands calculation in order to gather the data, and design our own python program to read and graph it by referencing our DOS program.