Electronic Structure Calculations of Boron Nitride Monolayer

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Introduction

Modern Material Science:
- Interdisciplinary field studying properties and interactions of real materials

Innovations in Computational Methods:
- Advanced computational methods drive research progress
- Enables sophisticated calculations and simulations

Methodology Development:
- Ground State Calculations:
  - Finds properties of materials in their organic, non-modified state
- Excited State Calculations
  - Finds properties of materials under a stressor or modifier (often light)
- Many types of methods have been developed each specializing in distinct system size, time, and output

Applications and Impact:
- Contributes to technological advancements and innovations

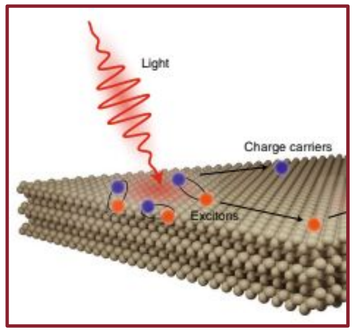

Figure 1. Light being shone on a material to examine its excited-state properties. Adapted from "Discovering and understanding materials through computation".[1.]

Objective & Impact of Professor's Research

The Li Group:
- Research focus: First principle approaches for studying excited-state properties of materials.
- Enhancing knowledge of materials through advanced computational techniques
- Interested in GW Perturbation theory and time-dependent GW
  - High-performance quantum computation methodologies used to describe electrons
- Identifying ways to control or modify quantum excitations.

Research & Learning Process

Learning Process:
- Studied research papers on fundamental concepts in quantum physics
  - Developed a foundational understanding of the subject
- Gained proficiency in lab-specific skills
  - Python, Bash, Linux operation, Quantum Espresso, Discovery supercomputer

Main Project:
- Explored distinct materials: Graphene and Boron Nitride
- Nearly identical molecular structures but inverse conductive properties
- Each material assigned to a lab partner for investigation; Boron Nitride given to me

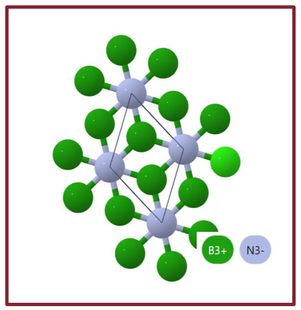

Figure 2. Boron Nitride (BN) Molecular Structure.

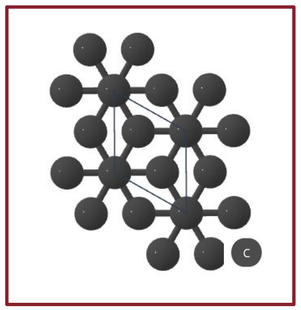

Figure 3. Graphene Molecular Structure.

Discovery supercomputer:
- Materials have intricate interactions, with many force and factors at the atomic level
- Requires intricate simulations and advanced computing resources
- Employed USC's Discovery supercomputer to host calculations

Quantum Espresso (QE):
- Free integrated software based on open-source code.
- Specialized in first-principle electronic-structure calculations and modeling

Methods & Results

QE Calculations:
- ❖ **Relax** - calculates ideal positions for atoms
- ❖ **SCF** - calculates the energy of a single point
- ❖ **SCF Convergence** - repeatedly run SCF calculations, changing the value of a parameter, to find its ideal value
- ❖ **Band** - calculates electronic bands
- ❖ **Band Post Processing (PP)** - adjusts and formats **Band** output
- ❖ **Band Structure Code** - uses **Band PP** output to plot the band structure

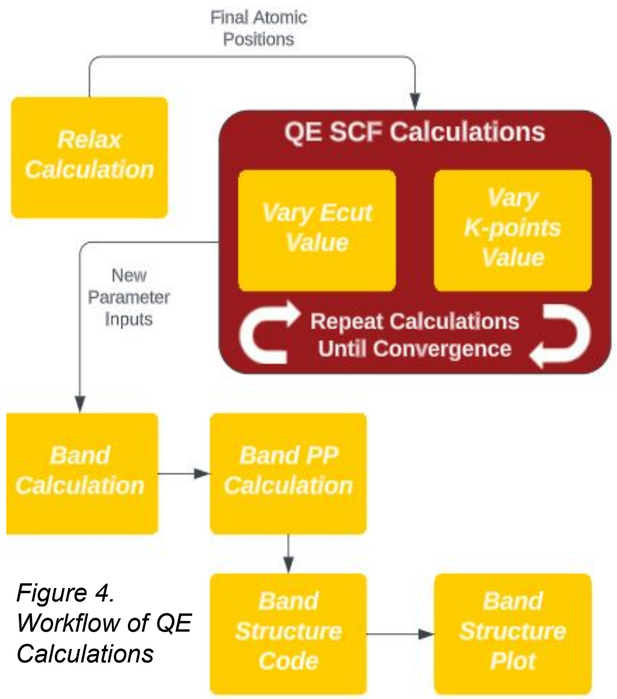

Figure 4. Workflow of QE Calculations

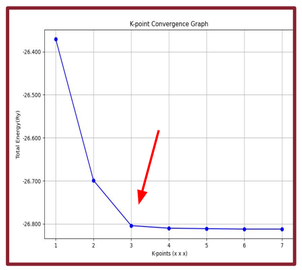

Figure 5. K-point Convergence Graph

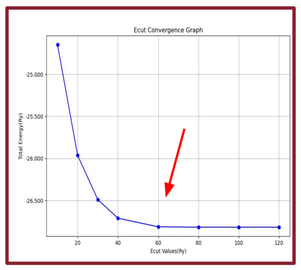

Figure 6. Ecut Convergence Graph

Result Analysis

Boron Nitride (BN) vs. Graphene:
- **Band Structure** - visualizes the ranges of energies electrons can occupy in a material
- BN's band structure has a band gap (red circle) where electrons cannot occupy this energy
- Graphene does not have this gap, which explains its conductive properties and BN's insulative ones

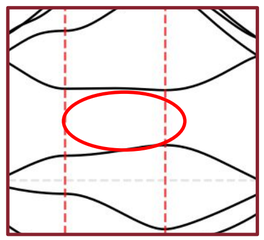

Figure 7. Boron Nitride (BN) Non-zero Band Gap

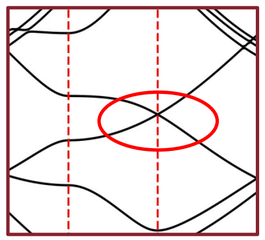

Figure 8. Graphene Zero Band Gap. (Graph by Carter Lee)

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Citations

1. *Louie, S., Chan, Y., da Jornada, F., Li, Z., & Qiu D. Discovering and understanding materials through computation. Nat. Mater.* ***20****, 728-735 (2021).*
2. *Chen, Chuu, C.-P., Tseng, C.-C., Wen, C.-K., Wong, H.-S. P. Wafer-scale single-crystal hexagonal boron nitride monolayers on Cu (111). Nature (London),* ***579****(7798), 219–223 (2020).*