First-Principles Study of Graphene

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Introduction

- Graphene is a material made of a monolayer of carbon atoms in a hexagonal lattice
- Discovered in 2004 by Andre Geim and Konstantin Novoselov
- Regarded as world's thinnest, strongest, and lightest compound
- Best conductor of electricity and heat at room temperature.
- Unique versatility makes Graphene a highly promising material in electronics

Objective of Professor's Research

- Professor Li specializes in computational materials science on quantum scale.
- Research uses DFT (density functional theory) computational programs to simulate material properties.
- Quantum Espresso on USC supercomputer run simulations, revealing material function and practicality.
- Goal is to discover new material applications in technologies such as superconductors.

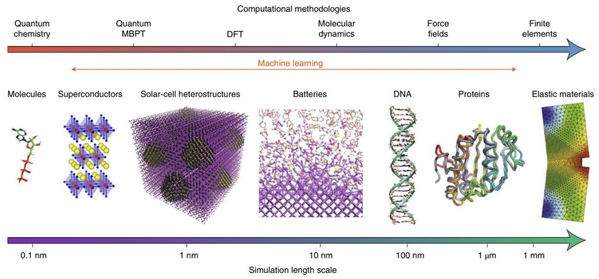


Fig1. Simulation methods and scales in computational materials science

Citations

Steven G. Louie, Yang-Hao Chan, Felipe H. da Jornada, Zhenglu Li, Diana Y. Qiu. (2021). Discovering and understanding materials through computation. Nature Materials, vol 20, 728-735

Novoselov, Kostya S., et al. "Electric field effect in atomically thin carbon films." *science* 306.5696 (2004): 666-669.

Research & Learning Process

- Analyzed characteristics and properties of Graphene through constructing its band structure.
- Relied on computational methods, which required proficiency in Linux, Vim, and Quantum Espresso
- Linux: terminal that uses bash commands to navigate and manage computation files.
- Vim: text editor that used commands to navigate code files themselves.
- Quantum Espresso: software that uses a material's parameters to calculate its properties and structure.

Fig2. Quantum Espresso Logo

- Learned various Quantum Espresso input categories such as the kinetic energy cutoff and k-points.
- Three main computational programs developed to construct the final band structure.

Methods & Results

- Three calculations: self-consistent field (SCF), relaxed, and band structure.
- SCF calculation: determined total energy of Graphene system (approximately -24.7 Ry) with ecut of 70.00 Ry.

```
total energy              =     -24.70902496 Ry
estimated scf accuracy    <       0.00000032 Ry

iteration #  8     ecut=    70.00 Ry     beta= 0.70
Davidson diagonalization with overlap
ethr =  4.06E-09,  avg # of iterations =  4.2
```

Fig3. Details of Total Energy Calculated by SCF

- Relaxed calculations: utilized total energy value to predict optimized positions (where external forces on atoms reach 0) of the two carbon atoms in monolayer.

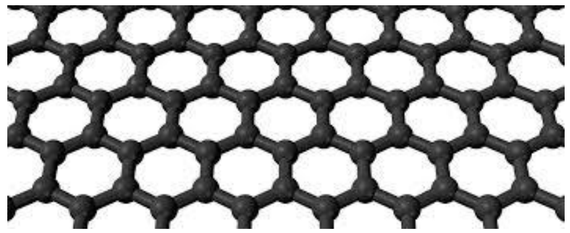
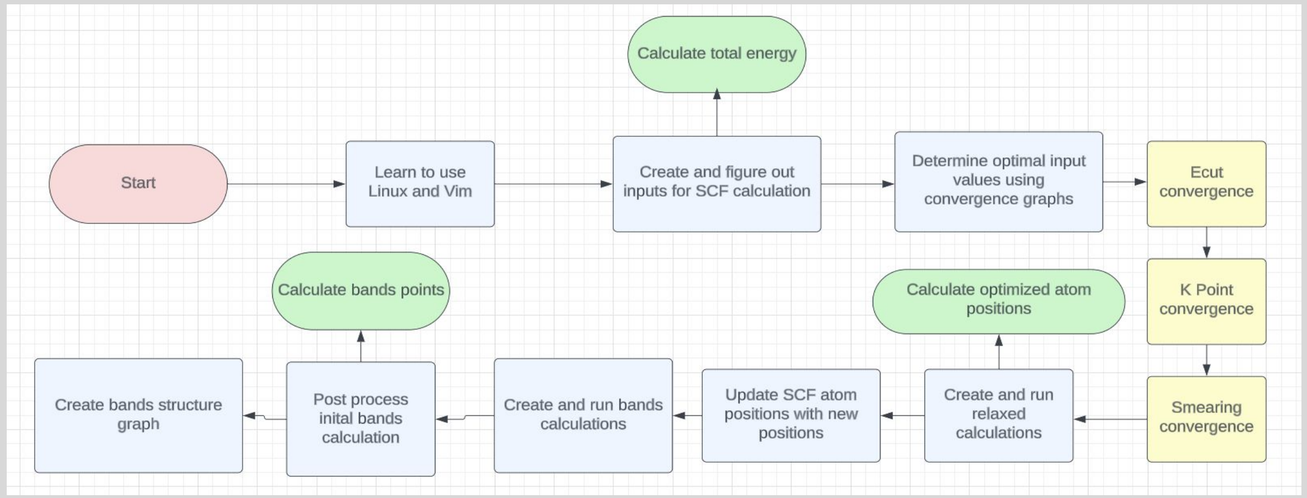


Fig4. Simulated hexagonal lattice of Graphene

- Band Structure Calculation: Yielded series of cartesian points using optimized positions applied to the SCF. These depicted the behavior of electrons in Graphene at various energy levels.

Workflow Diagram



Results Analysis

- Graph reveals semi-metallic nature because of intersection of bands at 0 energy level (absence of a bandgap).
- Semimetal classification from simulations reveals Graphene's high conductivity and durability.

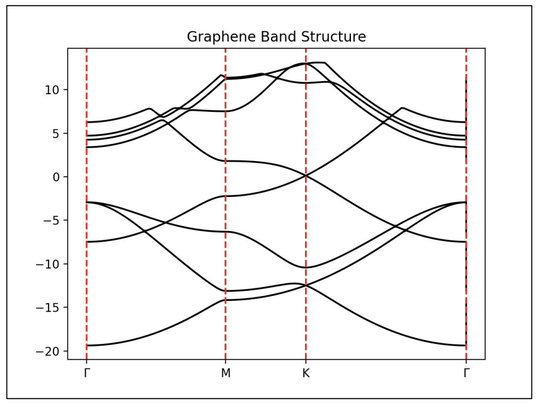


Fig5. Band Structure Graph with Lines of High Symmetry

Advice for Future Students

My advice for future SHINE students is to be confident in your abilities. For me, I came into this lab feeling like I did not belong. This research dealt with complicated topics and even the name "quantum materials science" sounded intimidating. Though as time went on, I realized that it wasn't as daunting as it first seemed and that I could indeed succeed in this lab. Afterall, I had been selected to be apart of it for a reason. So, I want to let incoming SHINE students know that even if they feel a similar way at the beginning, they should trust themselves and try to make the most of what SHINE has to offer.

Acknowledgements

I would like to thank both my advisor Professor Li and mentor Jimy for all of their help in working through this research. A lot of this material was new to me, though they both took the time to help me truly grasp these concepts so I could make the most out of my time at SHINE.