

Title: Predicting New Graphene - Boron Nitride 2D Nano-Materials: Structure Electron Bands Optical Response and Vibrations

Date: May 07, 2014 12:25 PM

URL: <http://pirsa.org/14050048>

Abstract: The goal of this research is to investigate theoretically the possibility of creating graphene-based semiconducting 2D heterosystems that allow tailoring of the band gap and creating states inside the gap by demand. Such systems are created in our computational experiment by depositing graphene on a layer of hexagonal boron nitride and adding hydrogen on top and bottom of the systems to passivate the dangling bonds and create covalent bonding between the layers of the system of interest. Apart from the atomic structure the thermal stability of the heterosystems their optical and vibrational properties were also studied. In this research four different bilayers and their properties are presented.

Goal of this Research

What

The goal of this research is to analyze theoretically how to create graphene and BN based **semiconducting** 2D heterosystems and to offer a tool for tailoring the band gap and/or creating states inside the gap by demand.

How

Such systems are created in our computational experiment by "numerically" depositing graphene on a hexagonal boron nitride monolayer and adding hydrogen on top and bottom of the systems to passivate the dangling bonds and form covalent bonding between the layers. At the same time, the intralayer covalent bonding opens the band gap of the bilayer, thus making the material semiconducting.

Properties

Apart from the atomic structure and DOS, the thermal stability of the heterosystems, their optical and vibrational properties were also studied using ab-initio molecular dynamics tools.

2D Electron Band
Engineering:
Application of High
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Computing to
Quantum
Nano-Systems

Wiki

Motivation and Goal of
this Research

Background

Computational
Methods

Specific Structures and
Their Density of States

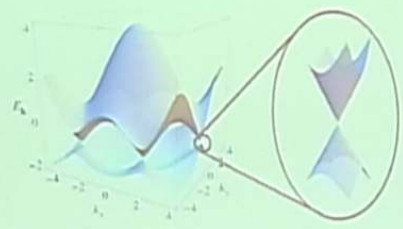
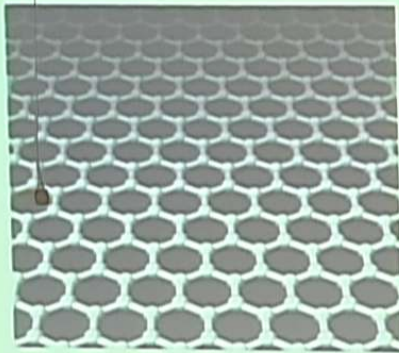
Thermal Stability and
Frequency

Conclusion

Graphene

What is this revolutionary material?

This discovery was awarded the 2010 Nobel Prize in Physics [K. S. Novoselov, A. K. Geim, S. V. Morozov, et. al. Science 306, 666 (2004)]. Graphene is a sp^2 bonded 2D sheet of carbon in a dense honeycomb crystal lattice. This leads to an extremely strong material with record high electron mobility due to linear band dispersion. However, it also has a zero band gap, making it a semi-metal.



2D Electron Band Engineering: Application of High Performance Computing to Quantum Nano-Systems

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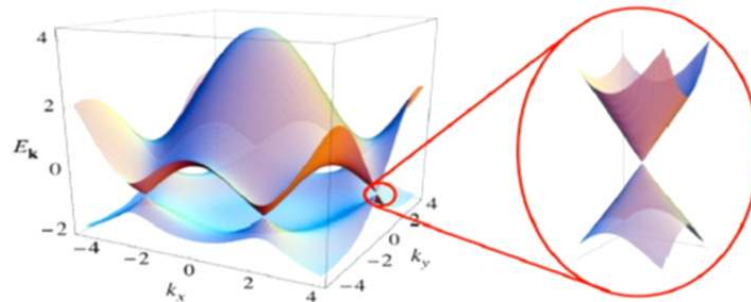
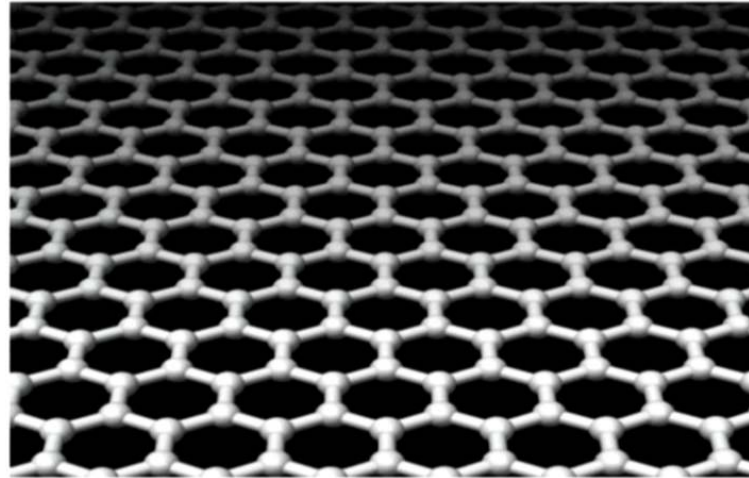
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Wilk

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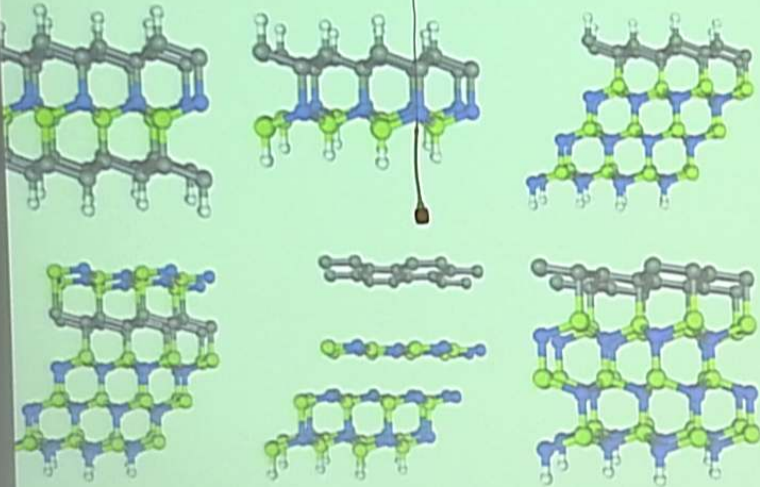
Computational Methods

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Structures Considered



We simulated more than 40 structures, including 2D bilayers and trilayers as well as BN bulk substrates and different levels of hydrogenation on each. Note that hydrogen is white, carbon is grey, boron is green and nitrogen is blue.

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Shifted Hydrogenated Bilayer (AB Stacking)

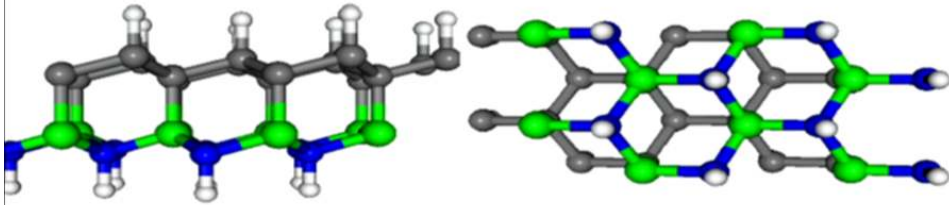


Figure: Side View

Figure: Top View

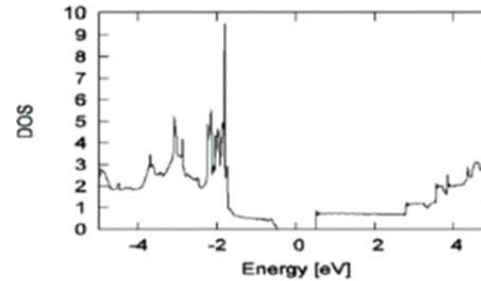


Figure: DOS

The AB stacked hydrogenated bilayer

The so-called AB-stacked hydrogenated bilayer is shifted in the x -direction by a quarter of the length and in the y -direction by a half of the width from the AA stacked version, in which atoms are located on top of each other. This follows the stacking sequence of the cubic structure. The change in structure from AA to AB sequence lowered the energy by 0.038 eV per unit cell of 6 atoms. Due to the similarity of the structures, the difference in band gaps is 0.1 eV, with 1.0 eV for the AB-stacked bilayer.



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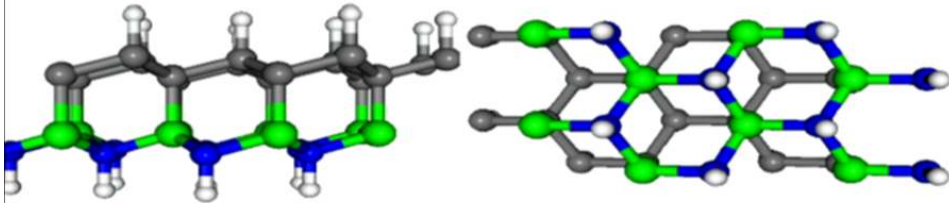


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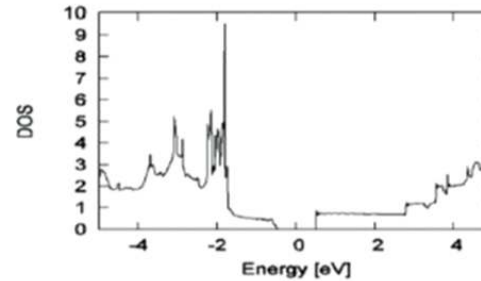


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