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

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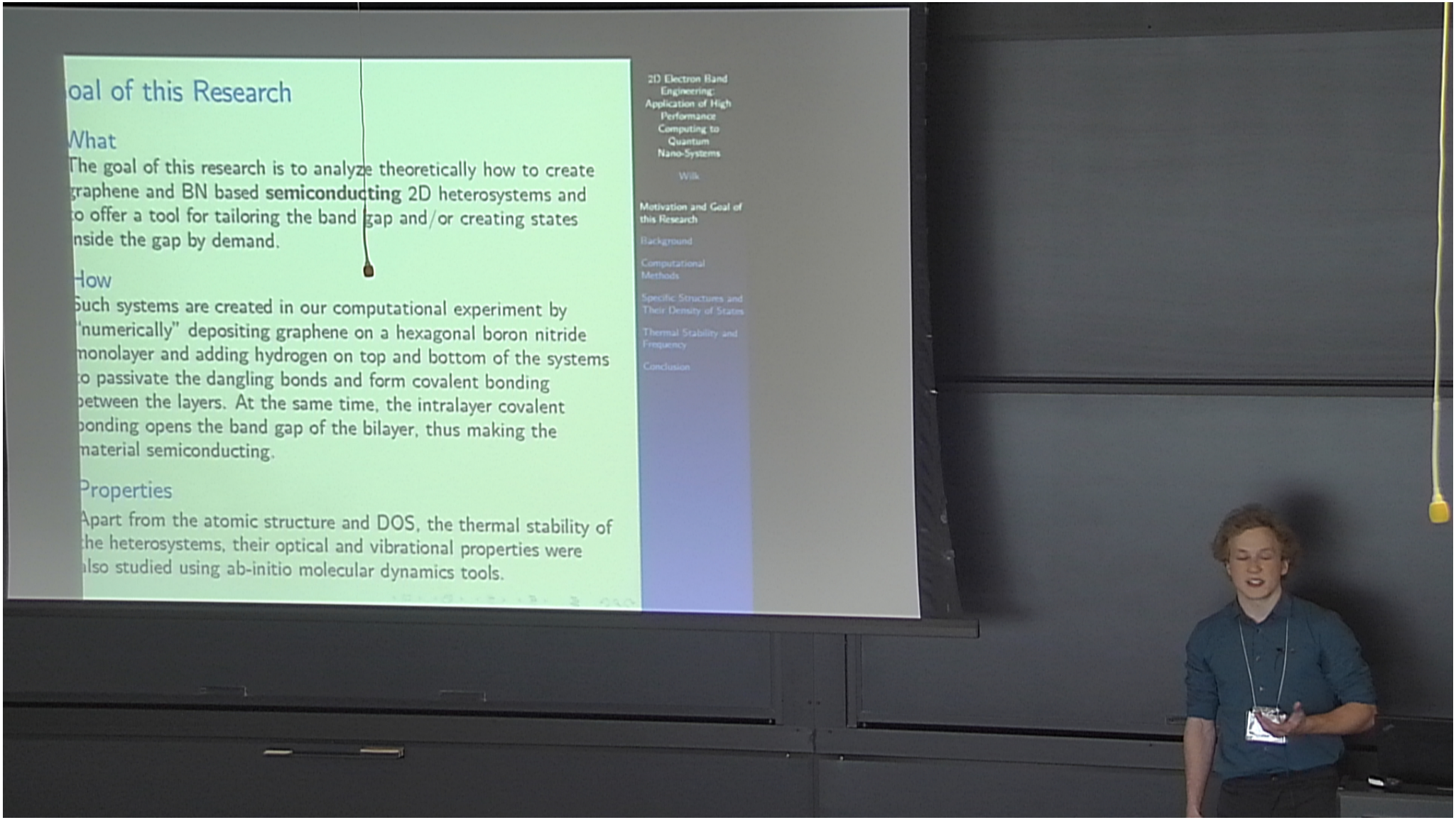
Abstract: The goal of this research is to investigate theoretically the possibility of creating graphene-based semiconducting 2D heterosystems that allow tailoring of the band gap and creating states inside the gap by demand. Such systems are created in our computational experiment by depositing graphene 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 dierent bilayers and their properties are presented.


oal 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 Performance Computing to Quantum Nano-Systems
Wilk
Motivation and Goal of this Research
Background
Computational Methods
Specific Structures and Their Density of States
Thermal Stability and Frequency
Conclusion

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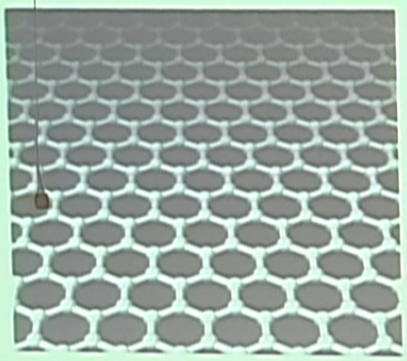

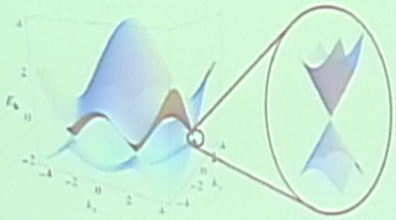

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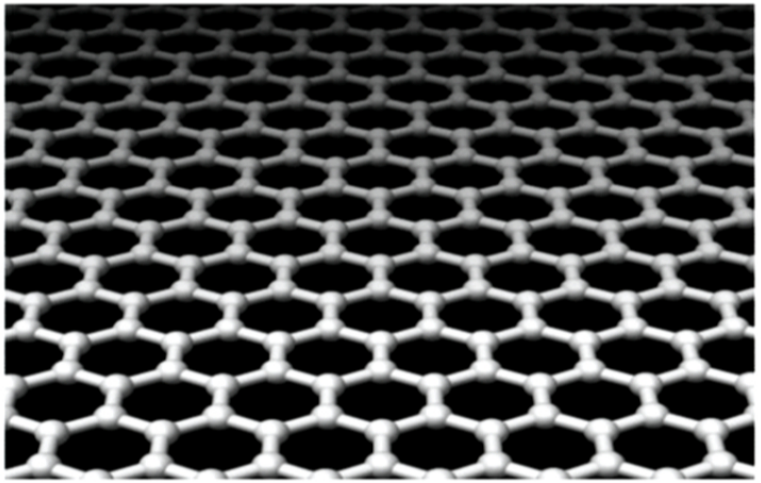

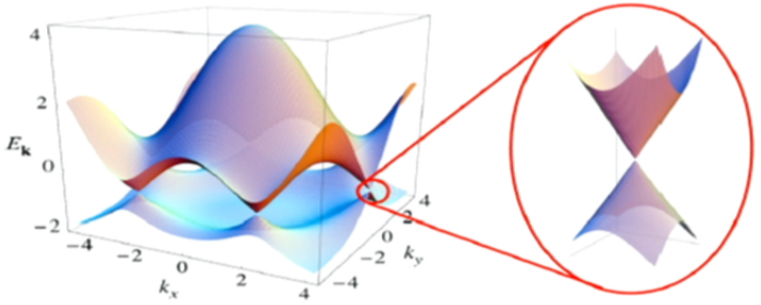

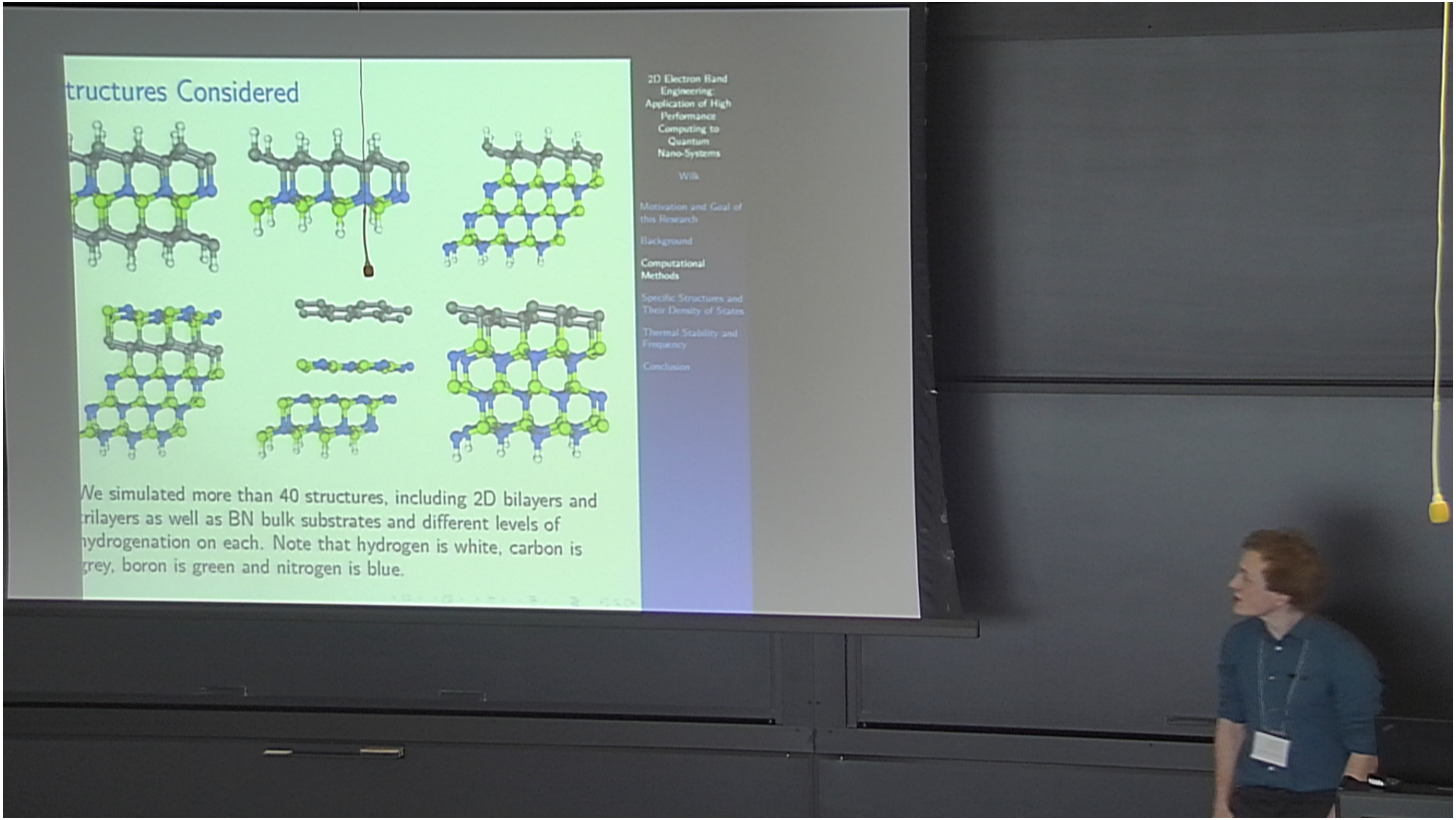
tructures Considered
We simulated more than 40 structures, including 2D bilayers and
rilayers as well as BN bulk substrates and different levels of
ydrogenation on each. Note that hydrogen is white, carbon is
rey, boron is green and nitrogen is blue.
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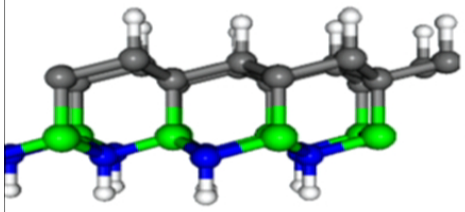

Figure: Side View

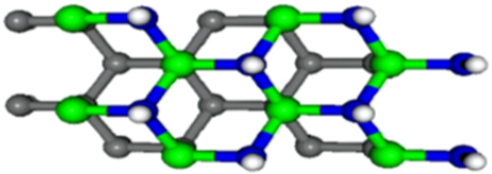

Figure: Top View

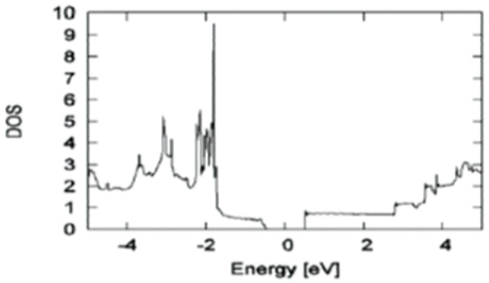

Figure: DOS

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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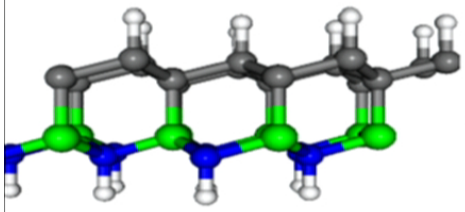

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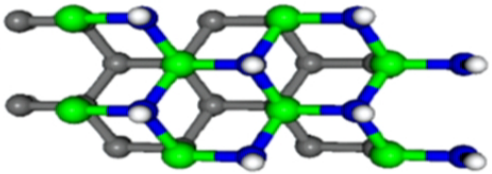

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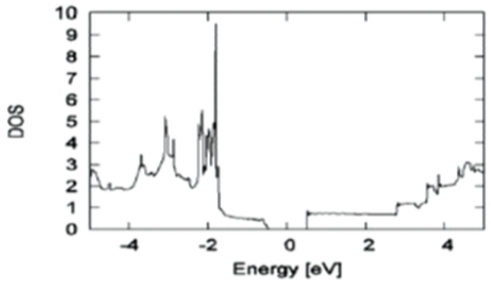

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