Spintronic Applications of Doped Graphene Ribbons

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INTRODUCTION

- Graphene (two-dimensional sheets of carbon atoms) has unique electronic properties such as the Dirac cone band structure.
- With new manufacturing techniques, the demand for uses of graphene has increased.
- Computational chemistry can find spintronic applications. Graphene could be used for solid-state devices with ternary processing and information storage.
- By doping graphene (embedding transition metals) we change properties such as band structure and magnetization. Calculating the embedding energy allows us to determine the difficulty of forming these materials.
- The goal is to find structures with an ideal magnetization to store data without corruption, yet at a low energy cost.

GRAPHENE RIBBON STRUCTURE

Graphene ribbons only tessellate along the x axis.
This produces unique properties - edge states and jumping orbitals.

This is a diagram of a pristine graphene ribbon.

This is a single supercell, which would tessellate infinitely horizontally.

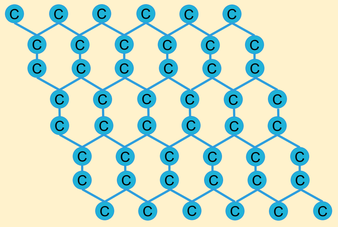


FIGURE 1

METHODOLOGY

Plane-Wave Density Functional Theory using Quantum Espresso (PWSCF v5.0.1)

1. Run a relaxation calculation to find the optimal geometry.
2. Calculate electron density, magnetization, and band structure.
3. Find the enthalpy of formation of the doped system.

Parameters

Pseudopotentials Rappe-Rabe-Kaxiras-Joannopoulos (RRKJ) ultrasoft pseudopotential

Perdew-Burke-Ernzerhof (PBE) generalized gradient approximation (GGA)

Supercell Dimensions 14.76 Å x 29.52 Å x 14.76 Å

Monkhorst-Pack K Point Grid 4 x 1 x 1

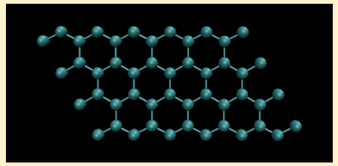
Planewave Cutoff Energy 30 Ry

Charge Density Cutoff 240 Ry

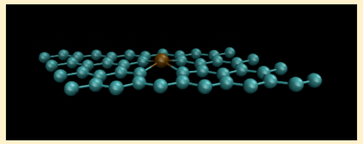
DATA

INITIAL WARPING

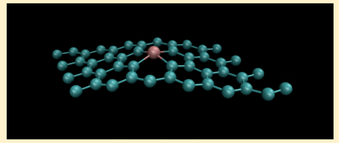
Our original ribbon systems were 6 x 2 unit cells, and warper significantly.
We restarted our data collection with stronger 6 x 4 unit cells.



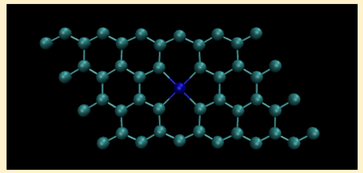
Pristine



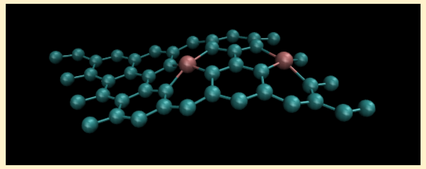
Co single



Fe single



Ni single



Fe double side1

Configuration	Final Energy (Ry)	Buckling Height (Å)	Total Magnetization	Absolute Magnetization
Fe-ribb1	-577.0191103716	0.88145671926087	12.02	19.97
Co-ribb1	-595.6217564590	0.47116490600000	13.00	17.67
Ni-ribb1	-607.1294070657	0.08944239000000	14.00	16.33
Pristine	-544.4707717939	n/a	14.25	16.26
Fe-ribbe2-side1	-609.5860263770	0.653641675 and 0.642406771	10.00	23.45

ANALYSIS AND RESULTS

Based on the data, we can see that the most magnetized configuration among the single metals is the Ni-ribb1. Such a high magnetization shows that this configuration has possible applications in spintronic devices; this magnetization, which is neither too high and too low, makes writing data into the material easy, but also strong enough so that there is no data leaking; in other words, it's within the goldilocks range to securely store data.
Also, we see that while most of the metals, with the exception of Nickel, had quite a high buckling height. The others look quite similar. Only the double metal configuration looks more severely warped than the other structures.
The low final energy of Fe-ribb1 suggests that the reaction for forming this configuration should be relatively exothermic, meaning it will form spontaneously without energy needing to be added.

APPLICATIONS

Our research problem focuses on one such application, the usage of 2D materials in solid-state electronics. As the world's information systems are digitized, being able to push the storage and computation power of computers is becoming more important. In the context of 2D materials, spintronics is the study of electron spin, and we are looking to see how the electron spin can be used to store data. Traditionally, digital systems are binary (using 0 or 1) but because electrons have three states (nonexistent, spin up, spin down), spintronic devices can store data with 0, 1, or 2, making data storage much more efficient.

ACKNOWLEDGEMENTS / REFERENCES

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Works Cited:

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"Band Theory for Solids." *HyperPhysics*, edited by Carl Rod Nave, Georgia State University, hyperphysics.phy-astr.gsu.edu/hbase/solids/band.html. Accessed 25 Sept. 2016. An introductory explanation on band structures. Also provides links to other resources for the associated topics. Covers solids, insulators, semiconductor, conductor, silicon, and germanium energy bands.

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