Chirality Genesis: Utilizing Graph Theory to Model Doped-Graphene-Ribbon Fullerene Growth

Micheal Chau[1], Tian Chen[1], Robert Cormia[2]

INTRODUCTION

- Graphene is a mono-layer carbon material; it is the most conductive material in the world, it is transparent, and it has a large surface area to volume ratio (Chen et al., Aug. 2011, p. 2799).
- Fullerene is a form of carbon that has a large spheroidal molecule consisting of a hollow cage of atoms
- One of the problems with producing graphene-based fullerenes is the various folding methods that cause the properties to differ on the particular type of material(Wang et al., Apr. 2009, p.102).
- Graph theory is a field of pure maths that studies that pairwise relationships between objects.
- This particular field has been used to study the topological characteristics of materials in chemistry and more recently the edge effect of graphene.

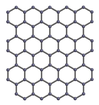


Fig 1. This represents a graphene sheet matrix configuration

AIM

What is the genesis of chirality, and can graph theory provide insights into modeling fullerene growth?

The subset research questions are:
-What are the echanisms of nanotube and graphene growth?
-Can Graph Theory describe graphene (CNTs, esp. chirality)?
-Can Graph Theory describe emergence properties of graphene?
-Can graphene be used to model the geometry of smaller sP2 domain growth?
-Can Graph Theory help categorize fullerenes and possible growth mechanisms?

METHODS

- *Quantum Espresso* (v. 5. 4. 0) using Density Functional Theory (open source)
- Hand Calculate coordinate of plain graphene sheet and ribbon
- **Inquiry Approach True Experimental Approach**
- **Data Collection Measurement (by simulation)**
- **Data Type Quantitative Data**
- **Data Analysis Descriptive statistics**

•When assigned the specific parameters and strings of our interest material, Quantum Espresso will use DFT and give its band structures and other molecular properties.

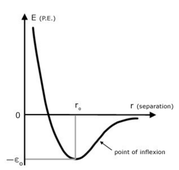
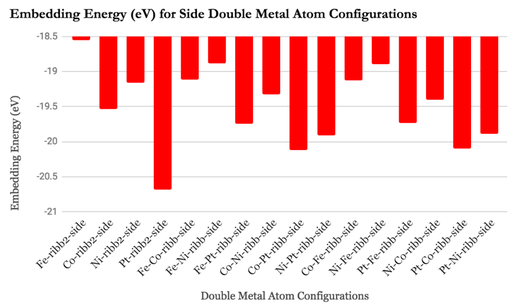


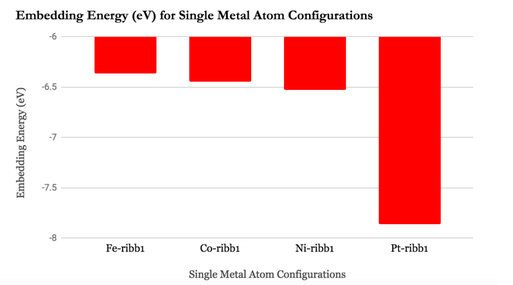
Fig 2. This is an atomic distance energy well

ENTHALPY ANALYSIS:

$$\Delta H^\circ = H_{calculated\ final} - \left(\sum H_{metal} + H_{hole}\right)$$

embedding energy and geometric data:





Geometry Ranking:
1.Structures with Fe
2.Structures with Ni
3.Structures with Co
4.Structures with Pt
5.Permeations are the range of H1-H2

- Similar geometric and energy trend as the Graph configuration
- Stronger repulsive forces between a larger electron cloud of metal atom pushes it further away from the neighboring carbon atoms,

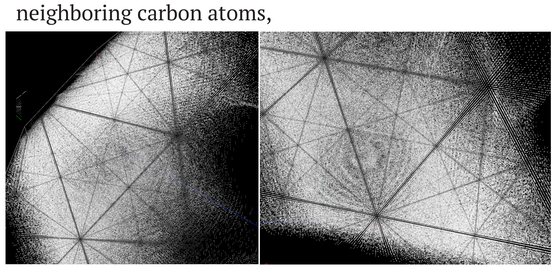
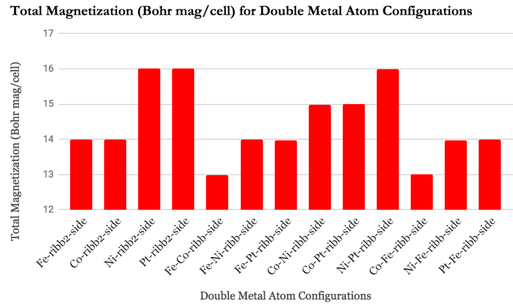


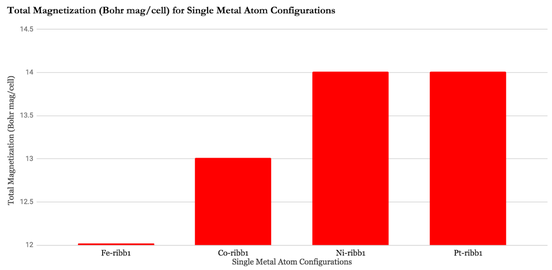
Fig 3. Image of electron density around doped area. The geometries can be generated and verified through graph theory

MAGNETIZATION ANALYSIS:

$$\mu_B = \frac{e\hbar}{2m_e}$$

magnetization data:





Ranking:
1.Pt-ribb2-side
2.Ni-ribb2- side
3.Structures containing one Co
4.Structures that do not contain any Fe
5.Structures that contain Fe and Co

- Pt-ribb2 , all of the magnetization was localized on the Pt metal atom, spread over the s and d orbitals.
- Ni-ribb2, all of the magnetization was also localized on the Co metal atom, mostly in the 3dz orbital.
- Pt and Ni embedded in graphene have the potential to store data due to magnetization preserved on the metal atom. Ni and Pt embedded in graphene have close to no magnetization, which makes it impractical to use for data storage.

CONCLUSION

- From this work, structures embedded with Ni seemed most promising.
- These data are organized by [atomic symbol]-[configuration]. In the first two graphs, we've collected magnetization data on the simulated materials (single metal and then double metal).

CONCLUSION (cont.)

- Magnetization is a measure of spin up electrons-spin down electrons, and is a indicator of how the electrons are being rearranged in the material/how attractive the metal atom is.
- The embedding energy is how much energy is needed to embed the metals we've selected into a "blank" clean slate of graphene.

FUTURE WORK

- We are still looking for data to compare, but the goal was to find experimental magnetization and embedding energy of these materials to compare with the data on our theoretical structure. If they are reasonably close, then we can conclude that our graph theory geometric model was in fact able to model chirality and fullerene growth. The next step is to find citable data to compare out collected data to.
- By analyzing band structures, we could further understand the magnetization properties of the material and calculate its momenta.
- We could also try more configurations with different metals, so metals with similar periodic properties could be compared with each other.

ACKNOWLEDGEMENTS

Special thanks to Dr. Robert Cormia and Ms. Angela Merchant of Palo Alto Unified School District for guiding our paper.

REFERENCES

Avdoshenko, S., Ioffe, I. N., Cuniberti, G., Dunsch, L., & Popov, A. A. (2011). Organometallic complexes of graphene: Toward atomic spintronics using a graphene web. ACS Nano, 5(12), 9939-9949. https://doi.org/10.1021/ nn203719a.
Burress, J. (2010). Graphene oxide framework materials: Theoretical predictions and experimental results. Angewandte Chemie International Edition, 49(47), 8902-8904. https://doi.org/10.1002/anie.201003328
Chen, L. (2011). First-principles calculation of the electronic structure and magnetism at the graphene interface. International Journal of Modern Physics B, 25(21), 2791-2800. https://doi.org/10.1142/S0217979211100746.
Density Functional Theory for Beginners. Density Functional Theory for Beginners, <http://newton.ex.ac.uk/research/qsystems/people/coomer/dft_intro.html.> Accessed 9 Oct. 2016.
Fan, L., Zhang, Q., Wang, K., Li, F., & Niu, L. (2012). Ferrocene functionalized graphene: Preparation, characterization and efficient electron transfer toward sensors of h2o2. Journal of Materials Chemistry, 22, 6165-6170. https://doi.org/10.1039/C2JM15411K .
Kaloni, T. P., N. Singh, and U. Schwingenschlögl. "Prediction of a Quantum Anomalous Hall State in Co-decorated Silicene." Physical Review B 89.3 (2014): n. pag. Web. <https://arxiv.org/pdf/1312.7127.pdf>.
Khludkov, S. (2012). Gallium nitride as a material for spintronics. Russian Physics Journal, 55(8), 903-909. https:// doi.org/10.1007/s11182-013-9899-5.
Li, D. (2008). Graphene-based materials. Science, 320(5880), 1170-1171. http://doi.org/10.1126/science.1158180.
Maassen, Jesse, et al. "Graphene Spintronics: The Role of Ferromagnetic Electrodes." Nano Letters, vol. 11, no. 1, Dec. 2011, pp. 151–155., doi:10.1021/nl1031919.
Nakada, Kyoko, et al. "Edge State in Graphene Ribbons: Nanometer Size Effect and Edge Shape Dependence." Physical Review B, 1 Dec. 1996, adsabs.harvard.edu/abs/1996PhRvB..5417954N.
Roche, Stephan, and Sergio O Valenzuela. "Graphene Spintronics: Puzzling Controversies and Challenges for Spin Manipulation." Journal of Physics D: Applied Physics, vol. 47, no. 9, Dec. 2014, p. 094011., doi:10.1088/0022-3727/47/9/094011.
Ruth, David, and Mike Williams. Cobalt Atoms on Graphene a Powerful Combo. Rice University News & Media, 16 Oct. 2012. Cobalt Atoms on Graphene a Powerful Combo, <http://news.rice.edu/2015/10/21/cobalt-atoms-on-graphene-a-powerful-combo/.> Accessed 9 Oct. 2016.
Strange Phenomena in Matter's Flatlands. Kungliga Vetenskapsakademien (The Royal Swedish Academy of Sciences), 2016. The Nobel Prize in Physics 2016, <www.nobelprize.org/nobel_prizes/physics/laureates/2016/popular-physicsprize2016.pdf.> Accessed 9 Oct. 2016
The Nobel Prize in Physics 2010. Kungliga Vetenskapsakademien (The Royal Swedish Academy of Sciences), 5 Oct. 2010, <www.nobelprize.org/nobel_prizes/physics/laureates/2010/press.pdf.>
Wang, Wei L., et al. "Topological Frustration in Graphene Nanoflakes: Magnetic Order and Spin Logic Devices." Physical Review Letters, vol. 102, no. 15, Apr. 2009, doi:10.1103/physrevlett.102.157201.

[1] PAUSD/Advanced Authentic Research
[2] Foothill College