Graphene Spintronics: Density Functional Theory Study of Fe, Co, Ni, and Pt Embedded Graphene

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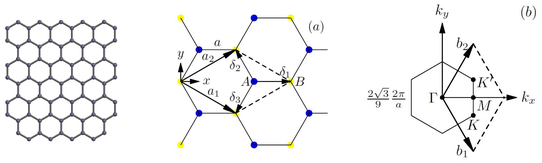
INTRODUCTION

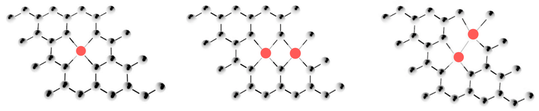
- Graphene, discovered in 2004 exhibits extraordinary characteristics. It is the most conductive material in the world, transparent, and large surface area to volume ratio.
- There is little known about embedding metals and metal complexes into 2D sheets.
- Band structures of Fe, Co, Ni, and Pt systems indicate spin polarization and have potential to be used in driving a spin current.
- Embedding ferromagnetic elements into graphene may be useful in the preservation and transport of spintronic information, similar to Co adsorbed silicene, for example.



AIM

Run relaxation calculations to determine ground state of Fe, Co, Ni, Pt atoms+dimers+combinations embedded graphene to investigate electronic and spintronics potential.

Single Atom, Double Atom (side), Double Atom (Diagonal)

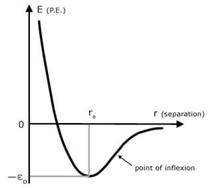


- *Fe, Co, Ni, Pt, (single)*
- *Fe2, Co2, Ni2, Pt2, FeCo, FeNi, FePt, CoNi, CoPt, NiPt (S + D)*

METHODS

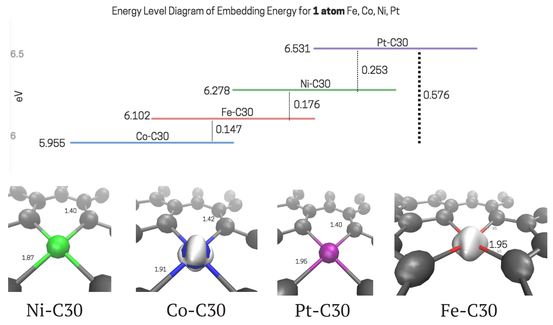
- *Quantum Espresso* (v. 5. 4. 0) using Density Functional Theory (open source)
  - *Rappe-Rabe-Kaxiras-Joannopoulos* (RRKJ) ultrasoft pseudopotentials
  - *Marzari-Vanderbilt* smearing
  - *Gaussian* spread of 0.001 Ry
  - Cutoff energy of 40 Ry for the planewave
  - 480 Ry for the charge density cutoff
  - *Visual Molecular Dynamics (*molecular visualization software) to obtain geometric data

- 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.



ENTHALPY DATA:

Single atom embedding energy and geometric data:



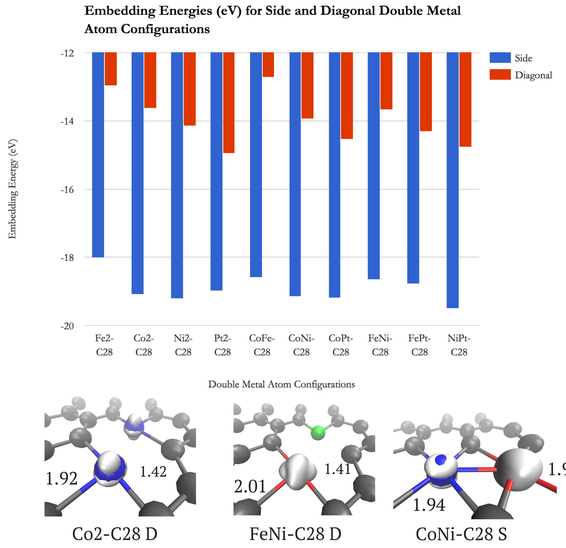
$$\Delta H^\circ = H_{calculated\ final} - \left(\sum H_{metal} + H_{hole}\right)$$

Ranking:

1. Co-C30 (-5.955 eV)
2. Fe-C30 (-6.102 eV)
3. Ni-C30 (-6.278 eV)
4. Pt-C30 (-6.531 eV)

Based on geometric data, the expected results is Fe-C30 or Pt-C30 having the highest embedding energy, Co-C30 having the second highest embedding energy, and Ni-C30 having the fourth highest embedding energy.

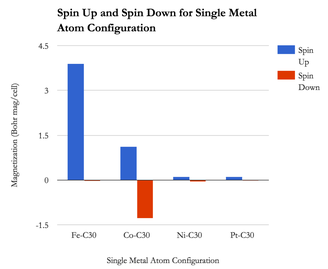
Double atom embedding energy and geometric data:



- Similar geometric and energy trend as the 1 atom configuration
- Stronger repulsive forces between a larger electron cloud of metal atom pushes it further away from the neighboring carbon atoms, which increases the metal-C bond length and buckling height.

MAGNETIZATION DATA:

Single atom magnetization data:



Magnetization Ranking:

1. Fe-C30
2. Co-C30
3. Ni-C30
4. Pt-C30

- Fe-C30, all of the magnetization was localized on the Fe metal atom, spread over the s and d orbitals.
- Co-C30, all of the magnetization was also localized on the Co metal atom, mostly localized in the 3dyz orbital.

- Based on the single metal atom configuration, Fe and Co embedded in graphene have the potential to store data because of its 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.

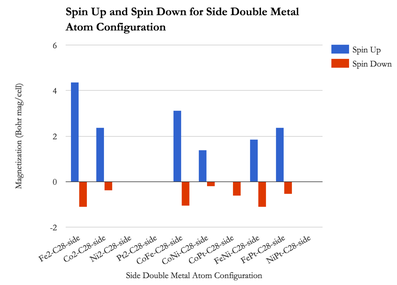
Double atom magnetization data:

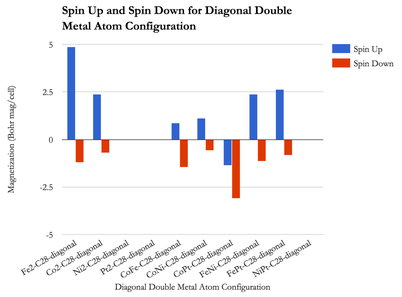
- Similar trend as the single metal atom configuration

Ranking:

1. Fe2-C28
2. Structures containing one Fe
3. Structures that do not contain any Fe
4. Structures that contain Ni, Pt, or both.

- Side configuration has a higher magnetization than the diagonal double metal atom configuration, with the exception of CoFe-C28.





Double atom magnetization data analysis :

Even when Ni or Pt is embedded with Co or Fe in a double metal atom configuration, the Ni or Pt consistently shows little to no magnetization. However, any double metal atom configurations that contain at least one Fe have a large enough magnetization to be considered for storing data.

CONCLUSION

- From this work, Ni and Pt embedded in graphene cannot be used for data storage, because of their lack of magnetization when looking at both the single metal atom and double metal atom configurations.
- Co and Fe embedded in graphene show potential for devices using spintronic data storage, because of its magnetization localized on the metal atom.
- Because the diagonal double metal atom configurations have lower embedding energies than the side double metal atom configurations, diagonal would more stable, so it is better for applying it in spintronic data storage devices.

FUTURE WORK

- 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

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