CALIFORNIA STATE SCIENCE FAIR
2017 PROJECT SUMMARY

Name(s)

Tian Chen; Frederick Nitta

Project Number

S0608

Project Title

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

Abstract

Objectives/Goals

By utilizing the plane-wave function of Density functional Theory, we performed relaxation calculations to investigate electronic and spintronics potential of Fe, Co, Ni, Pt atoms+dimers+combinations embedded graphene.

Methods/Materials

We used Quantum Espresso for all calculations; it is an open-source software that utilizes Density Functional Theory to study solid state systems. When given the necessary parameters in the input files for our various configurations, the software calculates charge density, band structure, density of states, etc. We also used Visual Molecular Dynamics, a molecular visualization software, to understand the geometric properties.

Results

Analyzing single atom complexes, we found Co-C30 had the lowest embedding energy, thus the most stable, followed by Fe-C30, Ni-C30, Pt-C30. The geometric data did not fully support the results of the embedding energy data. For the single metal, the geometric data showed that Fe-C30 or Pt-C30 had the longest metal-carbon bond, followed by Co-C30 and Ni-C30. Both double metal complexes had higher embedding energies than the single metal configurations, therefore, less stable. The diagonal configurations have lower embedding energies than the side configurations, so they would more stable and are better for applying it in spintronic data storage devices.

Magnetization data show that Co and Fe embedded in graphene have potential for spintronic data storage, because of its magnetization localized on the metal atom. However, 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.

Conclusions/Discussion

Graphene complexes embedded with Co and Fe show high potential for spintronic data storage, while Ni and Pt shows little promise. In the future, we will analyze band structures to further understand the magnetization properties of the material. More configurations with metals of similar periodic properties will be experimented to examine its properties.

Summary Statement

By utilizing the plane wave function of Density functional Theory, we performed relaxation calculations to investigate electronic and spintronics potential of Fe, Co, Ni, Pt atoms+dimers+combinations embedded graphene.

Help Received

We developed the idea of the project, and consulted Mr. Harman Johll of Singapore National Junior College to guide us through the theoretical nuances of Density Functional Theory and provide helpful tips when using Quantum Espresso. We were mentored by Dr. Glenn McGee of Palo Alto Unified School