The Effects of Single Vacancy Defects and Lithium on Single-Walled Carbon Nanotubes
Ross Kistler, Loyola University Maryland, 2011 SURF Fellow
Advisor: Prof. Dr. Seung Soon Jang  Graduate Mentor: Dr. Wonsang Koh

Introduction
Carbon nanotubes have been a subject of great interest in the recent years. This is because carbon nanotubes have immense potential in the field of nanotechnology due to their electronic and mechanical properties. One topic being explored is the adsorption of Li atoms on the surface of a single-walled carbon nanotube (SWCNT). The goal of this project is to determine the effects of doping a SWCNT with a single vacancy with a Li atom.

Procedure
First, DMol3 was used to create a simulation of a (5,5) SWCNT. A single C atom was removed from the structure, creating a defect known as a single vacancy. Geometric optimization, which uses quantum mechanics, was used to determine how the SWCNT restructures itself to compensate for the loss of the C atom. Next, the centroid feature is used to determine the x and y coordinates of the centroid of the CNT. By applying the z coordinate of the single vacancy to the (x,y) coordinates, the (x,y,z) coordinates describe the centroid closest that minimizes the distance between it and the single vacancy. With this centroid set as the origin and the coordinates of the single vacancy, the two points create a line that determines positions to set the Li atoms along. Because the z coordinate is the same as that of the centroid, there line is defined by x and y components. After positioning the Li atoms and using DMol3 to calculate the total energy of the CNT w/Single Vacancy and Li atom system, we can use the below equation to calculate the Adsorption Energy of the Li atom:

$$\Delta E = E[\text{Li+CNT w/vac}] - (E[\text{CNT w/defect}] + E[\text{Li}])$$

$$= E[\text{Li+CNT w/vac}] - (-2246.354356 \text{ Ha} - 7.458136 \text{ Ha})$$

By plotting the distance between the centroid of the CNT and the Li atom vs the adsorption energy of the Li atom, it was possible to determine the locations at which adsorption was minimized. By performing geometric optimizations upon these structures, the simulation determines what position is ideal for the Li atom. Moreover, the structures these geometric optimizations produce can be used to calculate Band Structures and Density of States.

Results and Discussion
The plot of Distance vs Adsorption energy, displayed in Figure 1, contains two relative minima that minimize adsorption energy. The Li atom has two minima in adsorption energy on both the interior and exterior of the CNT, at a distance 2.036 and 5.036 Angstroms from the center. DMol3 is then used to calculate and analyze the band structures and density of states of the structures. The subsequent geometric optimizations and band structures derived from these optimizations indicated that the CNTs w/Li retain metallic properties, as evidence by the very small band gaps in Figure 2.

Conclusions
The structures obtain through my project are viable for future use, and simulations indicate that doping CNT with Li lowers the adsorption energy and the total energy of the system as a whole. Furthermore, the CNT structures can still be classified as metallic materials.

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References