Lithium Doping of Single-Walled Carbon Nanotubes for Battery and Semiconductor Applications

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Abstract

The properties of lithium doped (5,5) metallic and (8,0) semiconducting carbon nanotubes are investigated using density functional theory. This is used to determine how lithium binds to carbon nanotubes and how this affects the band structure of the semiconducting carbon nanotube.

Introduction

When placed near carbon structures, lithium atoms perform charge transfer and bind. This process forms the basis of the graphite anode used in lithium-ion batteries. However, current lithium-ion batteries are limited by the formation of an oxidation layer over the anode, increasing the internal resistance over time and the fact that lithium must bond to at least six carbon atoms, a detriment to miniaturization. By replacing the graphite in the anode with metallic single-walled carbon nanotubes (CNTs), the growth of the oxidation layer is greatly retarded and the number of carbon atoms required is reduced.

In addition, the alteration of the Fermi level by the charge transfer alters the band structure of semiconducting CNTs. By doping the CNT with a select amount of lithium, it is possible to control the band structure to produce novel semiconductor materials. Using density functional theory (DFT), models of metallic and semiconducting CNTs were constructed and used to predict the properties of the systems.

Procedure

All calculations were conducted using generalized gradient approximation (GGA) with a Perdew-Burke-Ernzerhof (PBE) functional and double numerical and double numerical with polarization (DND) basis set. A (5,5) metallic CNT and an (8,0) semiconducting CNT were optimized using k-point sampling of 2x2x8. The metallic CNT used lattice parameters of 35.000 by 35.000 by 9.866 Å and the semiconducting CNT used lattice parameters of 35.000 by 35.000 by 8.535 Å. A lithium atom was placed at several distances from the center of the nanotube in the top, center, axial bridge, and zig-zag bridge positions. Specific point energy (SPE) measurements were taken to determine the total energy of the system using k-point sampling of 2x2x16.

The semiconducting CNT was then optimized with one lithium atom and two lithium atoms, both in the center position. In the two lithium system the lithium atoms were on opposite sides of the CNT. Both systems were optimized using gamma point sampling and had the band structure, density of states, electron density, and population analysis calculated using k-point sampling of 2x2x8.

Results and Conclusions

The SPE measurements were used to calculate the binding energy of the system. Binding energy was calculated with respect to the molecules at an infinite distance apart. Figure 1 shows the binding energies of the metallic and semiconducting CNTs. In both cases, the center position is the most stable.

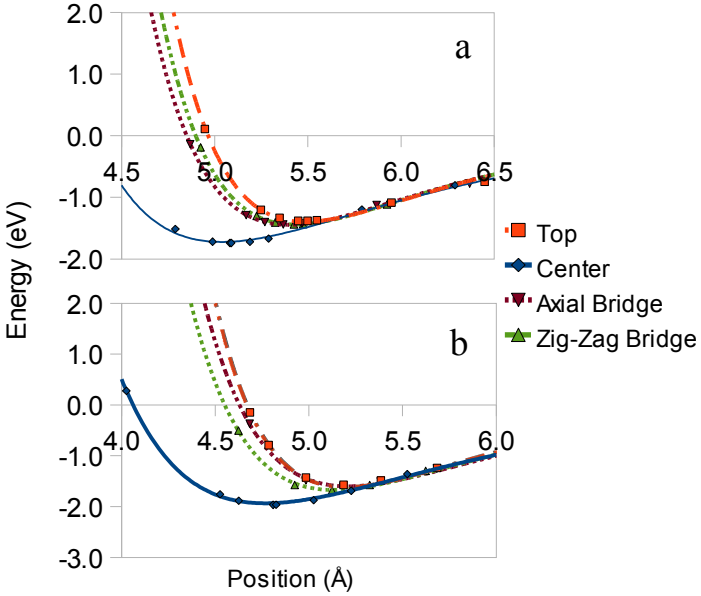

Figure 1: *Binding energy of a lithium atom with (a) a (5,5) CNT, and (b) an (8,0) CNT*

The original semiconducting CNT has a band gap of .599 eV. The one lithium system has a band gap of .517 eV, and the two lithium system does not have a band gap. This is shown by the band structures in Figure 2. This suggests that the band gap can be controlled through lithium doping.

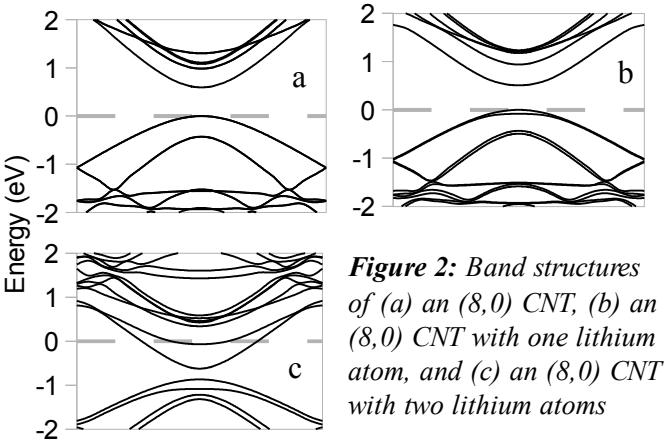

Figure 2: *Band structures of (a) an (8,0) CNT, (b) an (8,0) CNT with one lithium atom, and (c) an (8,0) CNT with two lithium atoms*

References

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