Predicting HOMO and LUMO Energy Gaps for Organic Semi-Conductor: A Theoretical Study

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Abstract

This poster presents a theoretical approach for characterizing the electronic properties of novel electron-deficient organic semiconductors containing variety of electron donor substituents. In treating these compounds, the following questions will be addressed:

- What effects do the substituents have on the bandgap?
- Will any of the substituents lower the bandgap to the desired range for solar cell applications (<2.0 eV)?
- Can we use the current, inexpensive and tractable computational methods as a predictive tool for guiding future experimental design of organic based solar cells, rather than depending solely on experimental procedures?

Introduction

Global warming is becoming one of the most serious problems of our generation. The average temperature of the Earth’s surface, air, and oceans is increasing as a result of an increased concentration of carbon dioxide and other greenhouse gases. Solar cells are devices that capture sunlight and convert this radiant energy into electricity. Unlike fossil fuels which release carbon dioxide and greenhouse gases into the atmosphere, solar power is clean, renewable, and sustainable, helping to protect our environment. Currently, inorganic semiconductor based solar cells are prevalent in the market place. These devices are typically both expensive and rigid. Conversely, organic molecules offer a cheaper and more flexible alternative for solar cell applications. Organic based solar cells can be created using strategic molecular design processes. One of the critical aspects for achieving high power conversion efficiency is to enhance light harvesting. To support effective light harvesting, molecules are required to have the small bandgaps (<2.0 eV). Computationally, the bandgap is defined as the difference between the HOMO (highest occupied molecular orbital) and LUMO (lowest unoccupied molecular orbital).

Results

HOMO and LUMO energies can be calculated using Density Functional Theory (B3LYP) coupled with modified basis sets 6-31G* and 6-31+G*. The target molecule (Figure 1) and (Figure 2) are generated using the Spartan electronic structure program. This program is used to visualize molecules as well as perform low-end calculations. In this study, HOMO, LUMO, and bandgap on an electron deficiency main core with various strong electron donating substituents such as benzene, thiophene, benzothiophene, dibenzothiophene, carbazole, and fluorene (Figure 2) will be calculated to assess which substituent will give the lowest possible bandgap. We will also ascertain whether computational results can predict experimentally observed trends (when experimental results are available).

Conclusions

Our ultimate goal is to understand how, electron-rich substituted on an electron deficiency main core affect electronic properties such as bandgap, HOMO, and LUMO values. After attaining the projected values of both the closed ring and open ring systems, we have seen that both systems follow the same general trend. The compounds thiophene and carbazole, in both systems, have the best values indicated by their low eV Fluorine, in the open ring system however, also has a lower eV so we are still investigating if its values are consistent. It is also worth noting, that all attained values are overestimated by 0.2 - 0.3 eV, so in an actual experimental procedure these values are expected to drop.

Future Plan

Since my passion and interest is in chemistry, I will continue to give my dedication to this project and attain the actual experimental values to further prove my thesis.

Reference

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