Optimizing Photovoltaic Molecules For Use as an Energy Source

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Why Photovoltaic Organic Molecules?

Photovoltaic organic molecules can harvest energy from the sun and turn it into electrical energy. These molecules have potential in solar panels as they are cheaper/easier to produce.

The Photovoltaic Molecule

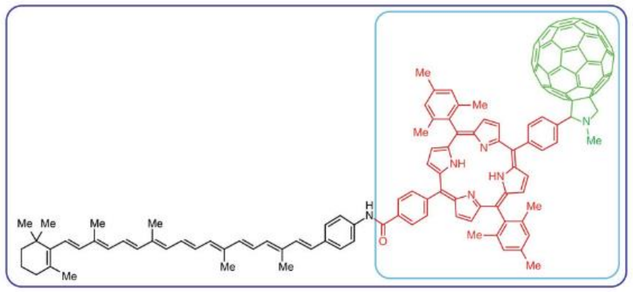
The Carotene-Porphyrin-Fullerene system consists of a polymer (carotene), a chromophore (porphyrin), and a buckyball (fullerene). The chromophore absorbs light and produces a charge pair (e^- and h^+). The polymer accepts the h+ and the buckyball collects the e^-, resulting in energy production.

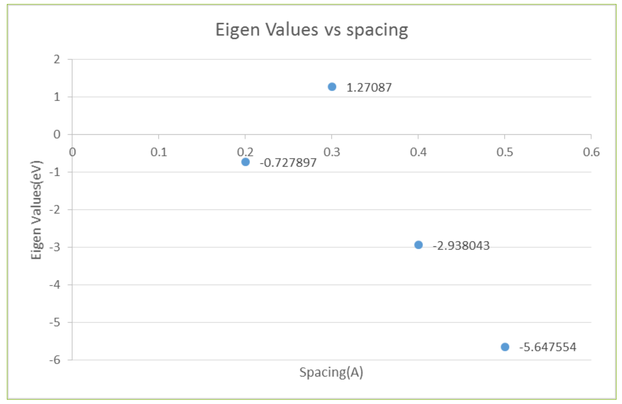
Optimizing Charge Transfer

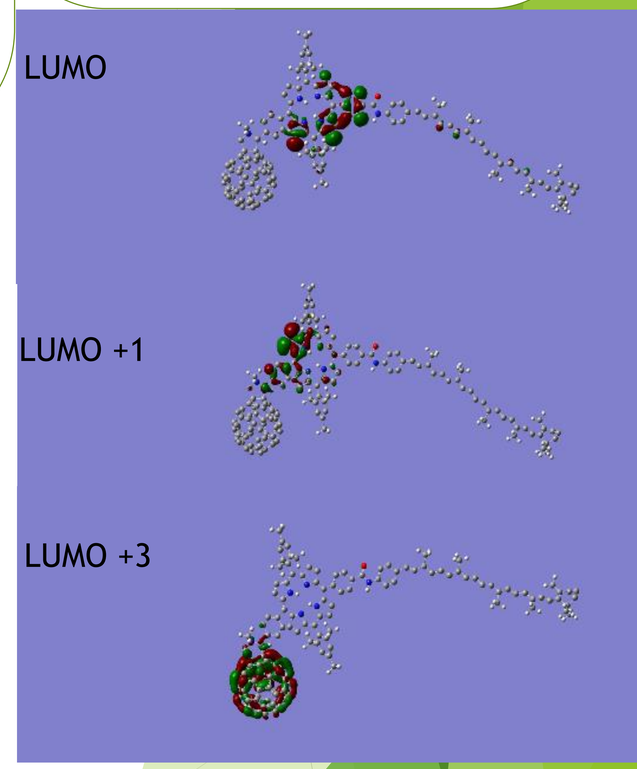
We modeled the Carotene-Porphyrin-Fullerene system in three steps: 1) Compute atom positions of the molecule using molecular dynamics[1], 2) Find the energy levels from quantum mechanics[2], and 3) calculate properties using time-dependent quantum mechanics[3]. We want to see what parameters allow for the optimal charge transfer once the chromophore collects sun light.

DFT: Molecular Orbitals

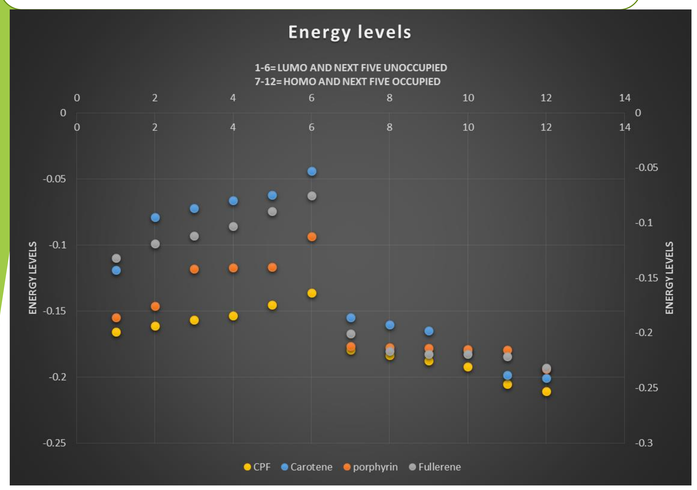
Using DFT, We found the electron density at various molecular orbitals of the molecule. Modeling where the charge would be located once the molecule is energized by the sun.







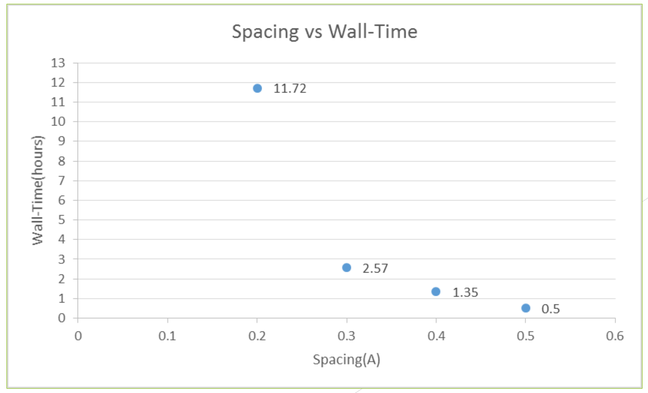
Energy levels according to Density Functional Theory



Time Dependent Calculations

Used the program Octopus to calculate the electron densities over time using a Time Dependent Density functional Theory (TDDFT)

Currently finding the appropriate spacing and wall time for final calculations.



Future Research

We plan on performing more TD-DFT calculations on CPF-like molecules. We will repeat this approach on other chromophore/polymer combinations. The goal is to find the system with the best charge transfer rate.

References

Rozzi, Carlo Andrea et al. "Quantum coherence controls the charge separation in a prototypical artificial light-harvesting system." nature communications 4.1602 (2013): 1-7. Print

http://laschoolreport.com/la-unified-close-to-completing-solar-power-systems/

Cowboy Cluster (HPCC)

Avogadro program[1] Marcus D Hanwell, Donald E Curtis, David C Lonie, Tim Vandermeersch, Eva Zurek and Geoffrey R Hutchison; "Avogadro: An advanced semantic chemical editor, visualization, and analysis platform" *Journal of Cheminformatics* **2012**, 4:17.

GaussView 5.0[2] GaussView, **Version 5**, Roy Dennington, Todd Keith, and John Millam, *Semichem Inc.*, Shawnee Mission, KS, 2009.

Octopus program[3] A. Castro, H. Appel, Micael Oliveira, C.A. Rozzi, X. Andrade, F. Lorenzen, M.A.L. Marques, E.K.U. Gross, and A. Rubio, *octopus: a tool for the application of time-dependent density functional theory*, Phys. Stat. Sol. B **243** 2465-2488 (2006)