UCA Department of Chemistry Seminar

February 7, 2014 2 pm Laney 104

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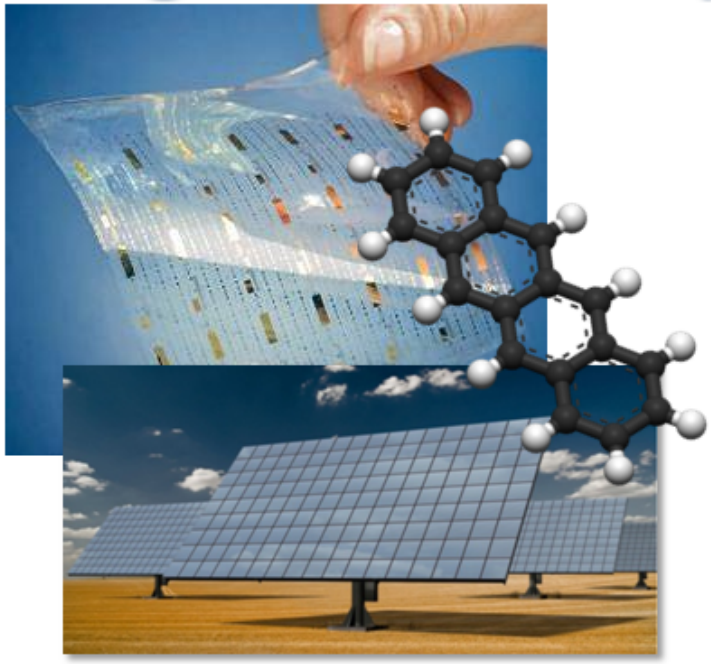

Understanding The Charge-transport Parameters In Organic Semiconductors

Presently, nearly 85% of the world's current 13-15 TW in total energy use comes from the combustion of fossil fuels. This global demand is expected to double by 2050 – potentially at a terrible cost to the environment; however, with ~ 1.2 X 10^5 TW of solar energy available at the Earth's surface, the development of efficient photovoltaic devices can provide a crucial renewable energy source.

Photovoltaic devices produced from inorganic semiconductor materials offer relatively large power conversion efficiencies; however, with a high production cost. If solar panels are to become viable as a major energy source, production costs have to be reduced, which requires innovative materials design.

Organic semiconductors can be manufactured at a lower cost, but at a lower efficiency than the current silicon-based solar panels. The performance of organic photovoltaic devices is integrally connected to the mobility of the charge carriers generated in the organic semiconductor, i.e., the rate with which the charge-carriers move through the π-conjugated materials. Charge-carrier mobilities in organic photovoltaic semiconductors (at best around 10 $cm^2V^{-1}s^{-1}$) are orders of magnitude smaller than that of crystalline silicon – a consequence of the localized nature of the charge carriers.

The electronic coupling (or transfer integral) and the reorganization energy are two key parameters that determine the rate of charge transfer, and therefore the overall charge mobility, in organic semiconductors. This work deals with the role of polarization and relaxation on the structures and energies of cluster anions of naphthalene, anthracene, and tetracene that have been experimentally investigated via photoelectron (PE) spectroscopy. The PE spectra for naphthalene clusters indicate a combination of localized and delocalized charged states. Therefore, we investigate the impact of polarization on the energies of electron charge carriers with a hybrid quantum-mechanics/molecular mechanics (QM/MM) approach. With an understanding of these structures as a bottom-up approach to understanding polarization and charge (de)localization in prototypical organic semiconductors, we then derive a connection between the electronic coupling (key to large mobilities) and non-covalent interactions present in organic semiconducting devices. Recent advances in understanding the effect of these non-covalent interactions on the charge carrier traps present in organic semiconductor devices will also be discussed.

Lunch provided for students with the seminar speaker from 12:00 – 1:15 pm in Laney Hall Rm 105.
Contact P. Desrochers (patrickd@uca.edu) for more information.