Seminar

Wednesday, September 20, 2017

11:00 AM – 206 Furnas Hall

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Regent's Professor

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Organic solar cells:

Characterization of interfacial charge-separation and charge-recombination processes

In this presentation, we will first introduce the working principles of organic solar cells and rationalize the need for the presence of both an electron-donor component (usually a conjugated polymer or oligomer) and an electron-acceptor component (often a fullerene derivative).

We will then discuss the impact that inter-molecular arrangements and interactions at the donor/acceptor (polymer/fullerene) interfaces have on the performance of bulk-heterojunction solar cells. We will describe the results of combined electronic-structure calculations and molecular-dynamics simulations. In particular, we will examine:

(i) the propensity of fullerene molecules to dock preferentially on top of the electron-poor moiety or electron-rich moiety of the polymer, as a function of the nature and location of the polymer side chains;

(ii) the impact that the packing arrangements have on the energetic distribution of the charge-transfer interfacial electronic states and their localization/ delocalization characteristics; and

(iii) the influence of molecular packing and electronic delocalization on non-radiative recombination processes.
We will end with a discussion of the prospects of the field of organic solar cells.

This work is supported by ONR (Award N00014-14-1-0580 for the Center for Advanced Organic Photovoltaics and Award N00014-17-1-2208).

Refreshments at 10:45

University at Buffalo
Department of Chemical and Biological Engineering
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