Organic Assemblies

Lightweight and flexible, cheap, environmentally-benign, and strongly absorbing, organic assemblies are promising for next-generation energy conversion applications. However, many organic-based solar energy conversion devices suffer from low efficiency and degradation. Improvement in either area relies on understanding the fundamental properties of these materials and hybrid interfaces with other organics (e.g. donor-acceptor) and inorganics (e.g. metal contact or photoabsorbing semiconductor catalyst). But that understanding is hindered by the challenges in characterizing the electronic structure of organic materials, both experimentally and theoretically, at nanometer length scales.

In ongoing work, we are applying many-body perturbation theory to compute structure and low-energy optical excitations for archetypal organic semiconductors pentacene (PEN), perfluoropentacene (PFP), and their composite donor-acceptor assemblies. We are extending existing methods to incorporate Stokes lattice couplings, finite-temperature effects and disorder, with the goal of exploring their significance on the nature and energetics of the excited state. This work will provide a foundation for long-term, time-dependent studies of exciton transport, with the aim of connecting with high-resolution near-field probe techniques and ultrafast time-resolved spectroscopy.

Open-Circuit Voltage of Organic Photovoltaics
Alison Hatt posted on Apr 04, 2012
Optimizing open-circuit voltage (Voc) remains a significant challenge for organic photovoltaics (OPV). In OPVs, where small molecules or polymers comprise donor and acceptor, Voc depends largely on atomic-level details of the donor-acceptor interface. This dependence is not well understood, however, because interfacial energetics are extremely challenging to probe experimentally.

To address this problem, we use a parameter-free density functional theory-based method to get quantitative insight into the electronic structure and morphology of OPV donor-acceptor interfaces.

Optical properties of pentacene and PTCDA
Alison Hatt posted on Mar 29, 2012
As prototypical organic systems, pentacene and PTCDA are central to the growing field of molecular-scale science, yet their electronic and optical properties are not well understood. Applying the tools of many-body perturbation theory to these systems, we study charge transport and optical absorption, and probe the nature of optically generated excitons.

Related Publications

Robert F Berger posted on Jun 24, 2013

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