

Introduction to OPV Materials, Mechanisms, and Devices

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Organic photovoltaic (OPV) and related approaches to solar energy harvesting are being intensely pursued at universities, national laboratories, and corporations around the globe. The long term goal of OPV research is to enable low-cost, high-throughput fabrication of photovoltaic modules on scales that are large enough to truly impact the world's energy supply lines. Encouraging advances in the efficiency of laboratory-scale devices have been made in the last several years, with multiple labs reporting certified AM1.5 power conversion efficiencies above 7%. This has in turn encouraged research into practical issues such as understanding the degradation mechanisms in the devices in order to increase their operational lifetime and developing fabrication strategies that are suitably robust for large-scale fabrication with minimal loss in efficiency compared to laboratory-scale procedures. Ultimately, OPV, as with all other approaches to photovoltaics, will be measured on an economic scale with the Levelized Cost of Electricity (LCOE) that it can achieve.

This talk provides an overview of the fundamental aspects of OPV materials and devices (Fig. 1), focussing largely on the polymer-fullerene blend, bulk heterojunction (BHJ) motif but also briefly addressing the small molecule approach. Of prime importance to the operation of an OPV device is the creation of meta-stable, charge separated states through ultrafast, photo-induced absorption between donor and acceptor molecules. This topic is discussed in the context of what properties of the donor-acceptor pair are needed for the metastable state, and what role ground state charge transfer plays in the process. Another critical issue in OPV is that of molecular morphology. How molecules or polymers are aligned or folded onto each other plays a central role in determining excitonic and charge transport properties in an organic semiconductor. Here the role of molecular ordering on charge carrier mobility and recombination is discussed.

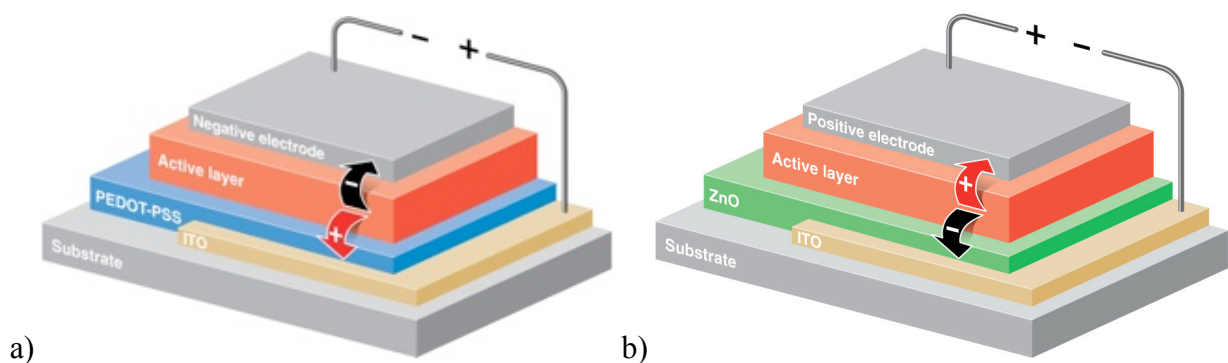


Figure 1. Geometry of typical OPV devices with a) “normal” geometry with a negative back/top electrode and b) “inverted” geometry with a positive back/top electrode.

An important part of the recent developments in OPV device efficiencies has been the progress made in designing and synthesizing low band gap polymers that absorb a more significant portion of the solar spectrum than was the case for earlier generations of polymers. Here the structure property relationship of pi-conjugated polymer is examined, and pathways to tuning the band gap are highlighted. As shown in Fig. 1, the use of computational chemistry techniques for calculating optical and electronic properties of molecules is briefly illustrated.

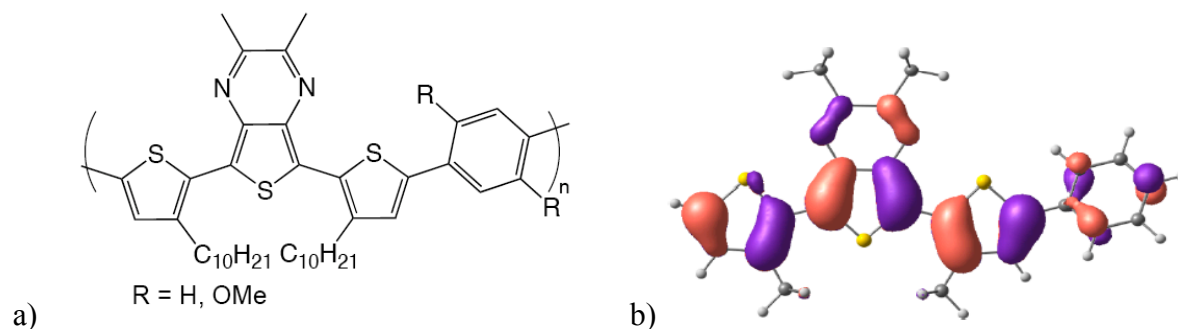


Figure 2. a) Molecular structure of an example low band gap polymer and b) the spatial distribution of its HOMO as calculated by density functional theory.

General principles of the operational physics of the devices, such as the origin of the V_{OC} and the band structure in the devices are discussed here. The simple band offset picture between donor and acceptor is being replaced in the community with more sophisticated models that take into account ground state interactions and carrier recombination. These are touched upon here. Also, a basic simulation of the JV characteristics of devices is presented and used to illustrate the effect of various parameters such as carrier mobilities, recombination rates, and doping densities on the device behavior. Lastly, pathways to achieving higher efficiencies are presented, and a synopsis of what is happening currently in the OPV industry is given.