Molecular Solar Cells Progress Report

Investigators
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Abstract
We have made progress toward organic solar cell device architectures that allow high efficiency solar cells to be built with organic materials despite the shortcomings of these materials. The device architecture makes use of a newly developed transparent electrode that is low-cost and laminatable. Progress was also made in the understanding of the physics of organic solar cells using low-temperature electrical measurements. These results indicate that high electric fields are necessary at most donor-acceptor interfaces.

Introduction
Organic solar cells are attractive because of their potential for very low-cost photovoltaics. Despite their promise, the efficiency of organic solar cells is still too low for applications. We are developing device architectures that overcome the fundamental limits of organic materials to reach power conversion efficiencies >10%.

An important reason for the low efficiencies of organic solar cells is our limited understanding of the physics that governs these devices. Unlike in inorganic solar cells, electrons and holes in organic semiconductors are strongly attracted to each other, leading to strong exciton binding energies (which necessitates the use of donor-acceptor junctions) and strong correlated motion between electrons and holes even after the excitons are dissociated, which leads to recombination. Using low-temperature current and capacitance measurements aided by computer modeling, we are building a detailed picture of the physics of organic solar cells on the relevant nanometer length scale.

Background
Progress is being made in the field of organic solar cells in terms of ensuring that the right nanostructures are formed to optimize efficiency and to tune the energy gaps of the materials. We are focused on making sure that these advances can be used to make more efficient solar cells by developing new device architectures that make use of these advances.

Results
Cost-Efficiency Analysis for Organic Solar Cells
In order for organic solar cells to be competitive with fossil fuel-based power generation and other photovoltaic technologies, it is important that their cost per square meter is sufficiently low. It is however also important to ensure a sufficiently high efficiency. We performed an analysis that calculates the cost per kWh produced using a solar cell technology for a large installation (1GWp), based on model developed by K. Zweibel [1]. Figure 1 shows the results of this analysis.
For a lifetime reasonable for organic photovoltaics (10 years), a module cost <$20/m² is required in order to produce electricity at a cost competitive with fossil fuel-based power. For efficiencies of 15%, the tolerable module cost can be as high as ~$40/m². This illustrates the importance of achieving high power conversion efficiencies. For a cost of $30/m², which many researchers believe is achievable with organic photovoltaics, a module efficiency of 13% is required to produce electrical power at 9.3c/kWh.

New Multijunction Device Architectures are Required

To achieve efficiencies of 13% on the module level, slightly higher efficiencies would have to be achieved in the lab. Multijunction architectures have been the major idea that is thought to allow organic solar cells to reach efficiencies >15%. However, due to the requirement that in a multijunction cell architecture the different junctions need to produce the same photocurrent and have distinct spectral absorption, multijunction cells with real materials are limited in efficiency. An analysis of a realistic 3-junction stack is shown in Fig. 2.

**Figure 1**: Levelized cost of electrical power from a 1GWp photovoltaic installation with a projected lifetime of 10 years (appropriate for organic photovoltaics).
Figure 2: Absorption characteristics of a 3-cell multijunction stack using organic semiconductors.

The power conversion efficiency of this stack (assumptions: internal quantum efficiency of 85%, fill factor of 65%, AM1.5G illumination) is 11.2%. This is only a fraction higher than the 8% efficiency limit achieved for a single junction organic solar cell, despite the use of three separate junctions.

A better approach is to use a multijunction architecture in which the cells are independently accessible rather than series-connected, as shown in Fig. 3. This architecture, despite using only two cells, has a realistic power conversion efficiency of 12.3%, close to what is needed.

Figure 3: Independently contacted multijunction cell with 2 cells.
Independent Tandem Cells with Laminatable Transparent Electrodes

In order to build the proposed independent tandem cells, several instances of conductive, transparent electrodes are required. These electrodes must not only be cheap (given that the overall module cost must be <$30/m² and because several instances of the transparent electrode must be used), but must also be deposited without damaging the underlying organic solar cells. For this purpose, we developed a laminatable electrode based on our earlier work on Ag nanowire transparent electrodes [2]. The lamination process is illustrated in Fig. 4.

![Figure 4: Schematic illustration of the Ag nanowire transparent electrode lamination process.](image)

Using the lamination process, we have demonstrated several types of tandem cells. A tandem cell that combines a polymer solar cell with a small molecular solar cell is shown in Fig. 5. This tandem cell employs a laminated transparent conductor between the two cells to eliminate the need for current matching.

![Figure 5: Characteristics of a 3-terminal organic multijunction cell.](image)
Our current work focuses on improving the efficiency of this type of cell towards world-record numbers by tuning of the top and bottom cell in the stack.

*Improved Understanding of the Physics of Molecular Solar Cells: Importance of Electrical Doping*

We have previously shown that electrical doping is essential for the operation of small-molecular weight bilayer solar cells. We suspect this is universally the case unless energy level gradients are present on the nanoscale to help separate electrons and holes. We have recently obtained further evidence of the importance of doping using low-temperature capacitance-voltage measurements on the archetypal CuPc/PTCBI molecular system.

Capacitance-voltage measurements can be used to estimate the doping concentration in a pn-junction. The concentration of free carriers can then be plotted as a function of temperature to estimate the doping density (number of donors or acceptors) and depth of the doping level (how much energy does it take to ionize the dopant). Figure 6 shows the results for CuPc/PTCBI bilayer solar cells. The doping density is estimated to be $4 \times 10^{17}$ cm$^{-3}$ and the doping level is 0.27 eV below/above the transport level.

![Figure 6: Analysis of electrical doping using the temperature-dependent capacitance-voltage method.](image)

These results can then be used to model the shape of the photocurrent vs voltage curves. At lower temperatures, the free carriers freeze out on their dopant sites, resulting in a reduced electric field at the interface which in turn leads to poorer electron-hole pair separation. This is indeed seen at low temperatures and this effect can be modeled accurately using Monte-Carlo carrier separation models that use the electric field (from capacitance-voltage measurements) as input. The agreement between measurements and our models are shown in Fig. 7.
Figure 7: Agreement between experiment (lines) and theory (open squares) as a function of temperature. The electric field determined via capacitance-voltage measurements and charge-separation model result in an accurate prediction of the shape of the photocurrent vs voltage curves.

Progress
The development of the multi-terminal multijunction architecture using laminated Ag nanowire transparent electrodes opens a path toward achieving record cell efficiencies, which will be the focus of our research program going forward. If we succeed in demonstrating record efficiencies, we will have propelled the organic solar field toward becoming a real technology with a potential for impacting how we generate our power. The improved understanding of the physics of organic solar cells and the role that is played by geminate recombination will help us pick and design materials.

Future Plans
Our future work will focus on demonstrating record efficiencies with the multi-terminal (or independent) multijunction cells. Since photocurrents do not need to be matched, higher conversion efficiencies can be reached using this approach.

Publications

References
1. NRELTechnical Report NREL/TP-520-38350

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