

# Molecular Solar Cells Progress Report

## Investigators

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## Summary

We have made progress in the understanding of small molecular weight organic solar cells and have identified geminate carrier separation as a key limiter to the efficiency of nanostructured organic solar cells. Our models, supported by experimental data, show that this efficiency bottleneck can be removed by carefully engineering the energy landscape for charge carriers on a nanometer length scale.

We have also made progress in ensuring that light that is incident on an organic solar cell is absorbed, despite the cells being thin. This is achieved through three novel light trapping techniques that are particularly effective for thin-film solar cells: V-shaped substrates, coherent light trapping using broadband cavities and grating coupled structures. We have shown that the upper limits of each of these approaches are equal to the thermodynamic limit of any light trapping approach.

We expanded on our research in transparent electrodes and have demonstrated organic solar cells with graphene electrodes in a collaboration with Prof. Zhenan Bao.

Finally, we have determined a practical upper limit for the efficiency of multijunction organic solar cells, including optical interference effects and the non-idealities of organic solar cells. For a triple-junction stack, we find that power conversion efficiencies of 23% are achievable. We have also shown an improved method to make such multijunction stacks based on metal nanowire electrodes developed in part under another GCEP project (Nanostructured Metal-Organic Composite Solar Cells, PI: Brongersma, co-PIs: Fan and Peumans). This approach removes the limitation that the photocurrent of each cell must be matched, greatly increasing our options to design and demonstrate more efficient multijunction organic solar cells.

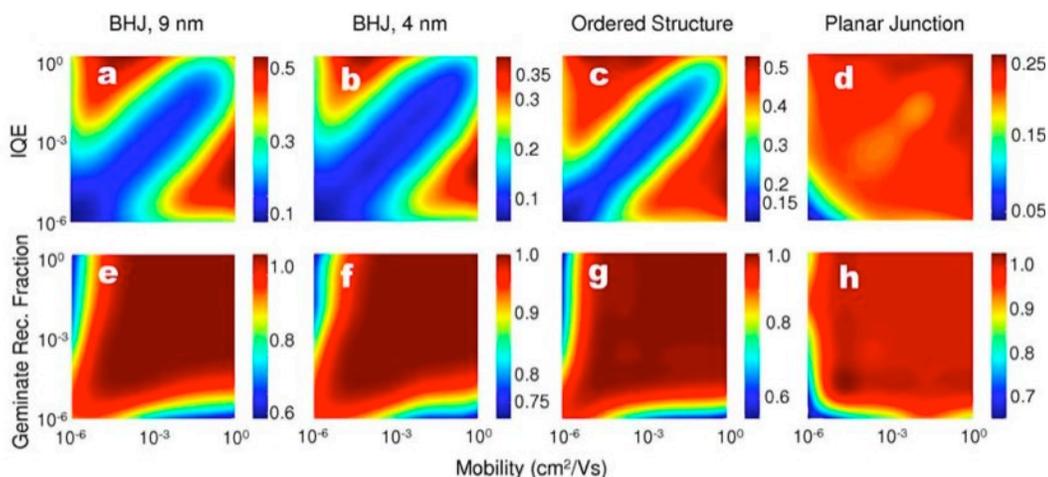
## Results

### A. New insight into geminate carrier recombination as an efficiency limited in nanostructured organic solar cells

We finalized an organic solar cell modeling tool that simulates the full dynamics of charge carriers in organic solar cells in nanostructured geometries. This is a major advantage over other modeling approach that use mean properties and ignore the nanostructured nature of organic solar cells. An important consequence of this work

is that we understand why many materials don't work efficiently when combined into a nanostructured organic solar cell (see **Fig. 1**). The basic reason is the strong Coulomb attraction between electrons and holes that prevents the carrier pairs from separating, especially in the presence of convoluted interfaces.

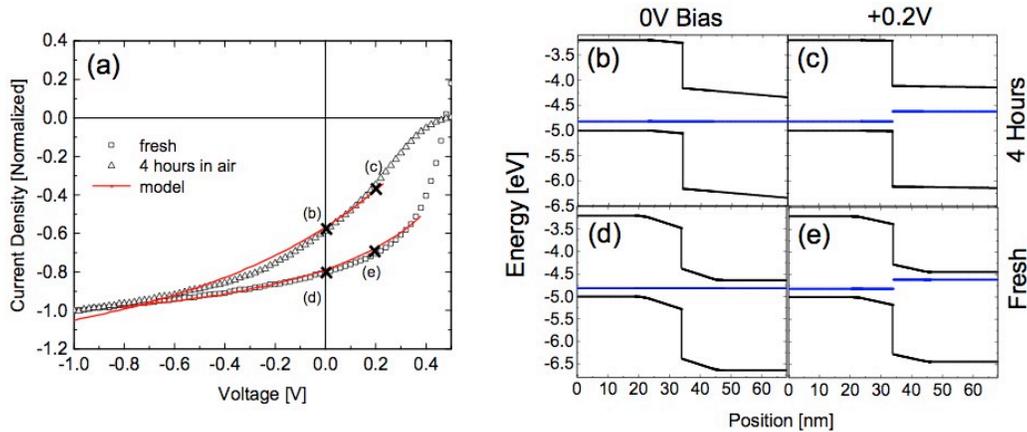
The work also indicates why fullerene acceptors (e.g. CuPc/C60, P3HT/PCBM) work well in random nanostructured solar cells. The fullerene acceptor's high polarizability funnels the electron into the bulk of the fullerene so that it is no longer available for recombination. When this effect is included, our models predict device performance accurately.



**Fig. 1.** Modeled internal quantum efficiency and fraction of electron-hole pairs that recombines before separating.

Based on the above analysis, establishing a strong electric field at the donor-acceptor interface in organic solar cells, is important. We profiled the electric field present in efficient organic cells and found that all efficient cells exhibit high fields because of unintentional electrical doping. This doping is present as an artifact of the synthesis process and can in many cases not be removed from the source material. This new insight explains a number of observations in the literature.

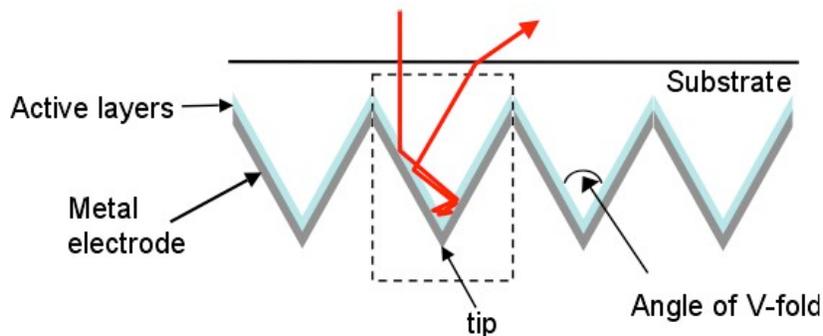
We discovered cases where the electrical doping can be removed by careful purification or exposure of the devices to air (which selectively deactivates the dopants), yielding further insight into what happens when doping is absent. As shown in **Fig. 2a**, the device that lacks doping (labeled 4hrs in air) exhibits a shifted IV curve and a lower power conversion efficiency. CV profiling was used to extract the band diagrams shown in **Fig. 2b-e**, showing weaker electric fields in the undoped case.



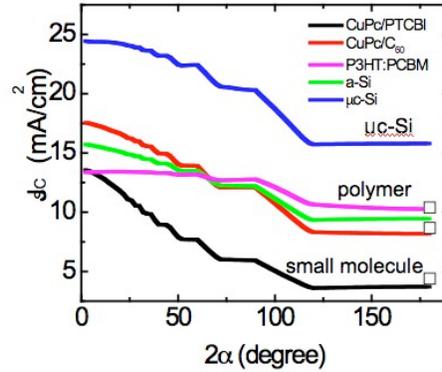
**Fig. 2.** Effect of electrical doping on the IV curves and band diagrams of organic donor-acceptor bilayer solar cells.

## B. Novel light trapping schemes for thin-film organic solar cells

We developed a light trapping approach that is particularly effective for thin-film solar cells such as organic and amorphous silicon solar cells in a collaboration with Prof. Mike McGehee. The approach uses a V-shaped substrate and multiple reflections in the V-shape to enhance the photocurrent. This method is more effective than textured surfaces for thin-film cells. The essential feature is that the film thickness is substantially smaller than the size of the V-shape, as shown in **Fig. 3**. The efficacy of this approach was analyzed theoretically for a number of thin-film solar cells (organic and inorganic) as shown in **Fig. 4**. An experimental demonstration using the polymer system P3HT/PCBM yielded a 52% improvement in efficiency.

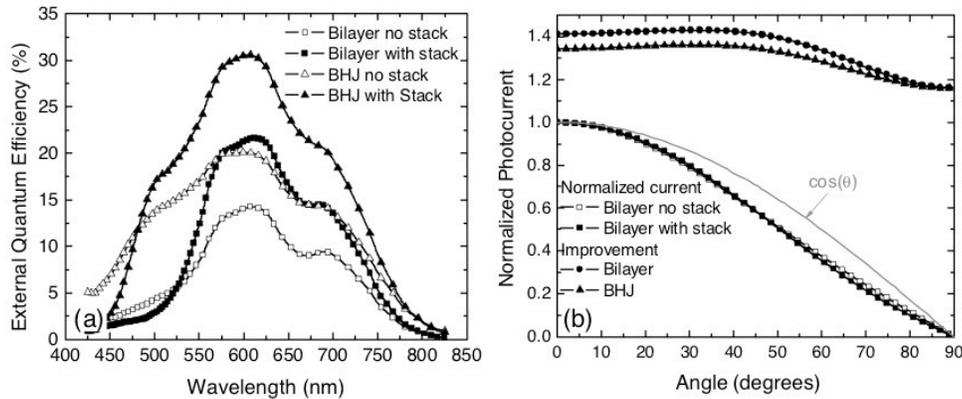


**Fig. 3.** Principle of the V-shaped light trap that is particularly effective for thin-film solar cells.



**Fig. 4.** Photocurrent as a function of the angle of the V-shape for 3 types of organic solar cells, an typical amorphous silicon solar cell and a microcrystalline silicon solar cell.

A second light trapping scheme that was investigated consists of a specialized coating that functions as an antireflection coating and cavity mirror at the same time. At wavelengths where the solar cell absorbs strongly, the coating behaves as a traditional antireflection coating. At wavelengths where the solar cell is only weakly absorbing, on the other hand, the coating is reflective to function as a cavity with enhanced absorption. The challenge is to design such a coating with the correct phase behavior, ensuring enhancement in absorption over the maximum possible spectral range. For a practical device structure, we were able to show that a custom coating can increase the power conversion efficiency by 40%, as shown in **Fig. 5**.



**Fig. 5.** (a) External quantum efficiency for a bilayer and bulk heterojunction device with and without custom coating (stack), (b) Angular dependence of the photocurrent showing that the enhancement is uniform for angles up to 50 degrees from normal.

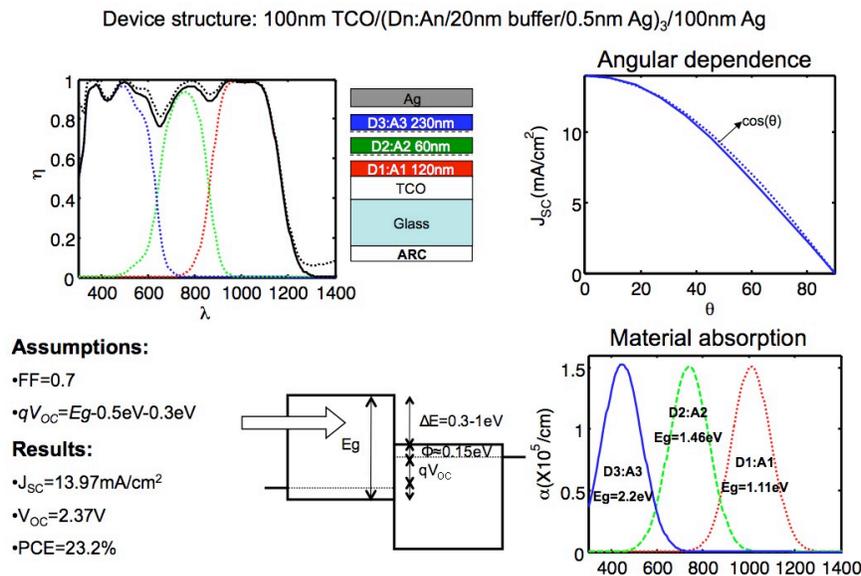
Finally, a third light trapping scheme was explored in which light is coupled into waveguided modes using a two-dimensional grating. We found that this approach, when rigorously optimized, yields a performance similar to the limits determined in the geometric optical domain. The performance of our structures far exceeds that of any other similar structures demonstrated in the literature so far.

### C. Transparent electrodes

Last year, we demonstrated transparent electrodes based on metal nanowires in a collaboration with Prof. Yi Cui in another GCEP project. This year, we worked with Prof. Zhenan Bao to demonstrate that graphene films, obtained by the reduction of solution-processable graphene oxide flakes, can also be used as a transparent electrode.

#### D. Multijunction organic solar cell practical limits and novel architecture

Using realistic assumptions about the properties of organic materials (optical and electrical) and using a concrete device structure, we estimated the maximum achievable power conversion efficiency of an organic triple-junction solar cell. The results are shown in **Fig. 6**. This structure achieves a power conversion efficiency of 23% under the approximation that  $qV_{OC}=E_G-0.8eV$ . It is likely that new materials will be able to develop a higher  $V_{OC}$  and therefore higher efficiencies.



**Fig. 6.** Efficiency limits of a triple-junction organic solar cell with realistic material and cell parameters.

#### Publications

- J. Wu, H.A. Becerril, Z. Bao and P. Peumans, "Organic solar cells with solution-processed graphene transparent electrodes," accepted in Appl. Phys. Lett.
- M. Agrawal and P. Peumans, "Broadband optical absorption enhancement through coherent light trapping in thin-film photovoltaic cells," *Optics Express* **16**, 5385-5396 (2008).
- Liu, S. Zhao, S.-B. Rim, M. Koenemann, P. Erk and P. Peumans, "Control of electric field strength and orientation at the donor-acceptor interface in organic solar cells," *Advanced Materials* **2008**, 1065-1070 (2008).
- S. Zhao and P. Peumans, "Geminate recombination at organic semiconductor heterojunctions," submitted.

- S.-B. Rim, S. Zhao, S.R. Scully, M.D. McGehee and P. Peumans, "An effective light trapping configuration for thin-film solar cells," *Applied Physics Letters* **91**, 243501 (2007).

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