

Photovoltaic Cells Based on Conducting Polymers and Perylene Diimides

Preprint

A. Breeze, A. Salomon, D. Ginley, and B. Gregg

*To be presented at the NCPV Program Review Meeting
Lakewood, Colorado
14-17 October 2001*



NREL

National Renewable Energy Laboratory

1617 Cole Boulevard
Golden, Colorado 80401-3393

NREL is a U.S. Department of Energy Laboratory
Operated by Midwest Research Institute • Battelle • Bechtel

Contract No. DE-AC36-99-GO10337

NOTICE

The submitted manuscript has been offered by an employee of the Midwest Research Institute (MRI), a contractor of the US Government under Contract No. DE-AC36-99GO10337. Accordingly, the US Government and MRI retain a nonexclusive royalty-free license to publish or reproduce the published form of this contribution, or allow others to do so, for US Government purposes.

This report was prepared as an account of work sponsored by an agency of the United States government. Neither the United States government nor any agency thereof, nor any of their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States government or any agency thereof. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States government or any agency thereof.

Available electronically at <http://www.osti.gov/bridge>

Available for a processing fee to U.S. Department of Energy
and its contractors, in paper, from:

U.S. Department of Energy
Office of Scientific and Technical Information
P.O. Box 62
Oak Ridge, TN 37831-0062
phone: 865.576.8401
fax: 865.576.5728
email: reports@adonis.osti.gov

Available for sale to the public, in paper, from:

U.S. Department of Commerce
National Technical Information Service
5285 Port Royal Road
Springfield, VA 22161
phone: 800.553.6847
fax: 703.605.6900
email: orders@ntis.fedworld.gov
online ordering: <http://www.ntis.gov/ordering.htm>



Printed on paper containing at least 50% wastepaper, including 20% postconsumer waste

Photovoltaic Cells Based on Conducting Polymers and Perylene Diimides

A. Breeze, A. Salomon, D. Ginley and B. Gregg

National Renewable Energy Laboratory

1617 Cole Blvd., Golden, CO 80401

ABSTRACT

NREL has recently begun investing polymer-based photovoltaic cells. We present initial results on a novel energy conversion device that uses both semiconducting polymers and organic small molecules as photoactive layers, using the advantageous properties of both classes of materials. By incorporating polymers into the device, we see results that are surprisingly good for a planar organic device with a notable increase in efficiency versus analogous devices constructed from only small molecule organics.

1. Introduction

During the last decade, semiconducting polymers have been developed as a novel class of optoelectronic materials with applications including both light-emitting diodes and photovoltaics. This is motivated in large part by their promise of low cost, less toxic manufacturing methods, tunable optical properties, and the possibility of lightweight, flexible large area panels. Polymer LED power conversion efficiencies are becoming comparable to those of their inorganic counterparts and are now on the brink of commercialization. An increasing research effort is now being directed toward polymer-based photovoltaics, leading to encouraging strides in both the basic understanding of device operation and improving device efficiency. As critical processes such as exciton dissociation become better understood, novel heterostructures such as presented below are being investigated and are leading to higher conversion efficiencies.

2. Polymer - Small Molecule Organic Composite Devices

As part of an internally funded effort, we have created polymer - small molecule organic composite devices in a layered structure that show promising improvements versus conventional cells constructed of either component alone [1, 2]. Electron conducting perylene benzimidazole (PBI) (Figure 1b) films are thermally evaporated to a thickness of 18 nm. The hole conducting polymer, poly[2,5-dimethoxy-1,4-phenylene-1,2-ethynylene-2-methoxy-5-(2-ethylhexyloxy)-1,4-phenylene-1,2-ethynylene (M3EH-PPV) (Figure 1a), is then spin cast from a solution in chlorobenzene to create films of 30 nm thickness. These photoactive layers are sandwiched between patterned indium tin oxide (ITO) and gold electrodes. We have achieved a power conversion efficiency of 1.4% with $V_{oc} =$

-0.58V, $J_{sc} = 6.06\text{mA/cm}^2$ and fill factor = 40% at one-sun incident light. Compared to other solid state planar organic devices, this is a promising efficiency. We discuss below approaches to optimize the device structure for higher efficiencies.

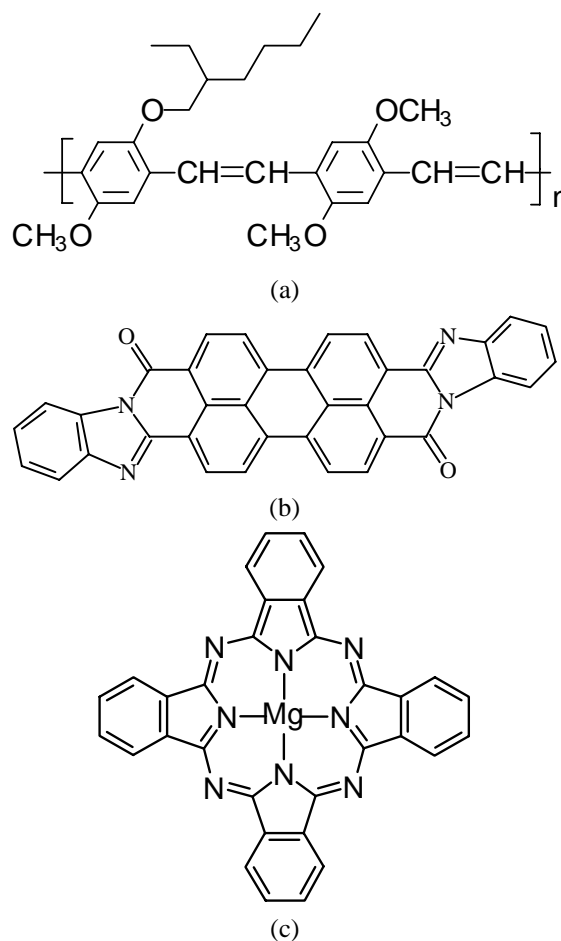


Fig 1. Chemical structures of (a) M3EH-PPV, (b) PBI, and (c) MgPc.

3. Comparison to Other Results

Figure 2 compares an ITO/PBI/M3EH-PPV/Au device to an analogous structure using magnesium phthalocyanine (MgPc) (Figure 1c), another small molecule commonly used in organic PV devices, in place of the polymer as the hole conducting media. The power efficiency of the organic molecule bilayer device is only 0.2%, a factor of seven less than the polymer composite cell.

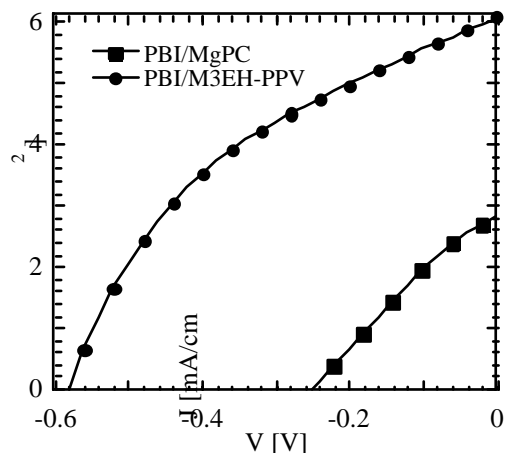


Fig 2. J-V characteristic for ITO/PBI/MgPC/Au (squares) and ITO/PBI/M3EH-PPV/Au (circles) devices under one-sun white light.

Figure 3 shows the absorption spectra for PBI, MgPc, and M3EH-PPV. The absorption spectra of PBI and MgPc are just as complementary, if not more so, as that of the PBI and M3EH-PPV. In addition, MgPc has a generally higher hole mobility than M3EH-PPV. Theoretically, this should lead to PBI/MgPC devices having the higher device efficiency. One possible explanation for the better performance in the polymer-based cells is the morphology of the polymer interface. The small molecule materials tend to form nanocrystals, which may lead to poor electrical contact across interfaces. Polymers, on the other hand, do not crystallize and therefore wet surfaces fairly well. This implies better electrical contact at polymer surfaces, which would lead to improved charge transport. It is also likely that exciton dissociation is more efficient at the M3EH-PPV/PBI interface than at the MgPC/PBI interface due to both the improved electrical contact and to a greater band offset between the polymer and perylene.

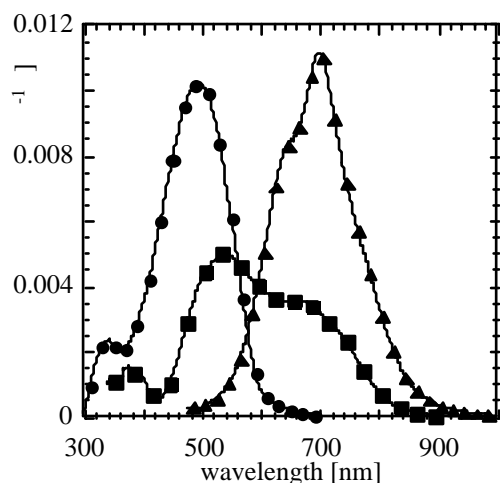


Fig 3. Absorption spectra for PBI (squares), MgPc (triangles), and M3EH-PPV (circles).

4. Photovoltage Determining Mechanisms

In single-layer polymer photovoltaics, the photovoltage is generally considered to be determined by an internal electric field that is created by the difference in electrode work functions. For our devices, however, this is not the case. The work function difference of 0.3V between ITO and Au is not consistent with our V_{oc} of up to 0.6V. In addition, when we reverse the order of the photoactive layers (ITO/M3EH-PPV/PBI/Au), we reverse the direction of the current flow. Although the electrode work functions likely contribute to the value of the photovoltage, the primary mechanism for its determination is probably the interfacial chemical potential gradient produced via exciton dissociation at the polymer/perylene interface.

5. Nanostructured ZnO Electrodes

One of the main factors limiting efficiency in polymer and other solid state organic solar cells is the short exciton diffusion length. In contrast to inorganic solar cell materials, photons absorbed in polymers create a neutral exciton (bound electron-hole pair) that must be dissociated in order to collect charge from the device. Excitons that do not reach a dissociation site recombine, decreasing efficiency. To circumvent this, we have initiated experiments to create high surface area doped zinc oxide (ZnO) films by electrochemical deposition to replace the planar ITO electrode. By coating this high surface area with very thin (~10nm) films, we can greatly increase the exciton dissociation surface area, while at the same time maintaining strong light absorption and decreasing the device series resistance and charge recombination. This should lead to strong increases in short-circuit current and fill factor, and therefore, device efficiency.

6. Conclusion

We have shown that polymer/perylene bilayer devices show substantial improvement versus photovoltaics made from phthalocyanine/perylene. Conversion efficiencies of 1.4% have been achieved for simple planar bilayer organic devices, and we believe that substantial improvements can be realized by developing nanostructured surfaces.

References

- [1] B.A. Gregg, "Bilayer Molecular Solar Cells on Spin-Coated TiO_2 Substrates," *Chem. Phys. Lett.* **258** (1996) 376-380.
- [2] A.J. Breeze, Z. Schlesinger, S.A. Carter, and P.J. Brock, "Charge Transport in TiO_2 /MEH-PPV Polymer Photovoltaics", *Phys. Rev. B*, in press.
- [3] R. Koenenkamp, K. Boedecker, M.C. Lux-Steiner, M. Poschenrieder, F. Zenia, C. Levy-Clement, and S. Wagner, "Thin Film Semiconductor Deposition on Free-Standing ZnO Columns", *Appl. Phys. Lett.* **77** (2000) 2575-2577.