Solution-Processed Bulk Heterojunction Solar Cells with Novel Acceptor Molecules

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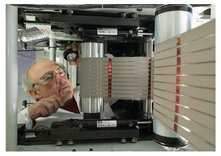
Organic Photovoltaics

Solar energy is a highly abundant, clean energy source. In 1.5 hours, enough solar energy hits the surface of the Earth to provide 100% of our global energy needs for an entire year (15 Tw × 1 year)

Why organic photovoltaics?

- *Using a 1.1V cell as a top cell in a tandem device with a CIGS cell could boost efficiency from 15% to 21%, cutting overall cost by ~ 30%*
  Beiley, Z. and McGehee, M.D., *Energy & Environ. Sci.*. **2012**, In press
- *Energy payback time for organic solar cells is only 2-3 months, compared to 2-3 years for other technologies*
  Roes et al., *Prog. Photovoltaics.* **2009** (17) 372-393
- *Roll-to-roll processing techniques are potentially very low cost*



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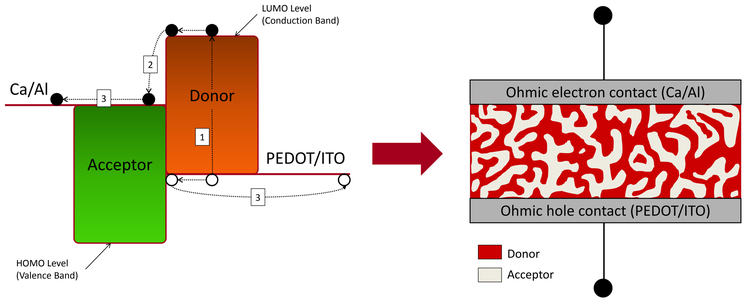
How do organic solar cells work?

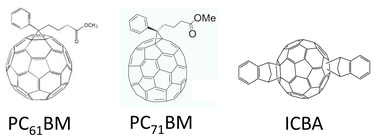


How current is generated

- *1) Photon absorption and exciton generation*
- *2) Charge transfer / exciton splitting*
- *3) Charge carrier collection*

Acceptor Materials in OPV

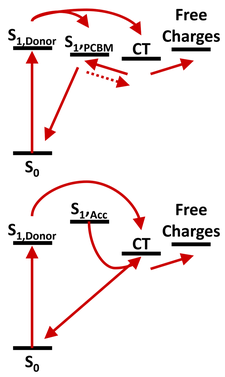
Fullerene Derivatives (Up to 8.8% efficient)



$PC_{61}BM$ $PC_{71}BM$ ICBA

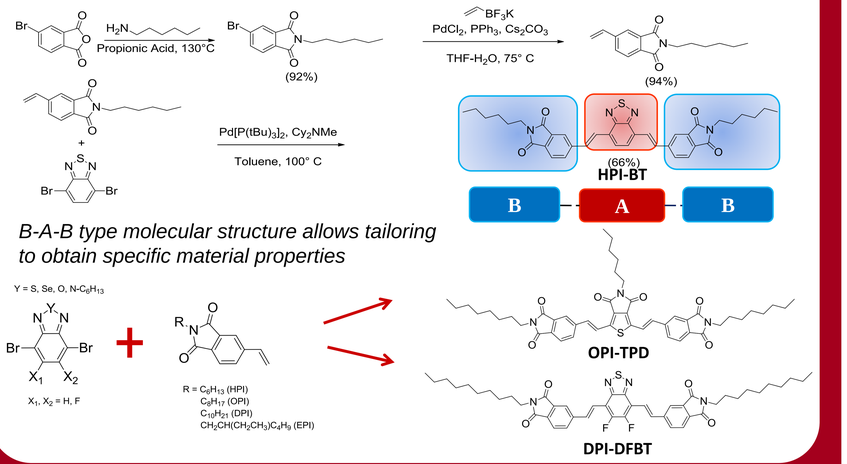
Drawbacks of Fullerene Derivatives

- *Low singlet state energy (1.7 eV) limits V_{OC} to 1.0 V*
- *Weak absorption of solar spectrum in visible region*
- *Higher cost ($50/g, $5.50/m², $0.06/W)*



- ***Alternative acceptor materials will be needed to produce high V_{OC} top cells in a hybrid tandem configuration***

Synthesis of New Acceptor Materials



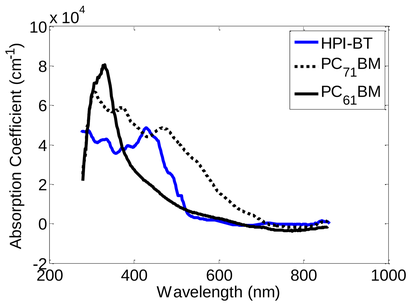
B-A-B type molecular structure allows tailoring to obtain specific material properties

Optoelectronic Properties of HPI-BT

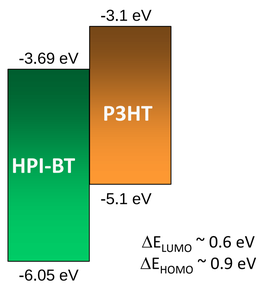
Material	Abs. Max. (nm)	Abs. Coeff. (cm^{-1})	$E_{g,opt}$ (eV) [a]	PL Max (nm)	HOMO/LUMO (eV)	T_m (°C)
HPI-BT	430	4.9 X 10^4	2.34	645	-5.8/-3.3[b] -6.1/-3.7[c]	156

[a] – Measured from onset of UV-Vis absorption signal.
[b] – Measured from cyclic voltammetry.
[c] – Measured with PESA (photoelectron spectroscopy in air)

Solid-State Absorption Spectrum



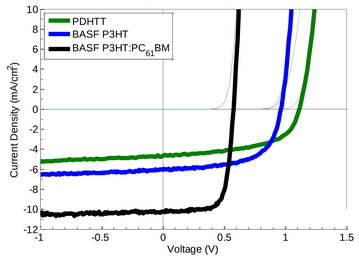
Energy Levels



- *Smaller electron affinity suggests larger V_{OC} values for HPI-BT than PCBM*
- *Acceptor materials absorb more than $PC_{61}BM$, but less than $PC_{71}BM$*

Device Performance

Current-Voltage Curves with HPI-BT

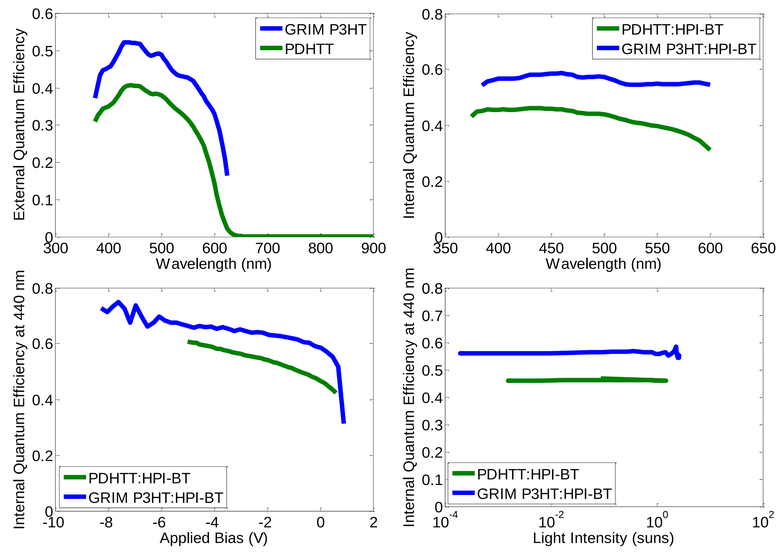


	BASF P3HT	GRIM P3HT	PDHTT	BASF P3HT
Acceptor	HPI-BT	HPI-BT	HPI-BT	$PC_{61}BM$
Jsc (mA/cm²)	6.1	6.1	4.8	10.3
Voc (V)	0.97	0.96	1.11	0.58
FF	0.61	0.57	0.64	0.73
PCE (%)	3.6	3.4	3.4	4.4

η = 3.6%

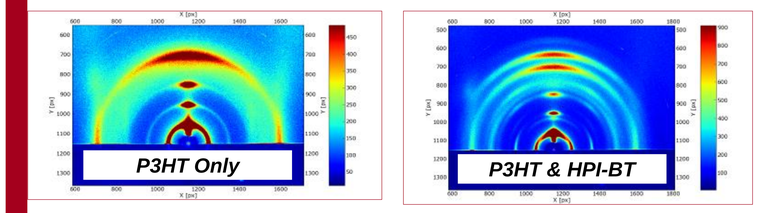
- *Believed to be highest efficiency using non-fullerene based acceptor with P3HT as donor material*

Current Lost to Recombination



- *Increase in internal quantum efficiency (IQE) with applied electric field, but not light intensity, suggests excitons are splitting efficiently, but not forming free charges (**geminate recombination**)*

X-Ray Diffraction



- *X-ray diffraction scan with P3HT & HPI-BT (right) shows additional peaks not associated with P3HT only (left)*

Summary

- *New small molecule electron acceptors fill some gaps left by fullerene derivatives*
  - *Open-circuit voltages as high as 1.11 V targeting top cells in tandem devices*
  - *Increased photocurrent from absorption in acceptor phase*
  - *Potentially lower cost synthesis*
- ***3.6% power conversion efficiency is believed to be the most efficient solution-processed bulk heterojunction device using P3HT as donor and a non-fullerene acceptor molecule***

Future Directions

- *Investigating effect of system energetics to drive down geminate recombination and enhance free charge formation using molecular design of acceptors*
- *Designing acceptor molecule to complement donors in newer, higher-efficiency devices*
- *Investigate presence and role of molecular mixing in D/A interfacial region on recombination and free charge formation*