Solution-Processed Bulk Heterojunction Solar Cells from Non-Fullerene Acceptor Molecules

Jason T. Bloking, Andrew T. Higgs, Xu Han, John P. Kastrup, Laxman Pandey, Joseph E. Norton, Chad Risko, Jean-Luc Bredas, Michael D. McGehee and Alan Selsing

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 Twh x 1 year)

Why organic photovoltaics?
• Roll-to-roll processing techniques are potentially very low cost
• Energy payback time for organic solar cells is less than other technologies

How do organic solar cells work?

How current is generated:
• 1) Photon absorption and exciton generation
• 2) Exciton diffusion
• 3) Charge transfer / exciton splitting
• 4) Charge carrier collection

Organic solar cells can be made from all organic materials, with the photosensitive layer typically a blend of a donor polymer or small molecule and an acceptor. This donor/acceptor pair is placed between two electrodes.

Here is a simplified schema showing the key features of a polymer/silicon solar cell:

- The donor absorbs light and generates free electrons
- The acceptor attracts holes
- The free electrons and holes diffuse to the contact electrodes

Acceptor Materials in OPV

- Fullerene Derivatives (Up to 7.4% efficient)
  - PCBM
  - PC71BM
  - ICB
- Drawbacks of Fullerene Derivatives:
  - Weak absorption of solar spectrum
  - Low-lying LUMO = Lower cell voltage
  - Higher cost ($50/g, $5.50/m², $0.06/W)
- Up to 10% of the entire module cost could be from fullerene material
- Need to find alternative acceptor materials

New Acceptor Materials

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

- Acceptor Material Building Blocks
  - Ethynylphenyl (EV)
  - Benzothiadiazole (BT)
  - Phenyl Imide (PI)
  - Naphthalene Imide (NI)

- Benzothiadiazole (BT)
  - EV-BT
  - HV-BT
- Phenyl Imide (PI)
  - EV-PI
  - HV-PI
- Naphthalene Imide (NI)
  - PI
  - NI

- Synthesis of PI-BT

- Properties of Acceptor Materials

<table>
<thead>
<tr>
<th>Material</th>
<th>Abs. Max. (nm)</th>
<th>Abs. Conc. (10^13 cm⁻²)</th>
<th>E_{LUMO} (eV)</th>
<th>PL Max (nm)</th>
<th>HOMO/LUMO (eV)</th>
<th>T_{onset} (°C)</th>
</tr>
</thead>
<tbody>
<tr>
<td>EV-BT</td>
<td>335, 442</td>
<td>3.33 x 10¹⁴</td>
<td>2.43</td>
<td>516</td>
<td>-6.0/-3.4</td>
<td>205</td>
</tr>
<tr>
<td>PI-BT</td>
<td>446</td>
<td>2.29 x 10¹⁴</td>
<td>2.34</td>
<td>525</td>
<td>-5.8/-3.3</td>
<td>156</td>
</tr>
<tr>
<td>NI-BT</td>
<td>467</td>
<td>3.85 x 10¹⁴</td>
<td>2.16</td>
<td>547</td>
<td>-5.7/-3.4</td>
<td>241</td>
</tr>
</tbody>
</table>

Current-Voltage Curves (P3HT as Donor)

External Quantum Efficiency (EQE)

X-Ray Diffraction

Summary

• New small molecule electron acceptors fill some gaps left by fullerene derivatives
  - Photocurrent from acceptor phase
  - Higher open-circuit voltage of 0.96 V
  - Potentially lower cost synthesis

- 2.5% 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

- Understanding of loss mechanisms in P3HT:PI-BT devices to find potential avenues for the design and synthesis of new acceptor molecules
- Selecting more suitable donor materials with complementary absorption spectra
- Investigation of new synthetic schemes to improve yield and purity

Device Performance

X-Ray diffraction scan with P3HT & PI-BT (upper left) shows additional peaks not associated with P3HT only (bottom left)
- NI-BT does not show extra crystal diffraction peaks – poor crystallization