Title
Characterization of Charge Transport Networks in Polymer/Non-fullerene Solar Cells.

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Characterization of Charge Transport Networks in Polymer/Non-fullerene Solar Cells

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Organic Photovoltaic Devices

- Synthetically tunable

  - Thin Films - (~ $10^{-7}$ meter) ~13% Solar-to-power conversion efficiency (PCE)
    - Compare to Silicon (~$10^{-3}$ meter) ~26% PCE
      - Less efficient but require less material AND LESS COST

- Transparent
- Flexible

- Solution processing
  - Paint-on or print roll-to-roll

plasticphotovoltaics.org

Archdaily.com
Photovoltaic Device

\[ E_{\text{photon}} = \frac{hc}{\lambda} \]

Polymer Donor
Ex. P3HT
“Fruit-fly”

Accepter Molecule PCBM
Organic Photovoltaic Device

**Bi-layer p-n Junction**

1. Absorb Light

2. Separate *Exciton* (electron/hole pair) - limited by diffusion length \(~10\) nm

3. Transport Charges to Opposite Electrodes

**Limited Donor/Acceptor (D/A) Interface**

**Minimal Free-Charge Generation**
Bulk-heterojunction Junction
- Increased D-A interface & Charge Generation
- Tortuous Charge Transport

Thermodynamically trapped donor-acceptor phase-segregation
Bulk-heterojunction
- Thermodynamically trapped donor-acceptor phase-segregation

Fine intermixing
Good charge separation,
Poor charge transport

Coarse intermixing
Poor charge separation,
Good charge transport
Fullerenes – why not?

Charge transport independent of intermolecular orientation

Absorbs narrow spectrum of light
Negligible contribution to photocurrent
Non-Fullerenes
Modify chemical structure
→ Influence nanometer scale device morphology?

PCBM
Quasi-sphere (3d)

Spiro-MeOTAD
twisted core - branched periphery

Perylene Diimide
2-d planar core
Non-Fullerenes

Modify chemical structure
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**PCBM**
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Roders, M., Pitch, G., Ayzner, A. *Manuscript in Progress*
Hierarchical Morphology Elucidation

Synchrotron Wide and Small-Angle X-ray Scattering

Statistical Information regarding size and shape of particles/aggregates

\[ q = \frac{4\pi}{\lambda} \cdot \frac{\sin \theta}{2} \propto \frac{1}{\text{particle size}} \]
Hierarchical Morphology Elucidation

Synchrotron Wide and Small-Angle X-ray Scattering

Scanning Transmission Electron Microscopy (STEM)
Energy Dispersive Spectroscopic (EDS) Imaging
Elemental Mapping

$\rho(\vec{r}) = \rho_0 + \Delta \rho(\vec{r})$
$\vec{q} = \vec{k}_f - \vec{k}_i = \frac{4\pi \sin(\theta)}{\lambda}$

A few nm - 100s nm structure


Hierarchical Morphology Elucidation

\[ q = \frac{4\pi}{\lambda} \sin\frac{\theta}{2} \propto \frac{1}{\text{particle size}} \]
Spiro series

~Subtle changes

(a) M

(b) Z

(c) E

(d)

(e)
Take-away

Morphological control with subtle changes to chemical structure

Roders, M; Pitch, G.; Ayzner, A. L. Manuscript in Progress
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