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**

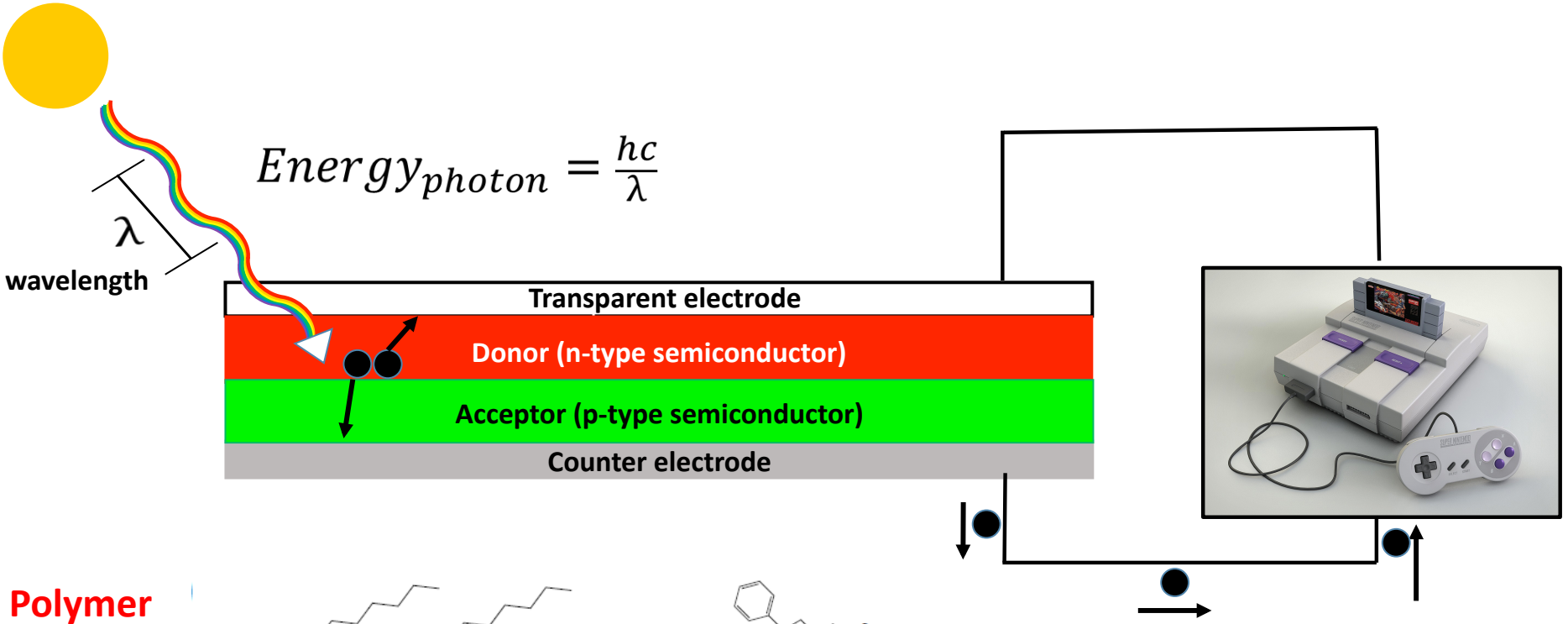
- **Transparent**
- **Flexible**

- Solution processing

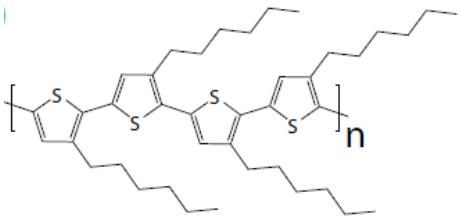
- Paint-on or print roll-to-roll

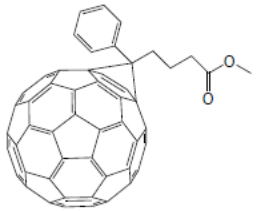
-

Photovoltaic Device



Polymer Donor Ex. P3HT "Fruit-fly"



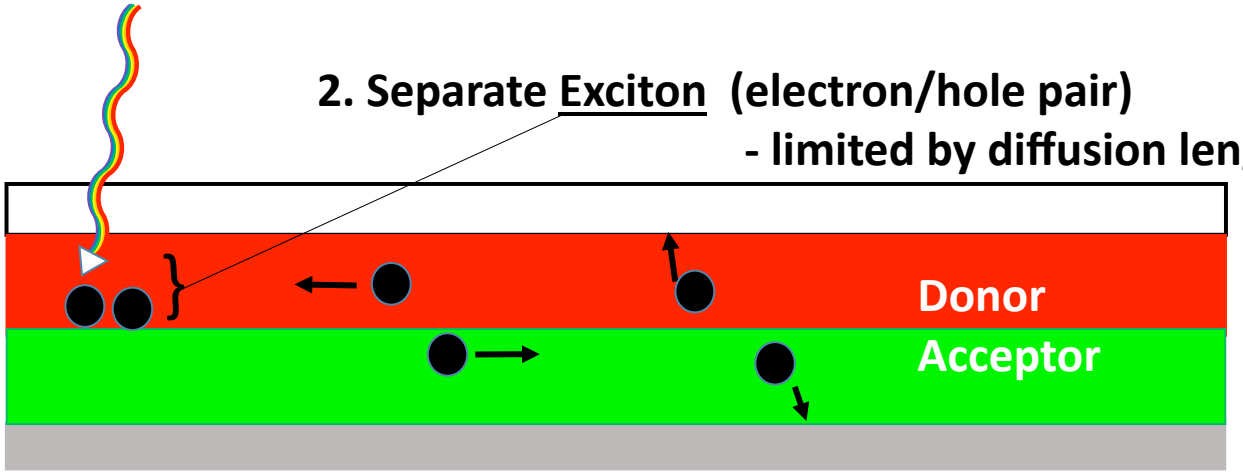


Acceptor Molecule PCBM

Organic Photovoltaic Device

Bi-layer p-n Junction

1. Absorb Light



2. Separate Exciton (electron/hole pair)

- limited by diffusion length ~10 nm

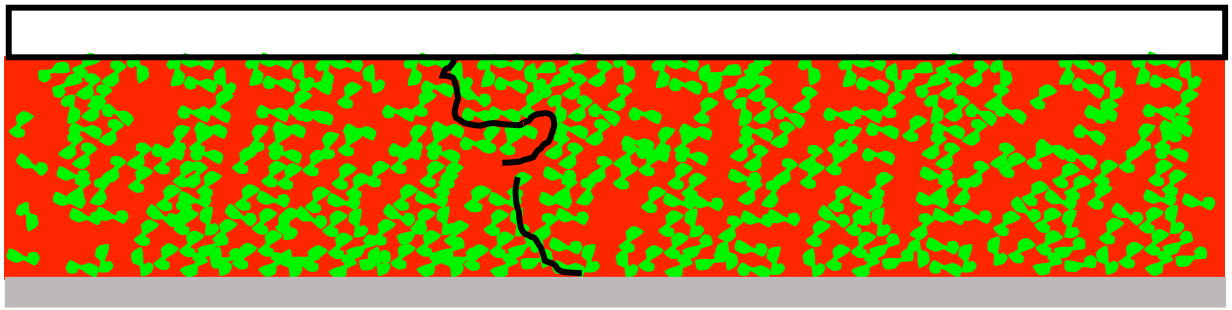
3. Transport Charges to Opposite Electrodes

Limited Donor/Acceptor (D/A) Interface

Minimal Free-Charge Generation

Bulk-heterojunction Junction

- Increased D-A interface & Charge Generation
- Tortuous Charge Transport

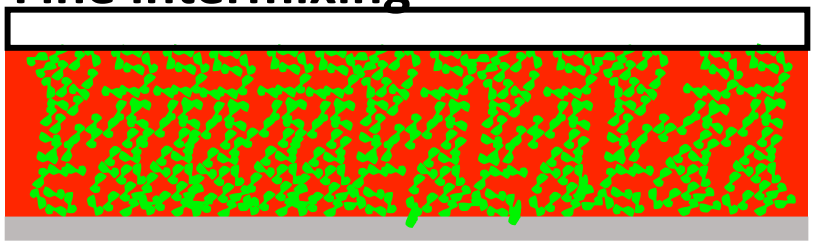


Thermodynamically trapped donor-acceptor phase-segregation

Bulk-heterojunction

- Thermodynamically trapped donor-acceptor phase-segregation

Fine intermixing



Good charge separation,
Poor charge transport

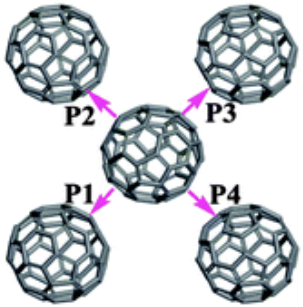
Coarse intermixing

Poor charge separation,
Good charge transport

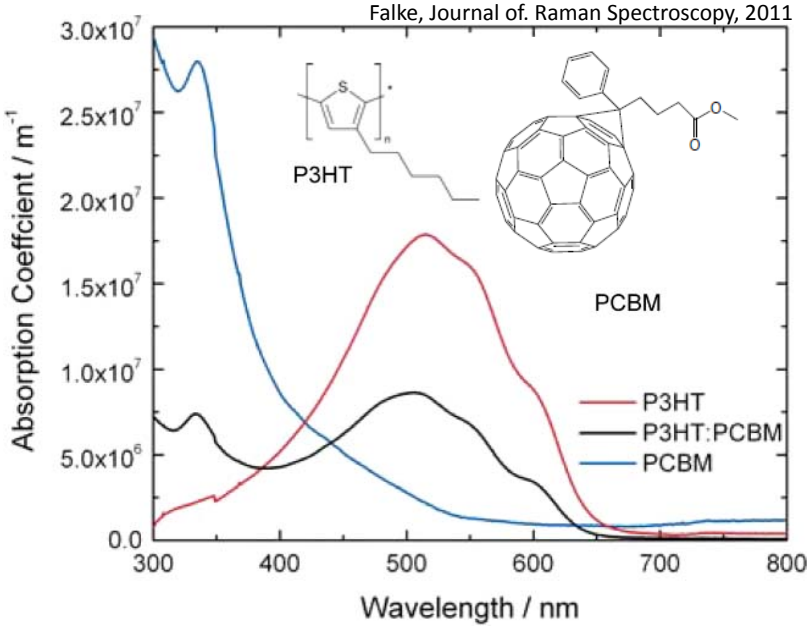
Fullerenes – why not?

Charge transport

independent of intermolecular orientation



Falke, Journal of. Raman Spectroscopy, 2011



Absorbs narrow spectrum of light

Neglible contribution to photocurrent

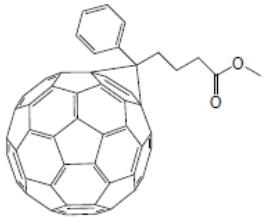
Non-Fullerenes

Modify chemical structure

→ Influence nanometer scale device morphology?

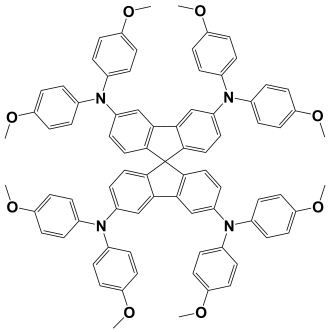
PCBM

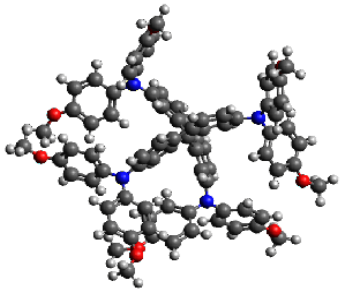
Quasi-sphere (3d)



Spiro-MeOTAD

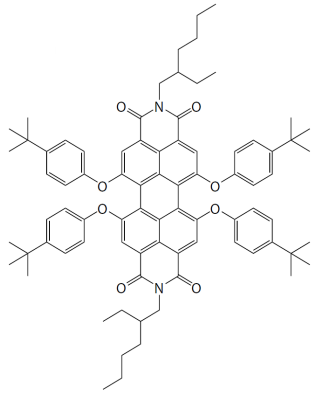
twisted core - branched periphery





Perylene Diimide

2-d planar core



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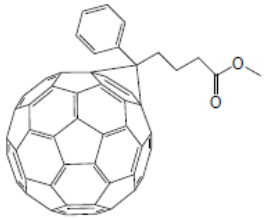

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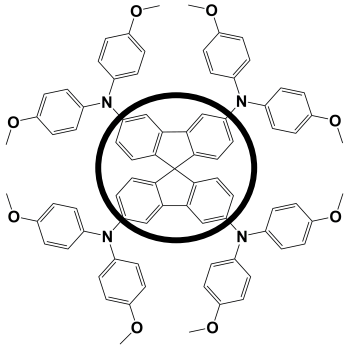

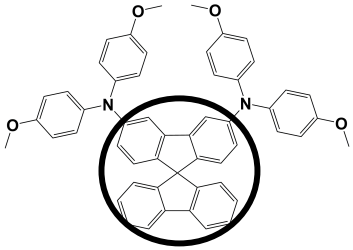

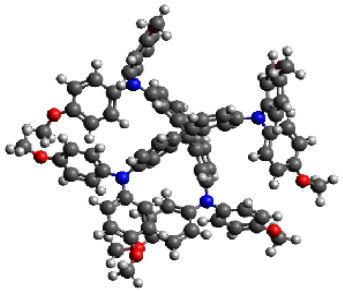

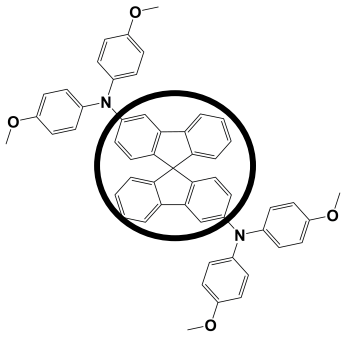

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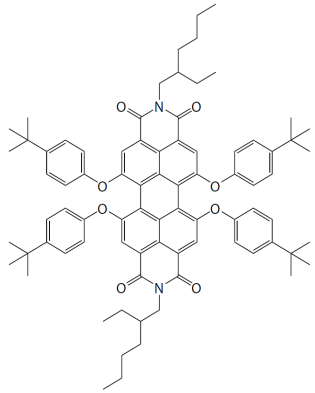
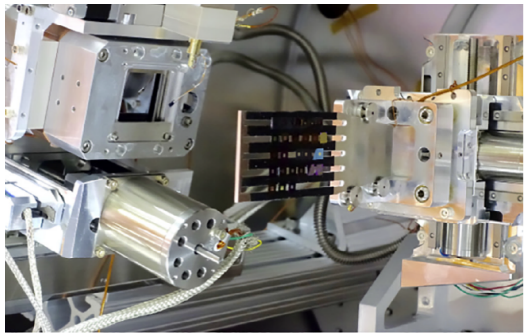
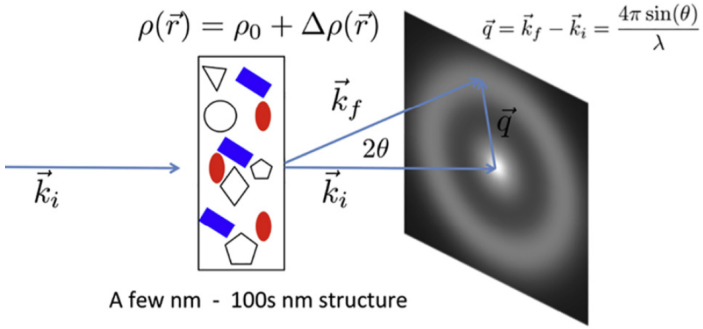


Roders, M., Pitch, G., Ayzner, A. *Manuscript in Progress*

Hierarchical Morphology Elucidation

Synchrotron Wide and Small-Angle X-ray Scattering



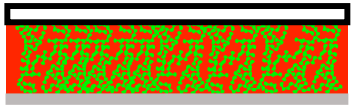


Liu; Bradey; Wang. Eur. Pol. Journ. 2016.

Statistical Information regarding size and shape of particles/aggregates

$$q = \frac{4\pi}{\lambda} \sin\frac{\theta}{2} \propto \frac{1}{particle\ size}$$

Hierarchical Morphology Elucidation



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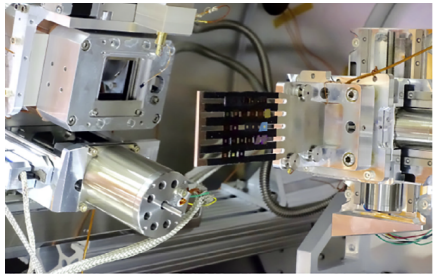

Statistical Information

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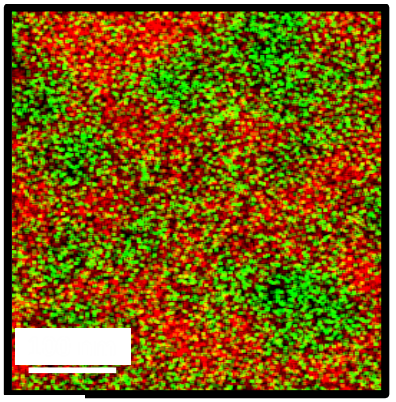
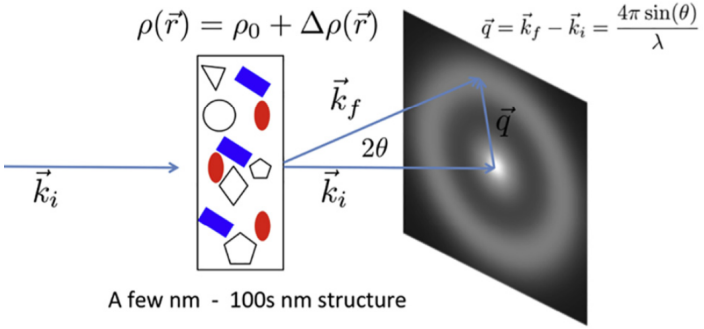
Visual Information

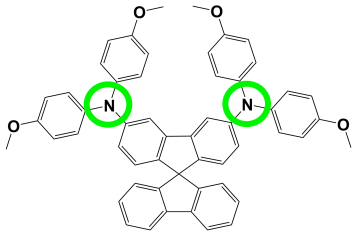
Scanning Transmission Electron Microscopy (STEM)
Energy Dispersive Spectroscopic (EDS) Imaging

Elemental Mapping

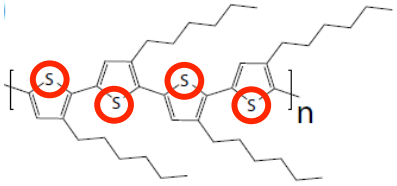




Nitrogen



Sulfur



Liu; Bradey; Wang. Eur. Pol. Journ. 2016.

Roders, M; Ayzner, A. L. *J. Mater. Res.* **2017**, 1-11.

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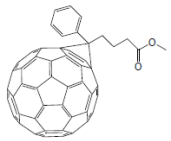

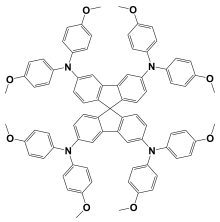

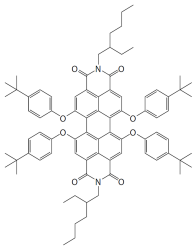

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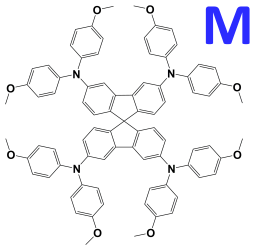
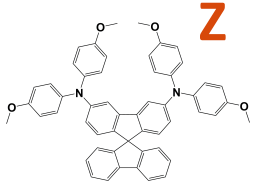
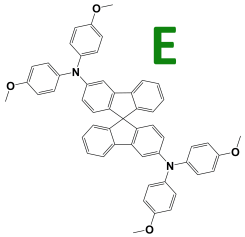


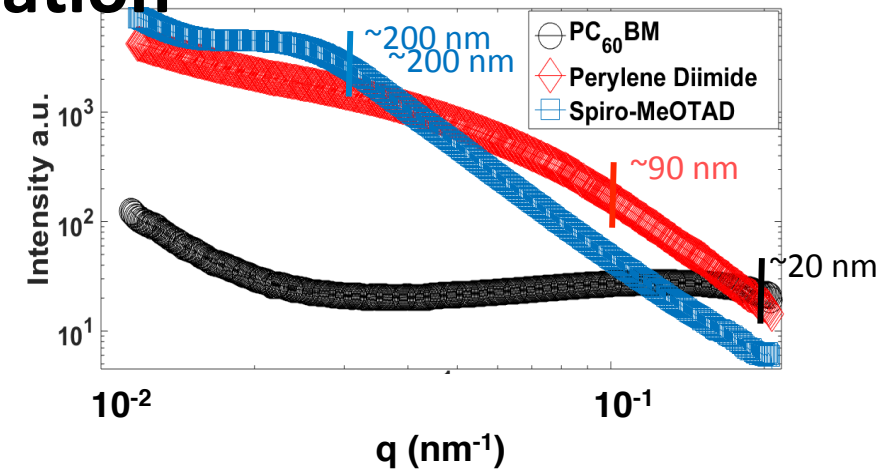
M

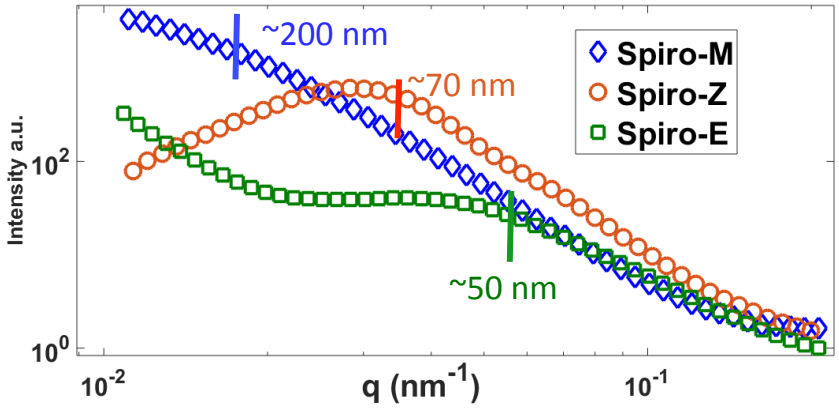


Z



E

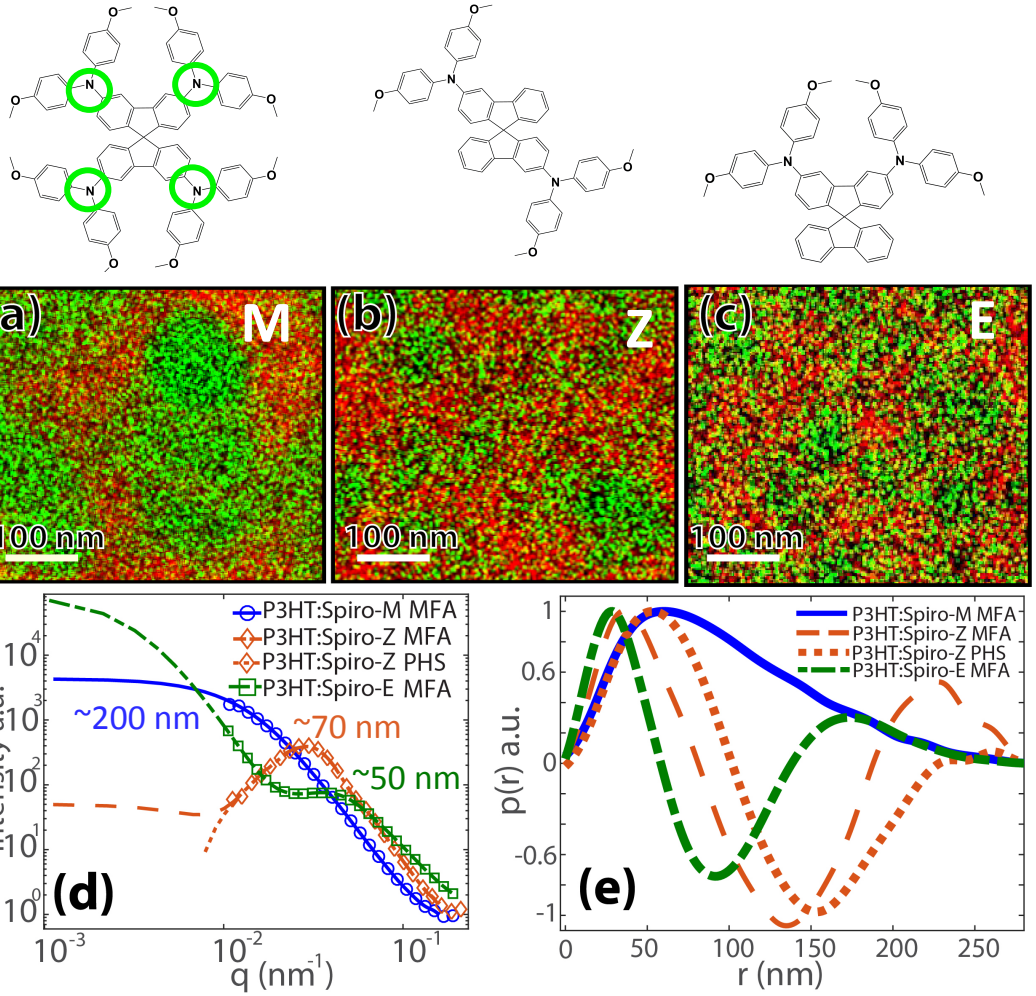


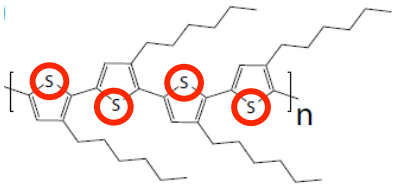


Liu; Bradey: Wang. Eur. Pol. Journ. 2016.

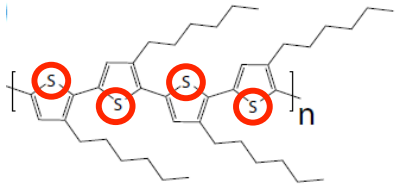
Spiro series

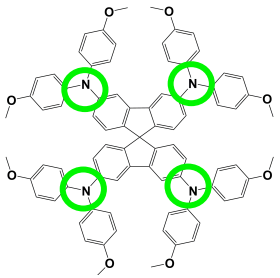
~Subtle changes

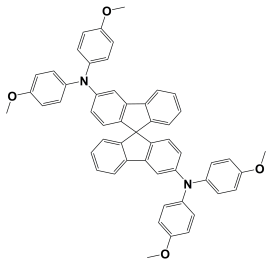


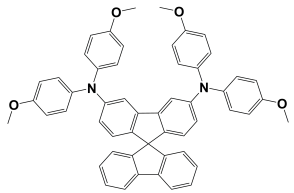


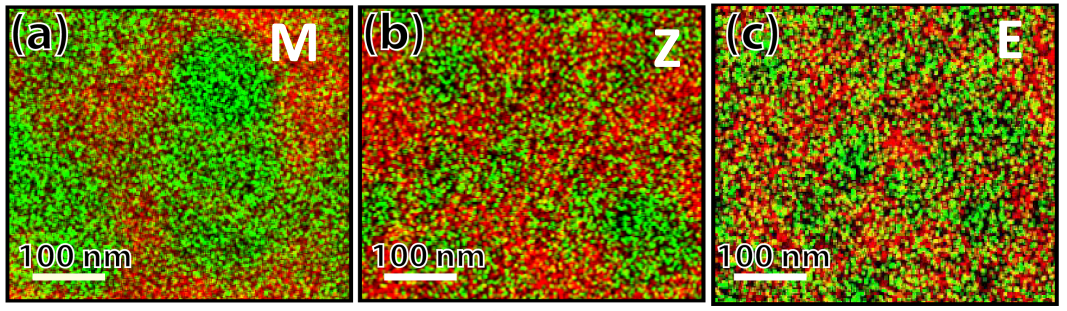
Take-away



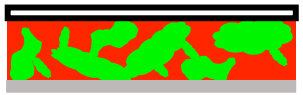




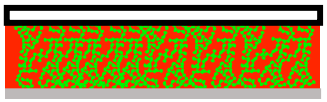




Morphological control with subtle changes to chemical structure



Better Charge **Transport**



Better **Charge Separation**

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

Acknowledgements

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- Diego Garcia
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