



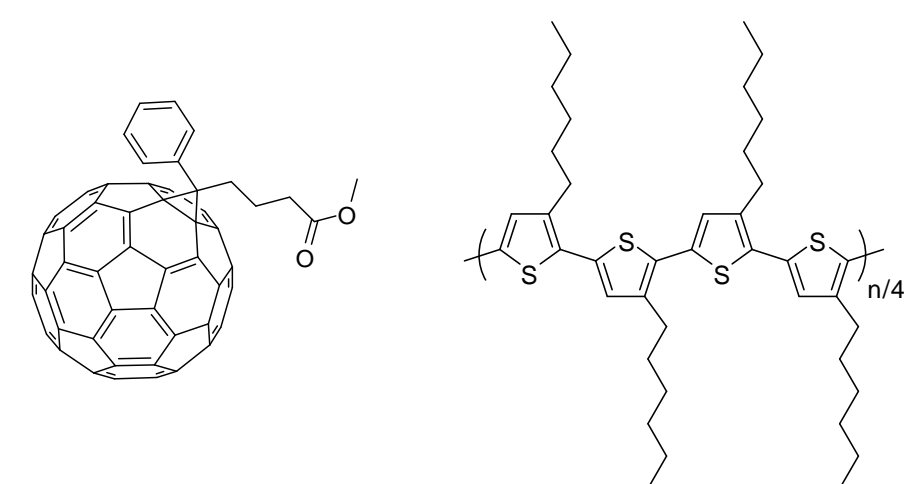
# Design of Conjugated Polymers for Ternary Blend Solar Cells

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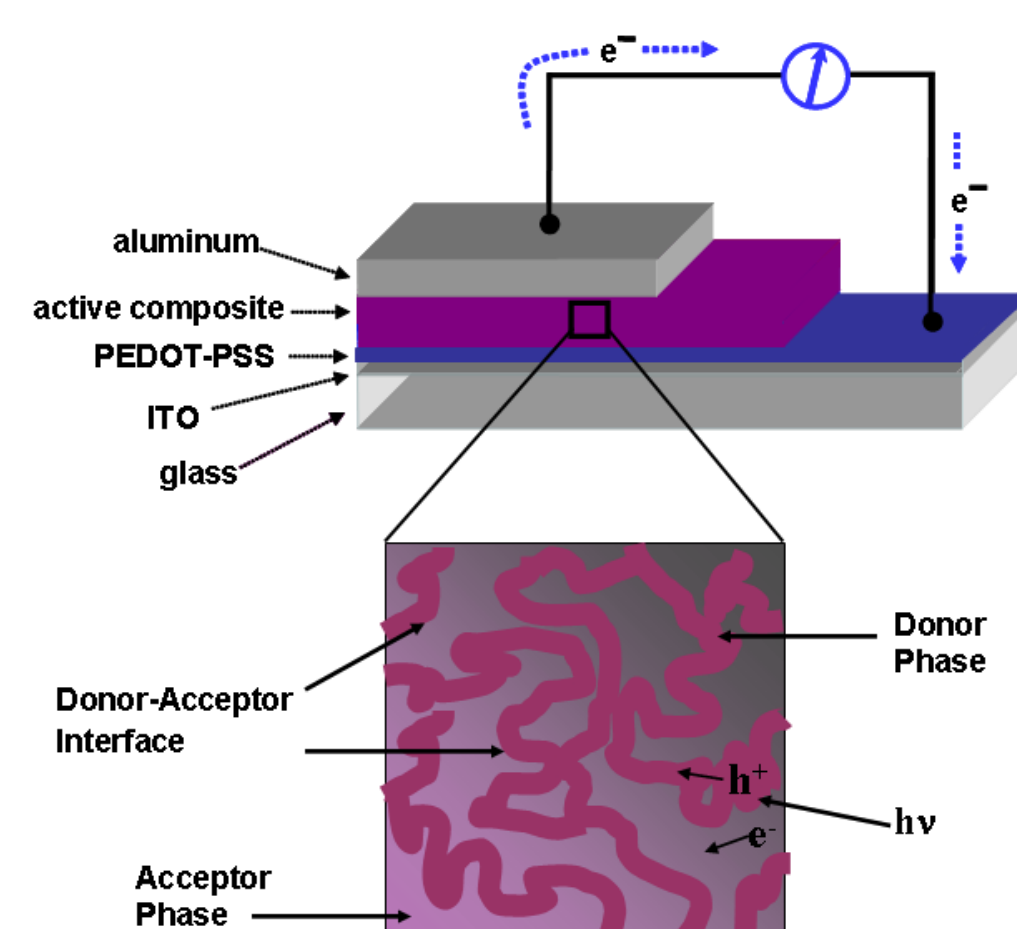
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## Polymer Based Solar Cells (Photovoltaics)<sup>1</sup>

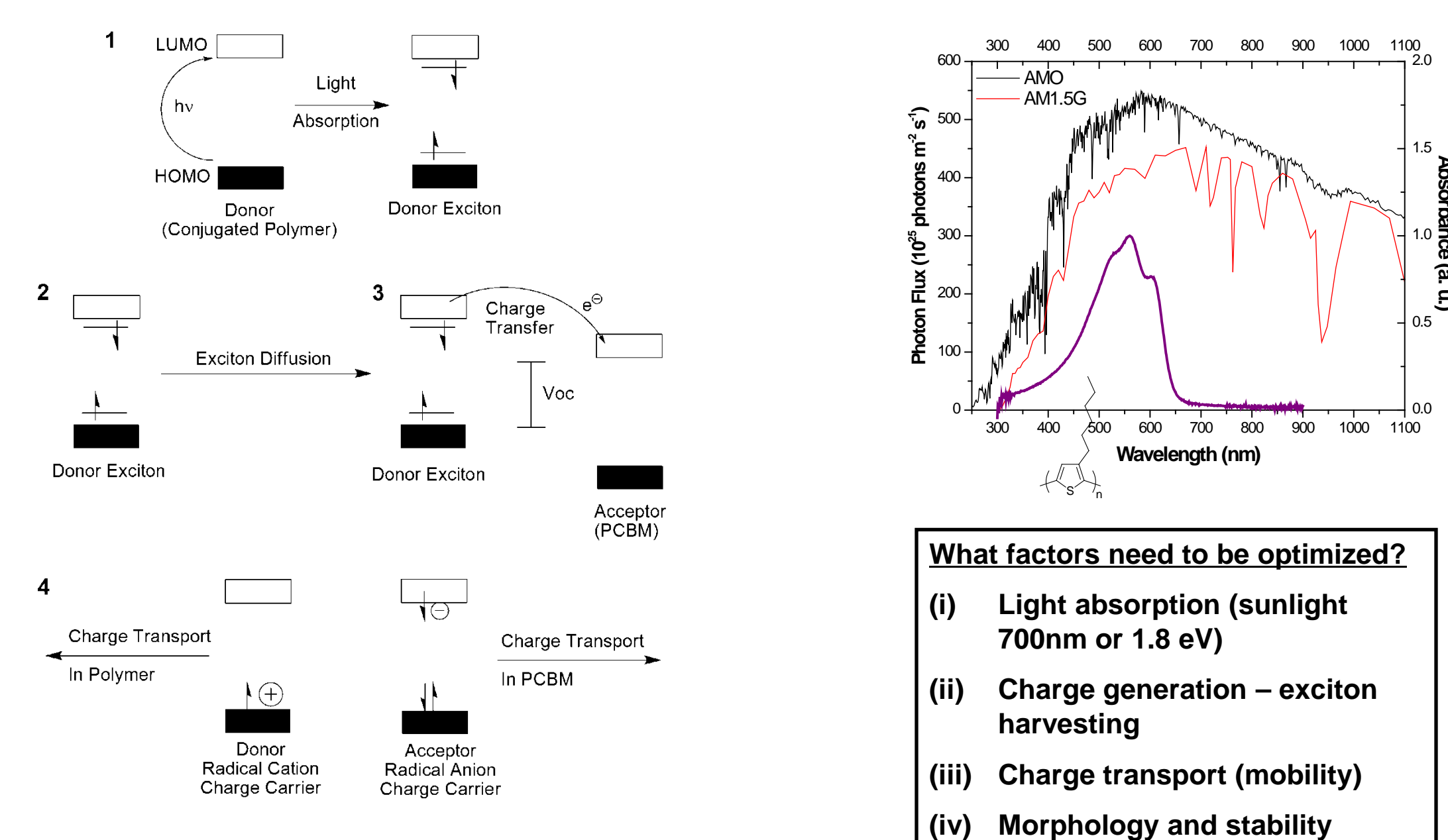
### Polymer-Fullerene Bulk Heterojunction Photovoltaics



-Polymer Donor Material (P3HT)  
-Fullerene Acceptor Material (PCBM)



### Mechanism of Operation and the Necessity for Optimization

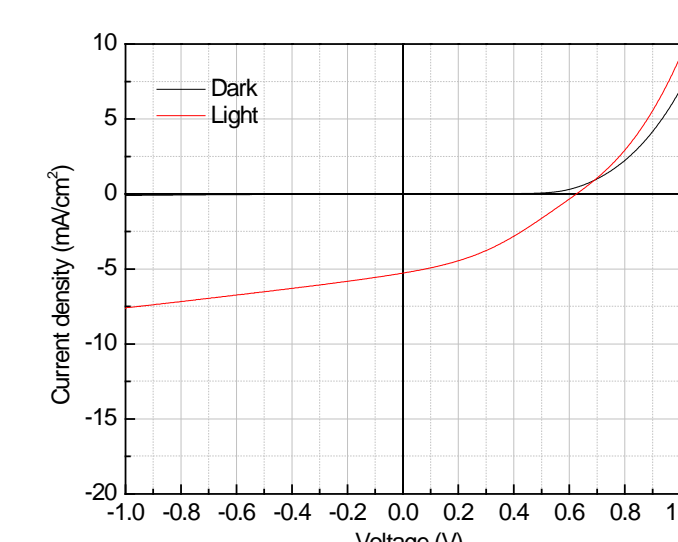
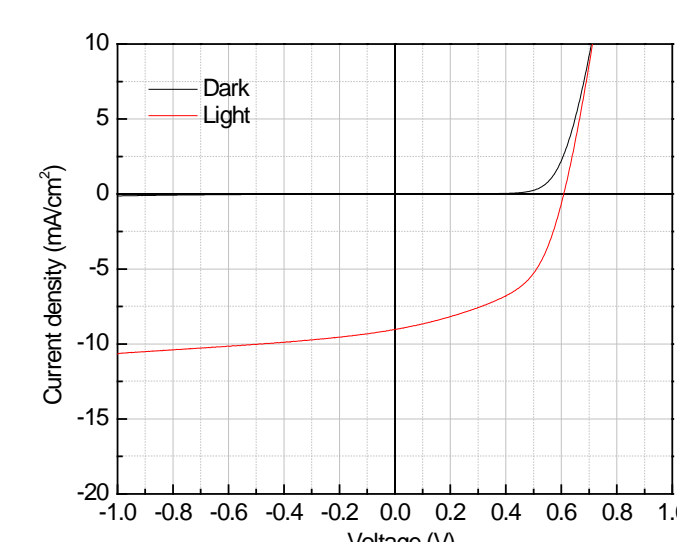


## Devices

### Coupling of with the fullerene [6,6]-phenyl-C<sub>61</sub> butyric carboxylic acid PCBA

### Model Dyes in Binary Blends Devices

### Data

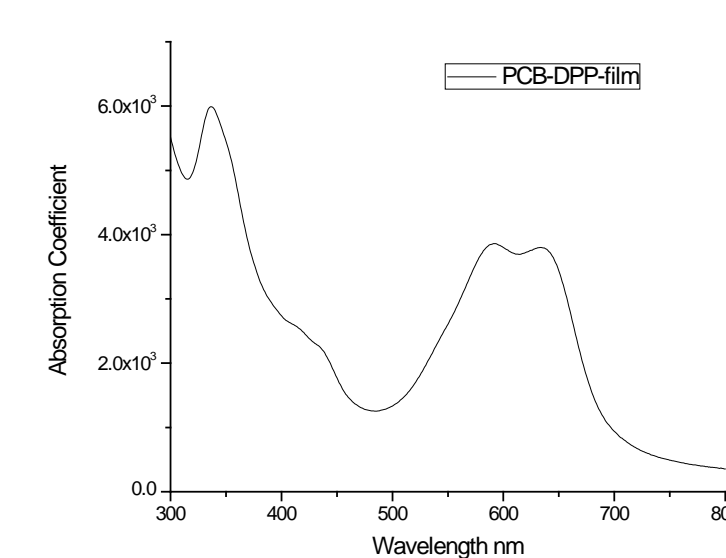
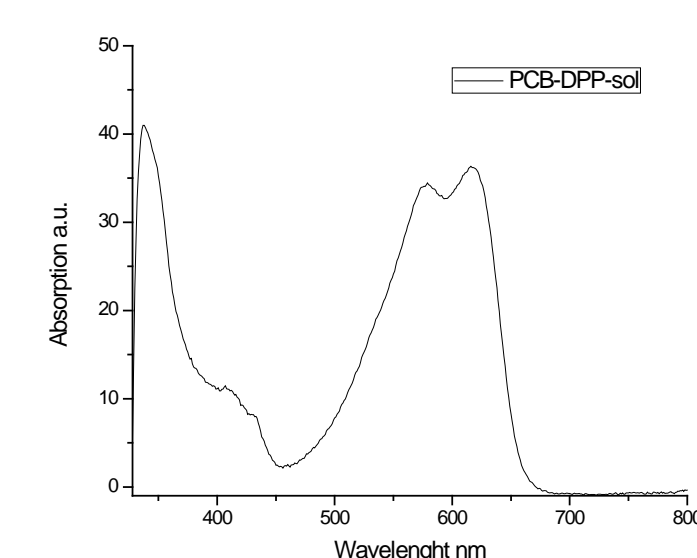
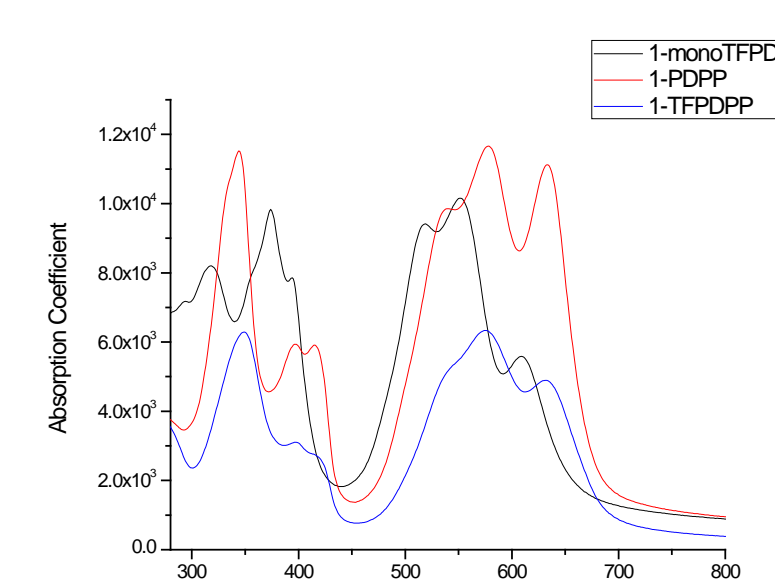
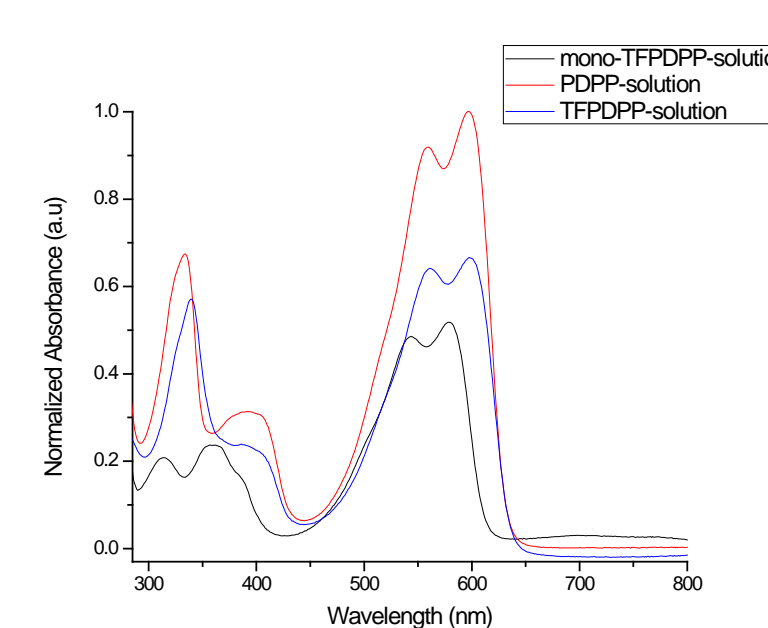


P3HT:PCBM (1:0.8)

P3HT:PCB-TFDPP (1:0.8)

|                        | $J_{sc}$ | $V_{oc}$ | FF   | PCE   |
|------------------------|----------|----------|------|-------|
| P3HT:PCBM (1:0.8)      | 8.82     | 0.61     | 0.51 | 2.71% |
| P3HT:PCB-TFDPP (1:0.8) | 5.14     | 0.62     | 0.34 | 1.09% |

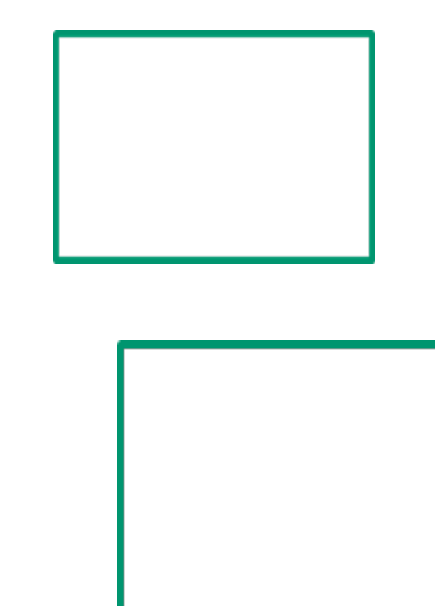
### UV/Vis Absorption



Future work will focus on ternary blend analogues based on P3HT and the free dye as donors, along with [6,6]-phenyl-C<sub>61</sub> butyric acid methyl ester (PCBM) as an acceptor. The relative importance of the energetic relationship between the three components is directly related to morphology and investigation towards the ideal composition will elucidate differences between simple mixtures and covalent attachments.

## Thiophene Monomers

### Synthesis of 3-hexylthiophene and 3-(oligoethylene oxide)-thiophene:

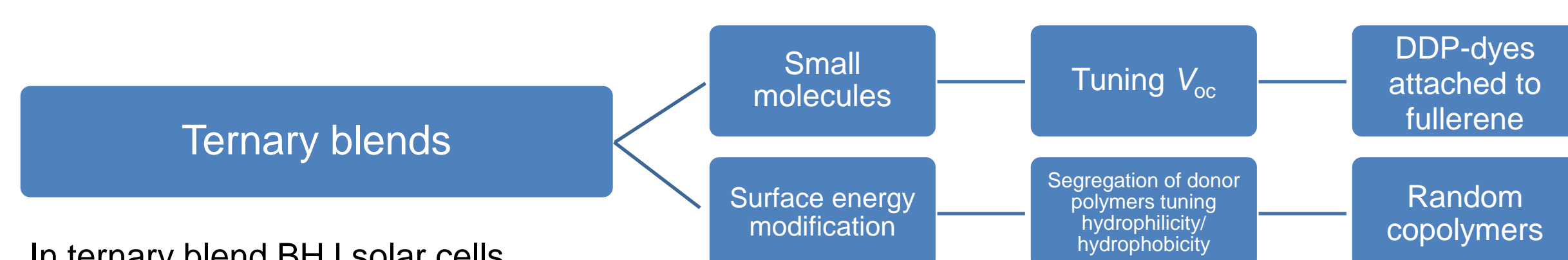


These monomers, along with 3-semifluorohexylthiophene and 3-(hydroxyl-oligoethylene oxide)-thiophene, provide:

- Basis for a new family of homopolymers, random copolymers, and semi-random copolymers with a range of electronic structures and surface energies
- Necessary control over phase separation to achieve desired morphologies by specific generation of donor polymers categorized as strongly hydrophilic, hydrophilic, hydrophobic, and strongly hydrophobic.

## Project Overview

Solar energy is among the most attractive forms of alternative energy. It has become apparent that utilization is best achieved through development of inexpensive strategies, such as solution-processable polymer-based photovoltaics. A ternary blend approach promises practical simplicity combined with the potential for performance exceeding that of tandem solar cells.



In ternary blend BHJ solar cells, the dye component:

- Can increase the spectral breadth of light absorption and thus  $J_{sc}$  (short circuit current)
- Provides a means to tune  $V_{oc}$  (open circuit voltage) through compositional control

The potential for simultaneous increase of both  $J_{sc}$  and  $V_{oc}$  corresponds to a higher  $J_{sc} \times V_{oc}$  product and efficiency that can rival or surpass that of a binary blend with same constituent components.

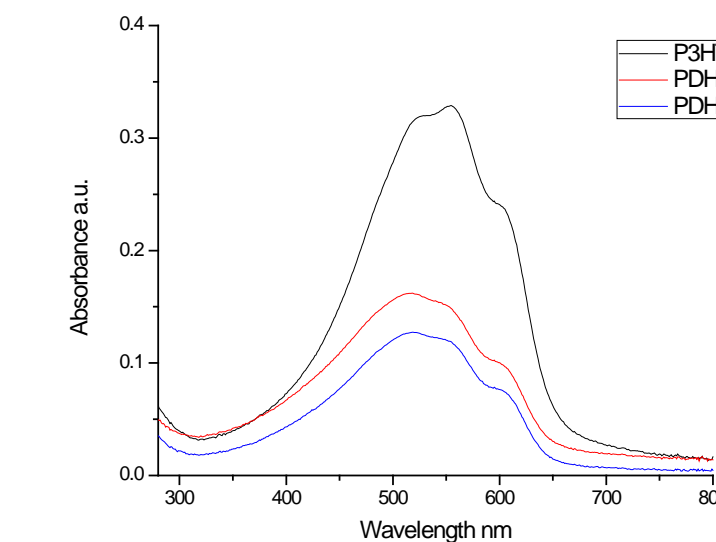
## Diketopyrrolopyrrole-based dye

### Synthesis of an ethanol-based precursor to trifluoromethylphenyl diketopyrrolopyrrole (TFDPP)



Copolymers with a range of electronic structures and surface energies can be used to explore the influences of morphology and electronic structure relationships in ternary blends.

### UV/Vis Absorption



## Outlook

- Define effect of the added dye compound
- Provide adequate explanation of how the addition strategy influences device properties

## References

<sup>1</sup> Thompson, B. C.; Fréchet, J. M. J. *Angew. Chem. Int. Ed.* **2008**, *47*, 58-77.