Utilizing Thiazole and Thioalkyl Side Chains in DPP-based Donor-Acceptor Copolymers for Organic Electronics

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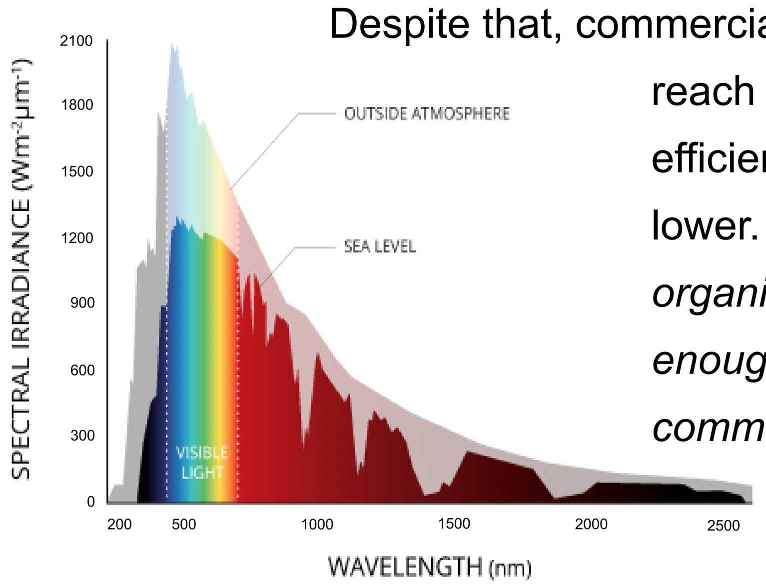
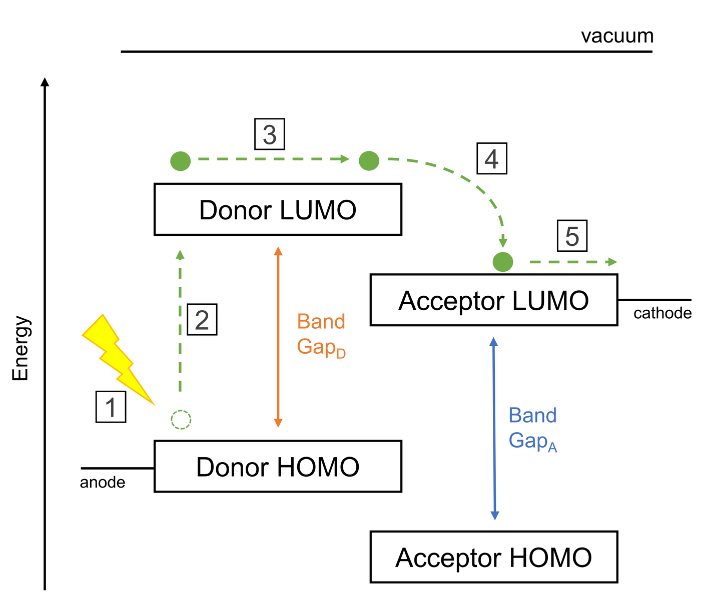
Motivation & Background

There is an ever-growing need for clean, renewable energy. Just one hour of unobstructed sunlight has enough energy to power the entire world for a year! So why don't we use this?

A large amount of solar radiation is lost to the atmosphere. Despite that, commercial silicon solar cells only reach up to around 20% efficiency. Organics are even lower. *The goal is to create new organic donor materials with high enough efficiencies to commercialize.*

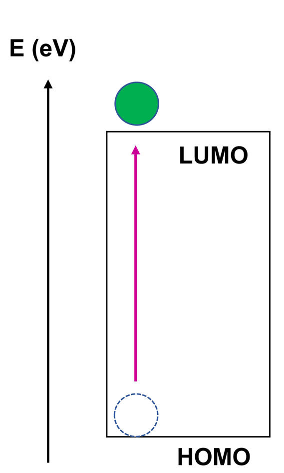


Basics of an Organic Solar Cell



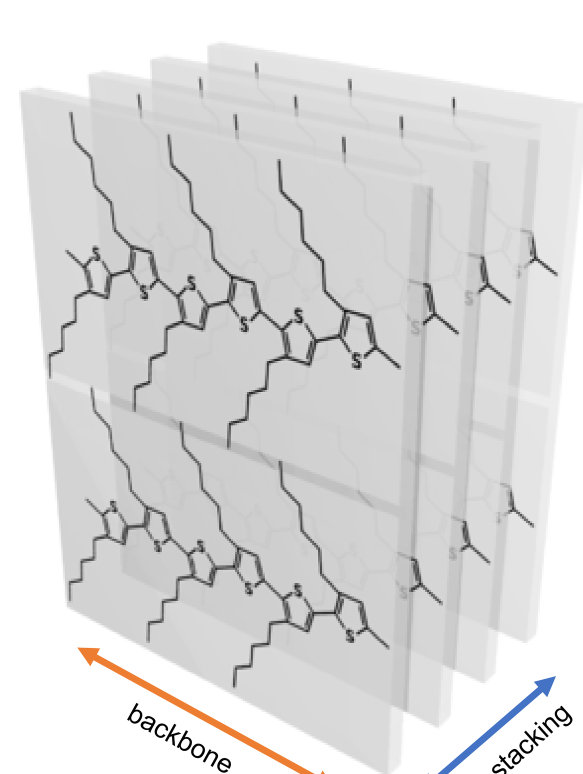
1. Photon absorbed
2. Electron excited
   - Leaves positive charge (*hole*)
3. Charges travel to D/A interface
4. Charge separation
5. Charges collected

Ideal Parameters

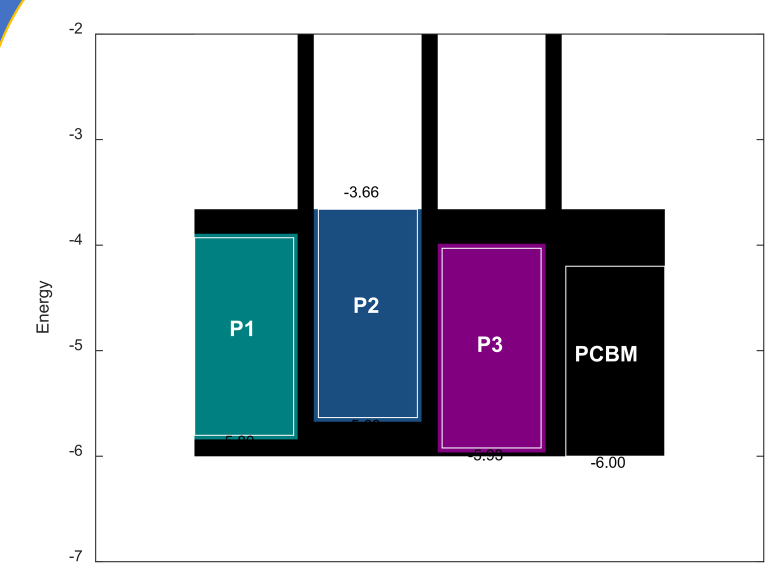


- Relatively stable LUMO energy levels (-3.8eV or lower)
- Small HOMO to LUMO gap (*band gap*) to limit the amount of energy needed to excite charges

- Soluble without compromising packing abilities
- Effective charge carrying capabilities (*conjugation*) both along the backbone and between polymer faces (*π-π stacking*)
- Ease of production



Electronic Data

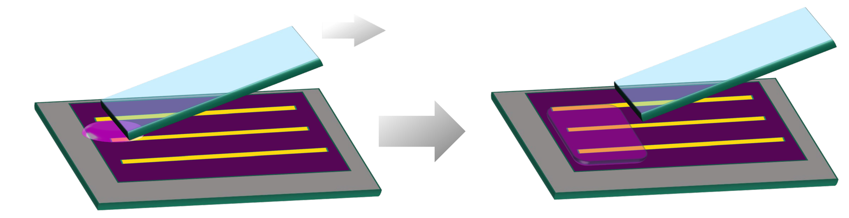


Estimated HOMO/LUMO levels of polymers against a common acceptor, PCBM.

	Hole Mobility ($cm^2/V \cdot s$)	Electron Mobility ($cm^2/V \cdot s$)
P1	1.21×10^{-5}	8.34×10^{-5}
P2	3.53×10^{-4}	-
P3	2.13×10^{-5}	8.45×10^{-5}

Mobility values based on solution in chloroform and heated 30min at 60°C.

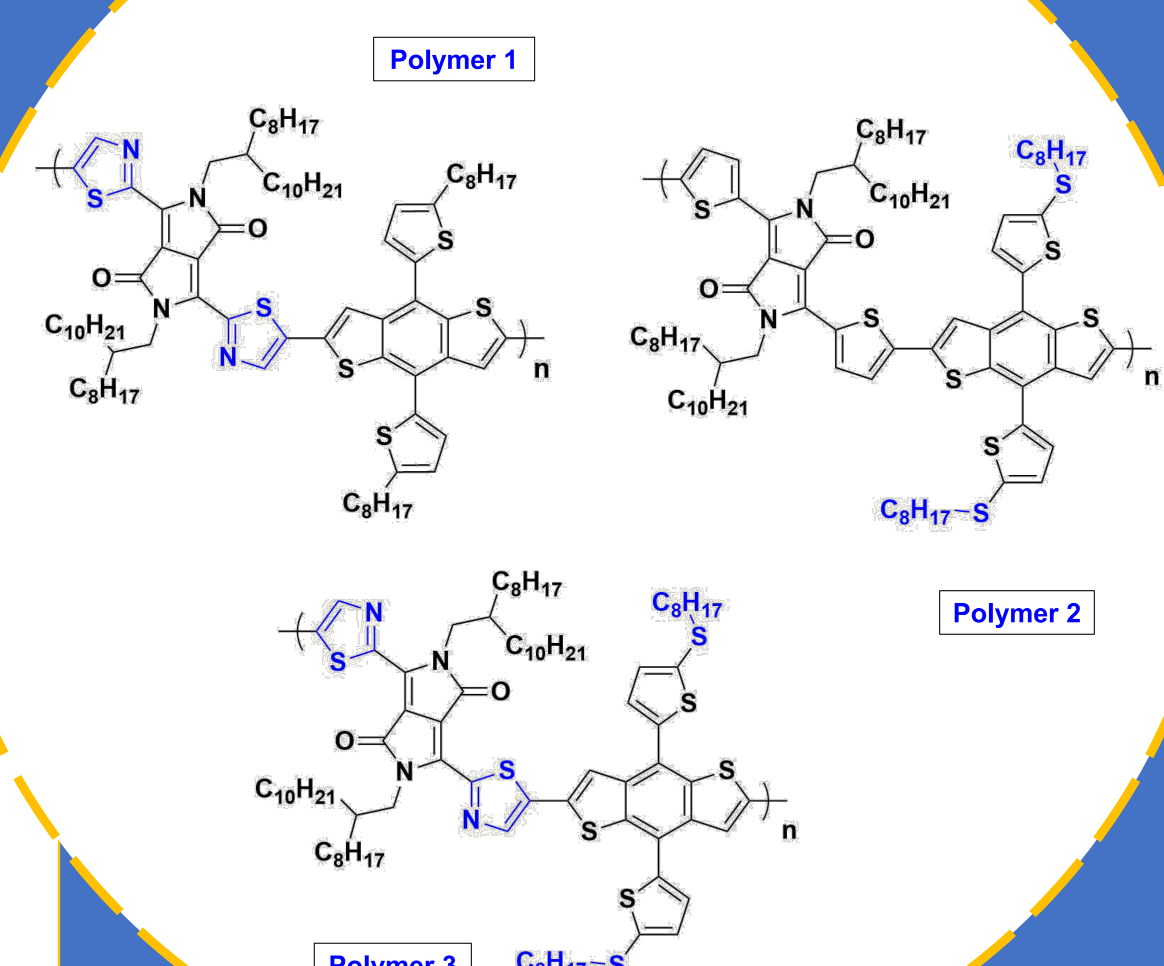
- Electronic tests suggest P2 has the largest band gap of 1.97eV, while P1 and P3 are at 1.87eV and 1.89eV.
- P2 has the highest energy levels, suggesting it could be a better donor material



Organic Field Effect Transistors (OFETs) are a simple method that determine the ability of a material to move charges. The polymer is blade coated, as shown in figure above, and a voltage is applied to read the current produced.

- P2 is an order of magnitude better at moving holes than the other two polymers
- P1 & P3 are four time or more better at moving electrons than holes

Polymer Design

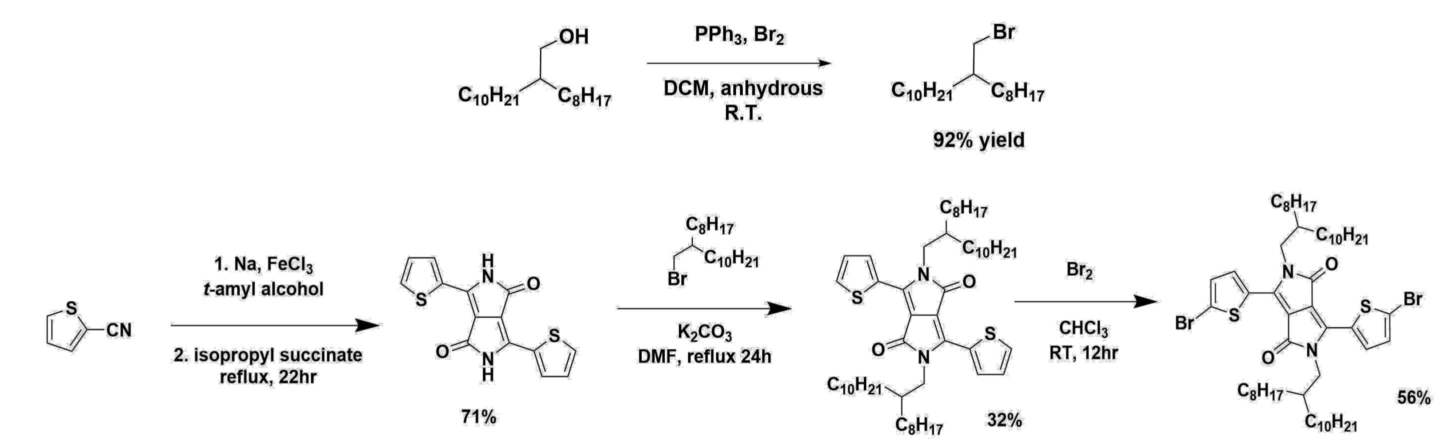


Key Components

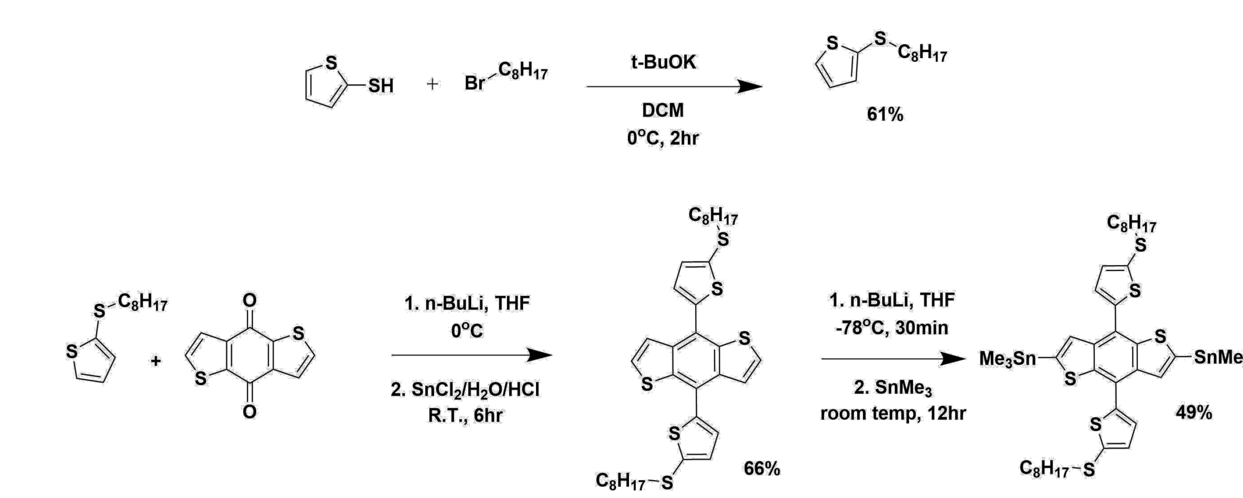
- Side Chain – needed for solubility but can reduce packing ability
- 2D Conjugation – possibility to extend conjugation into another plane
- Aromatic Linker – needs to maintain low torsional angle
- Octyl-thiol group – shown to stabilize HOMO/LUMO energy levels

Total Synthesis Example: P2

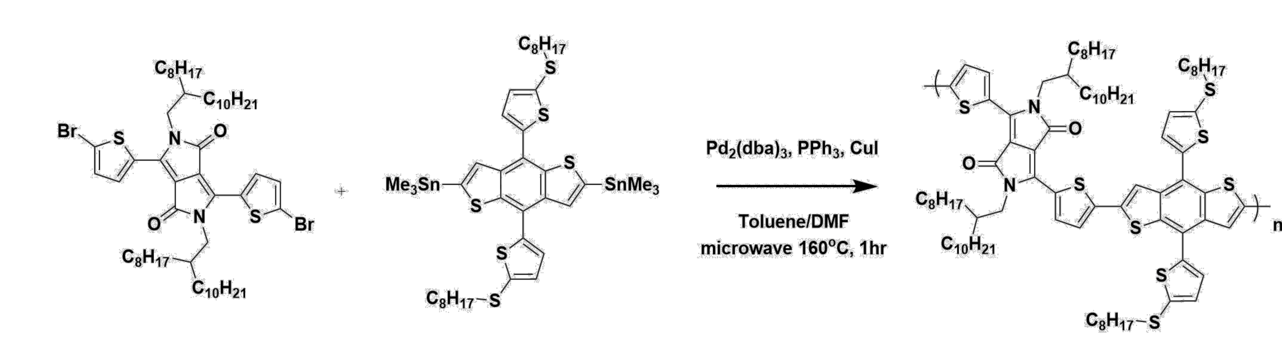
DPP-Tz Synthesis



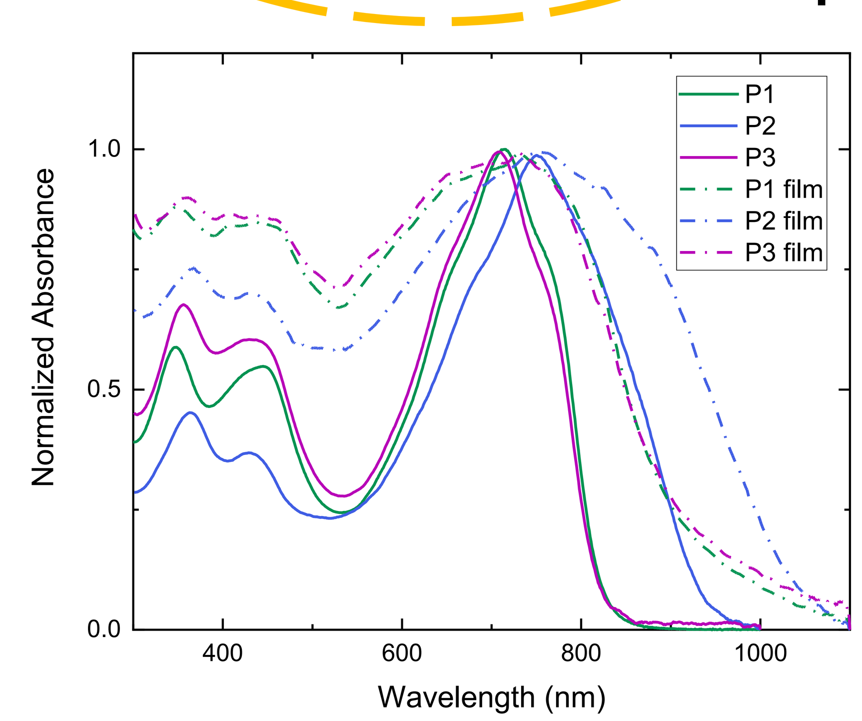
BDT-OSTh Synthesis



Microwave Stille Polymerization



Spectroscopic Data



UV-vis spectra of polymers in chloroform and film.

- P2 has the highest absorption onset, thus it has the smallest optical band gap (E_g^{opt}).
- P1 and P3 have roughly the same onsets and E_g.

	Solution		Film	
	Onset Abs (nm)	E_g^{opt}(eV)	Onset Abs (nm)	E_g^{opt}(eV)
P1	823	1.51	917	1.35
P2	941	1.32	1038	1.19
P3	824	1.50	930	1.33

Conclusions

- P2 has the smallest optical band gap, but the largest electronic band gap
- P1 and P3 transport electrons approximately four times better than holes, meaning they may work better as acceptors
- P2 is an order of magnitude better at moving charges than P1 and P3
- Preliminary solar testing of P2 with PC71BM has <1% efficiency

Future Work

- Test polymers as donors in solar cells with PCBM
- Test all-polymer solar cells

Acknowledgements

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