Synthesis and characterization of new electron-withdrawing moiety thieno[2,3-c] pyrrole-4,6- dione-based molecules for small molecule solar cells

傅磊 （10929037） 导师：陈红征 教授

MOE Key Laboratory of Macromolecular Synthesis and Functionalization, State Key Lab of Silicon Materials, & Department of Polymer Science and Engineering, Zhejiang University

Introduction

Organic photovoltaic (OPV) cells have become a promising alternative technology for producing clean and renewable energy due to their unique advantages, such as low-cost, simple manufacturing process and light weight. The imide moiety from thieno[2,3-c] pyrrole-4,6-dione (TPD) is a simple and common electron-withdrawing substituent which can be easily modified to improve the solubility and efficiently lower the HOMO of materials while maintaining or reducing band gap. Therefore new conjugated small molecules DTS(BTTPD)$_2$ and DTS(TTPD)$_2$ of the acceptor-π-donor-π-acceptor type end-capped with thieno[2,3-c] pyrrole-4,6-dione (TPD) units for small molecule solar cells have been prepared through coupling of dithienosilole (DTS) and TPD units bridged with thienylene and bithienylene[1].

Optical and Electrochemical properties

Compared to the solution, the absorption peaks of the thin films are broadened and exhibit red-shift by 20 nm and 30 nm for DTS(BTTPD)$_2$ and DTS(TTPD)$_2$, respectively, indicating good intermolecular interaction and that significant π-π stacking occurred in the solid state. Interestingly, when the thin film of DTS(BTTPD)$_2$ was placed for 2 min at the room temperature, the absorption maxima hypochromatic shifted to 511 nm, suggesting that H-aggregates might be formed in the solid state. These small molecules had very similar optical band gaps (1.87eV and 1.92 eV) and fairly close HOMO energy levels (-5.52 and -5.55 eV) for DTS(BTTPD)$_2$ and DTS(TTPD)$_2$, respectively.

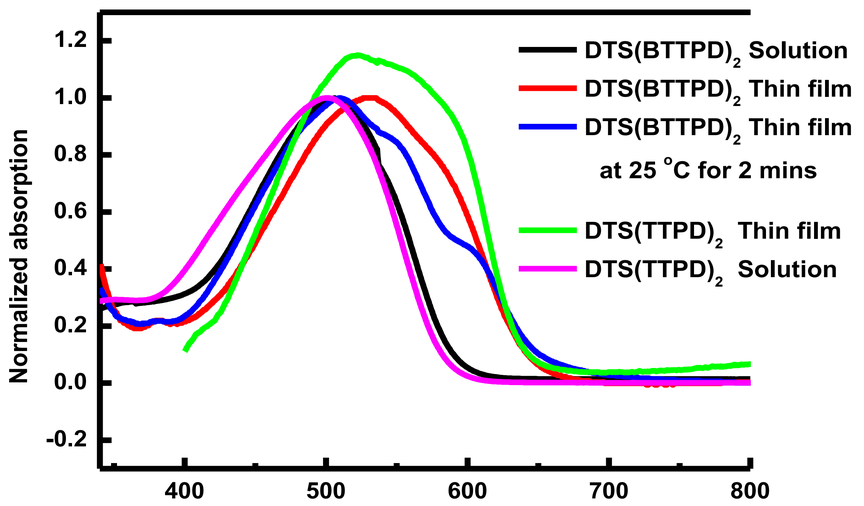


Figure 1. UV-vis absorption spectra of **DTS(BTTPD)$_2$** and **DTS(TTPD)$_2$** in $CHCl_3$ solution and the thin film.

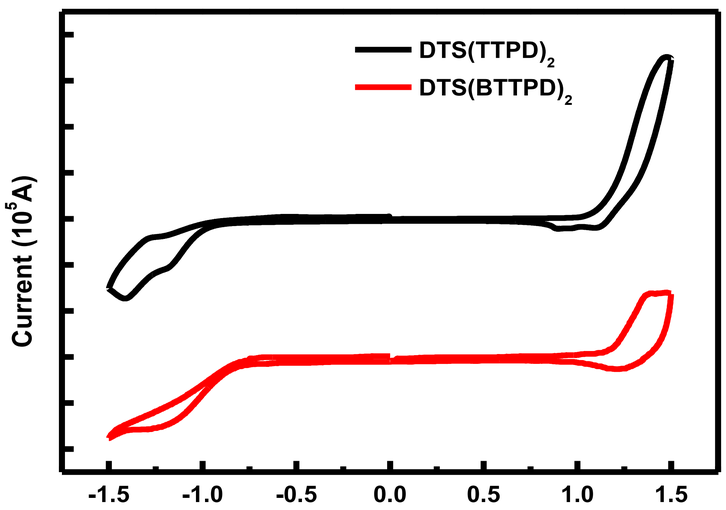
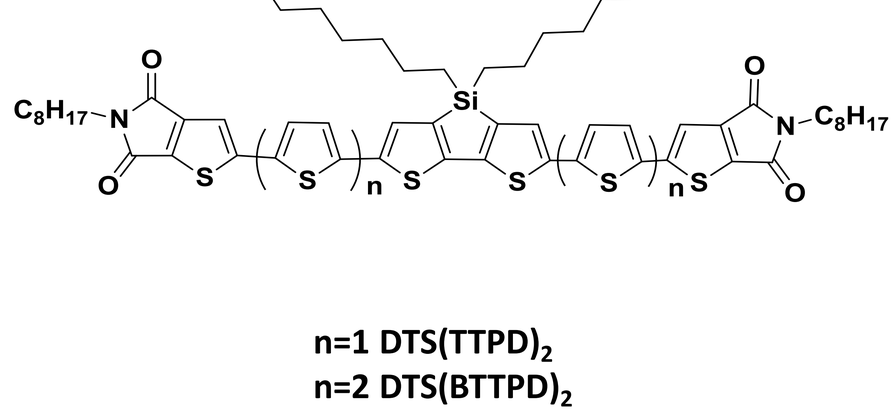


Figure 2. CV traces of **DTS(BTTPD)$_2$** and **DTS(TTPD)$_2$**



Photovoltaic property

Table 1. Optimized photovoltaic performance for normal geometry devices based on with **DTS(TTPD)$_2$** or **DTS(BTTPD)$_2$:PC$_{61}$BM** blends under illumination of AM 1.5G, 100 mW cm^{-2}.

Molecule	Donor: $PC_{61}BM$ (weight ratios)	V_{oc} (V)	J_{sc} (mA/cm^2)	FF (%)	PCE (%)
DTS(TTPD)$_2$	2:3[a]	0.99	2.28	31.01	0.70
	2:3[b]	0.97	2.60	47.58	1.20
DTS(BTTPD)$_2$	2:3[a]	0.88	2.59	32.90	0.75
	2:3[b]	0.67	1.20	27.11	0.22

a) as cast
b) annealed at 110 ° C

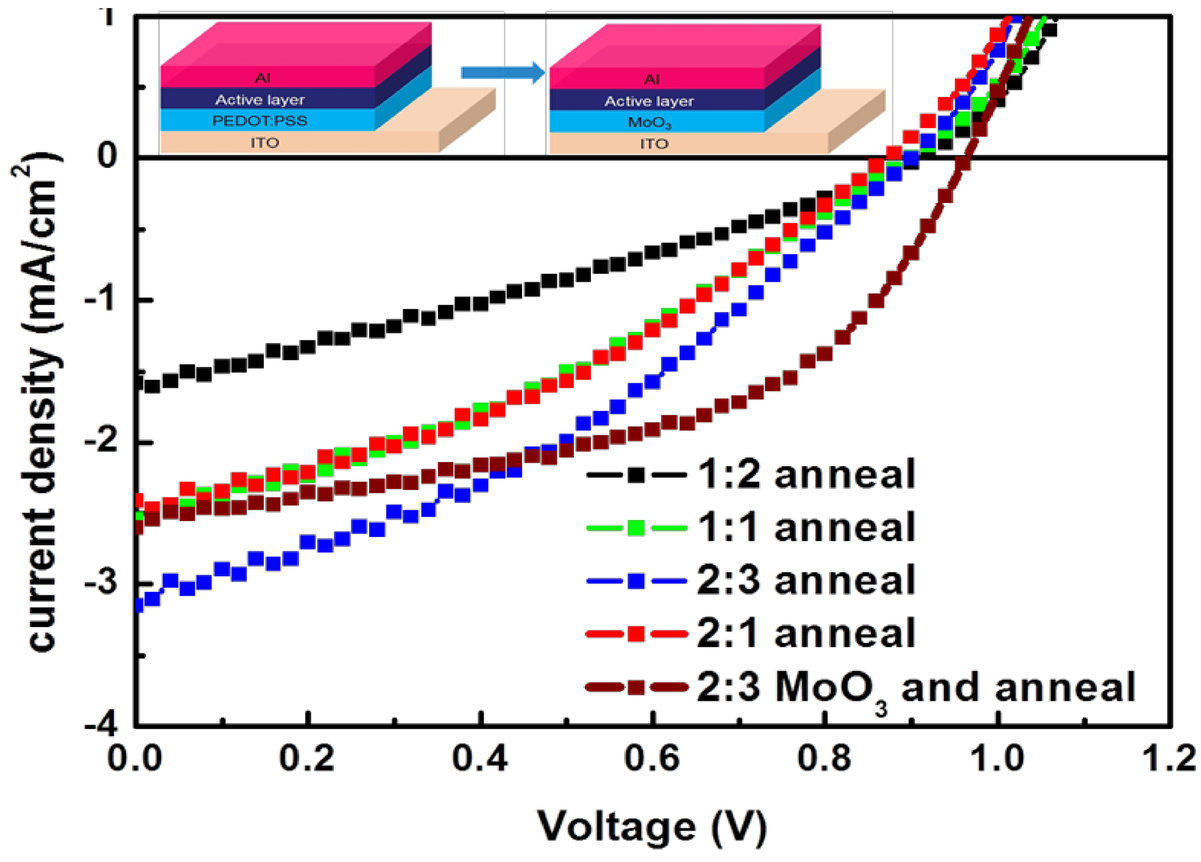


Figure 3. J–V curves obtained from normal geometry devices with different **DTS(TTPD)$_2$: PC$_{61}$BM** blends annealed at 110° C for 3 min.

Acknowledgements

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References

[1] L. Fu, H. B. Pan, T. T. Larsen-Olsen, T. R. Andersen, E. Bundgaard, F. C. Krebs, and H. Z. Chen, *DYES PIGMENTS*. 2012,92,1384-93.