Effect of end-groups on the photovoltaic property of diphenyl substituted diketopyrrolopyrrole derivatives

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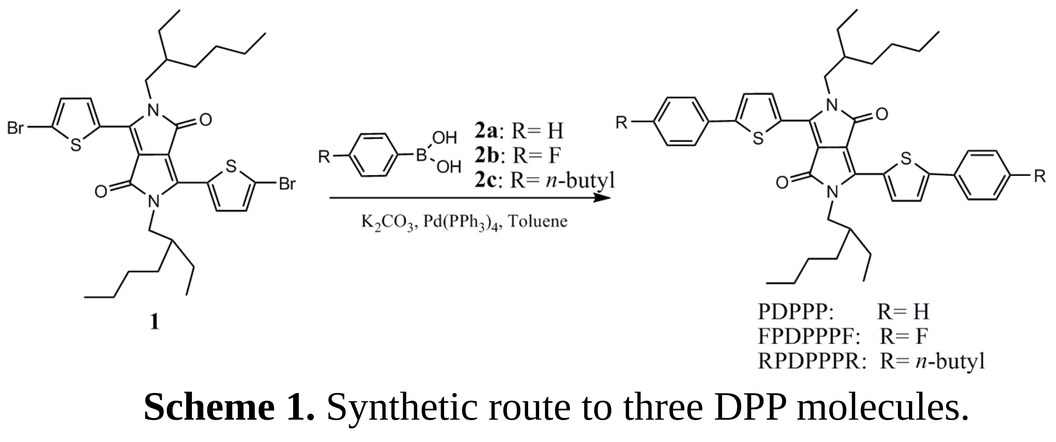
Introduction

Chemical modifications are normally employed for improving the solubility of diketopyrrolopyrrole (DPP)-based molecules and polymers by introducing alkyl side chains on the DPP core[1]. However, researches on the effect of different substituents on the aggregation structure and photovoltaic property of DPP-based small molecules, especially substituents as end-groups instead of side-groups, are few. In this work, we designed and synthesized a diphenyl substituted DPP molecule and its two derivatives end-capped with fluorine and n-butyl respectively. Their optical properties, electrochemical behaviors, and the morphologies of the blended films with $PC_{61}BM$ are fully investigated, in order to clarify how the end-groups influence the photovoltaic property of DPP derivatives.



Scheme 1. Synthetic route to three DPP molecules.

Result & Discussion

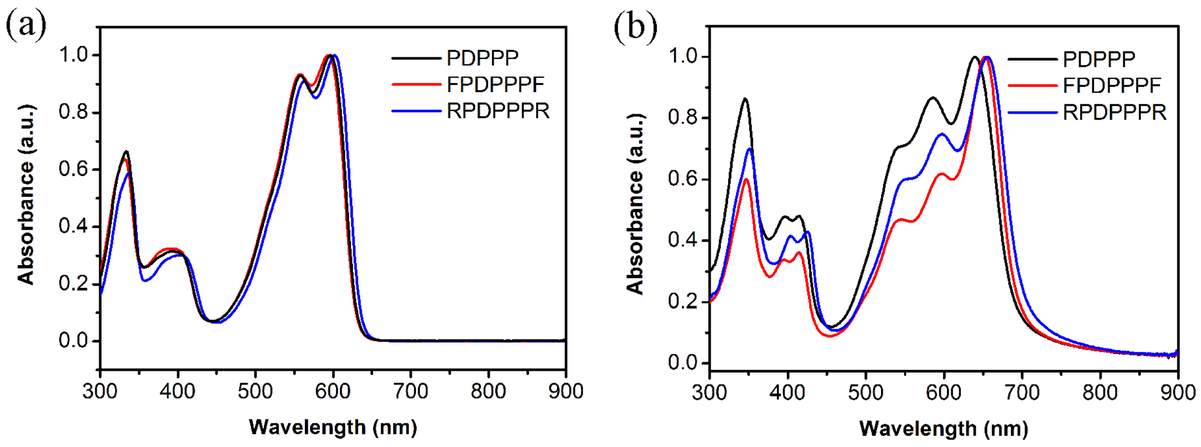


Fig. 1. UV-vis absorption spectra of three DPP molecules in (a) chloroform solutions and (b) solid films.

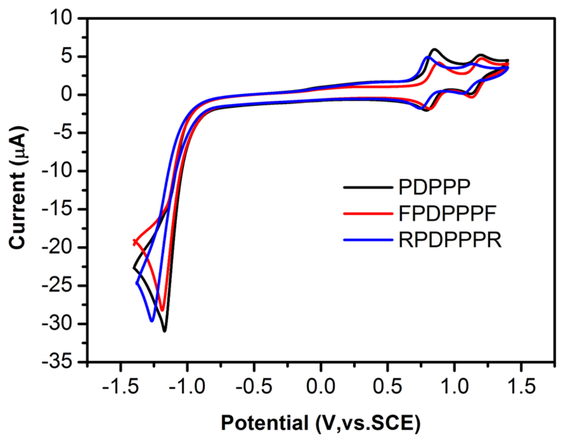


Fig. 2. Cyclic voltammograms of three DPP molecules at the scanning rate of 50 mV/s.

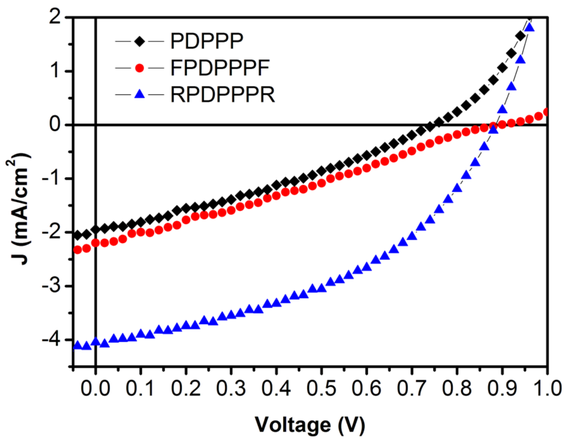


Fig. 3. *J-V* characteristics of the best OSCs based on three DPP molecules.

The three molecules exhibit similar energy structures, i.e. both relatively narrow optical band gaps (1.75~1.79 eV) and deep HOMO energy levels (-5.18~-5.25 eV). However, three molecules show different photovoltaic performances.

Table 1 Photovoltaic parameters of the devices based on DPP molecules.

Donor Material	D:A ratio	J_{sc} (mA/cm^2)	V_{oc} (V)	*FF*	PCE (%)
PDPPP	1:1	1.94	0.74	0.32	0.46
FPDPPPF	1:2	2.19	0.89	0.28	0.55
RPDPPPR	1:1	4.05	0.88	0.45	1.59

Through atomic force microscopy (AFM), space charge limited current (SCLC) and X-ray diffraction (XRD) characterizations, the prominent role of end-groups in the photovoltaic properties of DPP derivatives are disclosed.

Fig. 4. AFM images of DPP molecule : $PC_{61}BM$ blended films with the best photovoltaic performances.

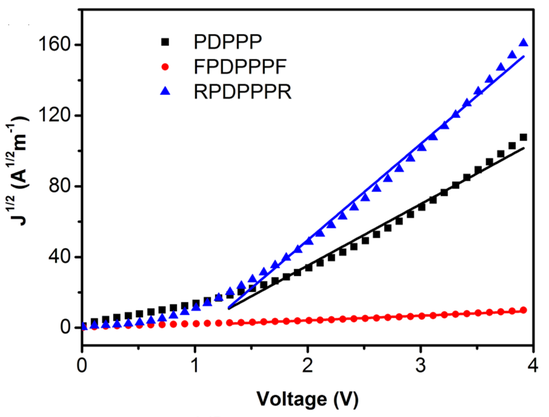


Fig. 5. $J^{1/2}$-V characteristics of electron-only devices.

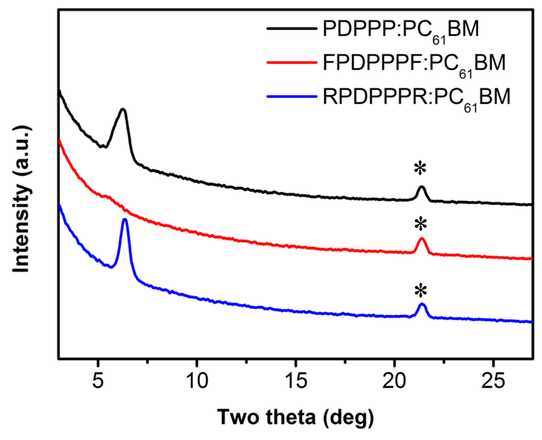


Fig. 6. XRD patterns of three active layers on the top of PEDOT:PSS and ITO.

Conclusion

Terminal alkyl chains in RPDPPPR can promote molecular crystallization and lead to the formation of finer phase-separation domains in the blended film, which are in favor of charge generation and transportation in the photovoltaic devices. Thus, RPDPPPR provides the best photovoltaic property among three DPP molecules.

Reference

[1] W. Li, K.H. Hendriks, W.S.C. Roelofs, Y. Kim, M.M. Wienk, R.A.J. Janssen, Adv. Mater. 25 (2013) 3182–3186.