# A spirobifluorene and diketopyrrolopyrrole moieties based non-fullerene acceptor for efficient and thermally stable polymer solar cells with high open-circuit voltage

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## Introduction

Fast development of polymer solar cells was made in the previous decades with the promise of eventually producing light weight, flexible and low-cost clean energy alternatives. The prospect material innovation has long been a strong driving force to move the field forward. However, the development of electron acceptors occurred at a relatively slower pace than that of donor components. This is because the fullerene derivative based acceptors were being widely used in devices with no rival alternatives, though their clear drawbacks, such as limited chemical and energetic tunabilities, poor light-absorption, high-cost purification, and morphology instability, have become the bottlenecks to constrain the further advancement of PSCs.

Recently, the exploration of non-fullerene electron acceptors have gained considerable attention and we report herein the design of a new non-fullerene acceptor, $SF(DPPB)_4$, which shows a cross-shaped molecular geometry to help suppress strong intermolecular aggregation. In addition, the energy levels of $SF(DPPB)_4$ match well with those of P3HT, which not only allows achievement of efficient exciton dissociation, but also ensures high $V_{oc}$ (1.14 V) and efficiency (5.16%) in P3HT:$SF(DPPB)_4$ PSCs. Moreover, the devices show excellent thermal stability. The abovementioned results demonstrate that the new design strategy of employing a high-performance non-fullerene acceptor has promising practical applications.

## Results and discussion

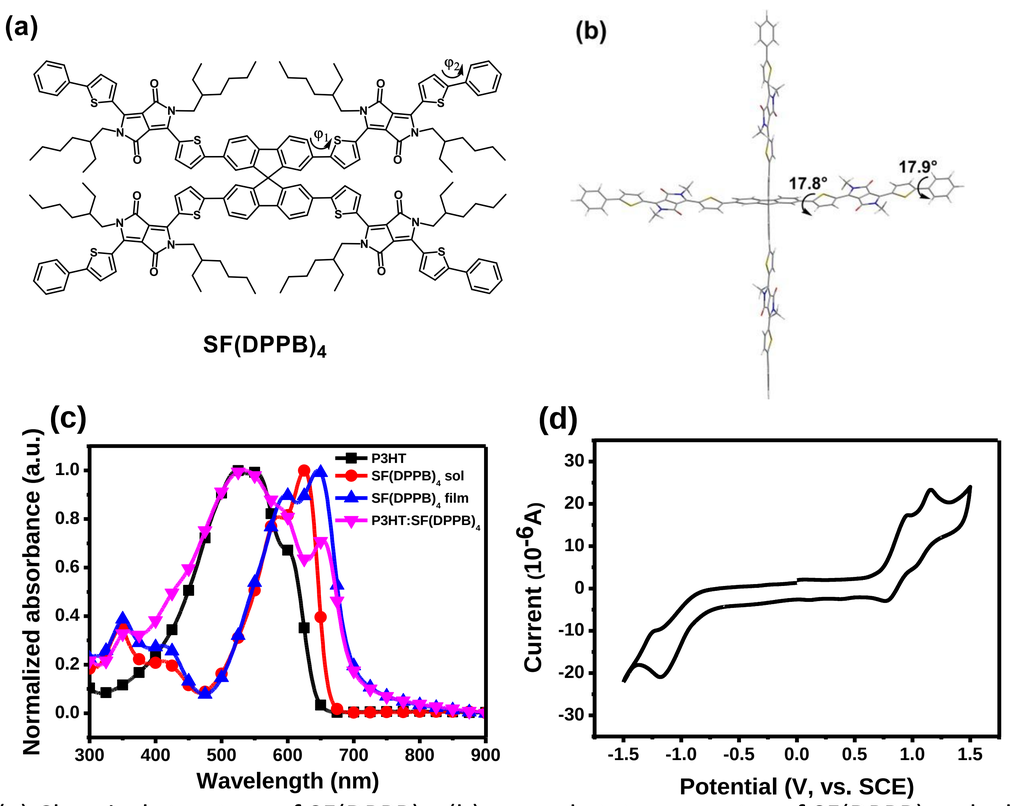


**Fig. 1** (a) Chemical structure of $SF(DPPB)_4$; (b) ground-state geometry of $SF(DPPB)_4$ calculated by DFT method; (c) UV-vis absorption spectra of P3HT film, $SF(DPPB)_4$ solution and film, and P3HT:$SF(DPPB)_4$ (2:1, by wt.) blended film; (d) cyclic voltammogram for $SF(DPPB)_4$ in dichloromethane solution.

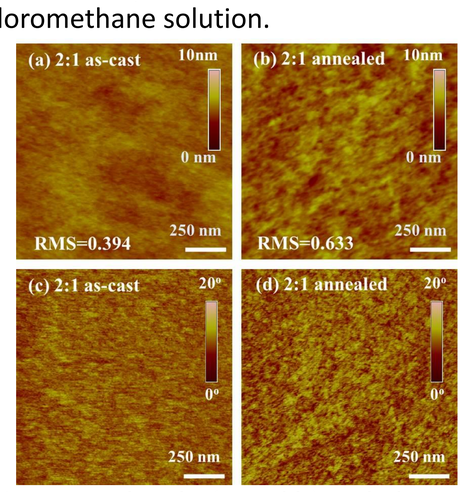


**Fig. 4** AFM height (a and b) and phase (c and d) images of the as-cast (aand c) and annealed (b and d) P3HT:$SF(DPPB)_4$ films.

**Table 1** The photovoltaic performances of the PSCs based on P3HT:$SF(DPPB)_4$.

| D:A (w/w) | $V_{oc}$ (V) | $J_{sc}$ (mA cm$^{-2}$) | FF | PCE (%) |
|---|---|---|---|---|
| P3HT:$SF(DPPB)_4$ (2:1)[a] | 1.20 | 1.91 | 0.28 | 0.63 (0.60)[d] |
| P3HT:$SF(DPPB)_4$ (1:1)[b] | 1.13 | 5.78 | 0.57 | 3.70 (3.57)[d] |
| P3HT:$SF(DPPB)_4$ (2:1)[b] | 1.14 | 8.29 | 0.55 | 5.16 (5.10)[d] |
| P3HT:$SF(DPPB)_4$ (3:1)[b] | 1.13 | 7.13 | 0.46 | 3.68 (3.55)[d] |
| P3HT:$PC_{61}BM$ (1:0.8)[c] | 0.62 | 8.27 | 0.62 | 3.18 (3.14)[d] |

[a] As-cast. [b] Annealed at 120 °C for 10 min. [c] Annealed at 170 °C for 10 min. [d] The values in the parentheses are the average PCEs from 10 devices.

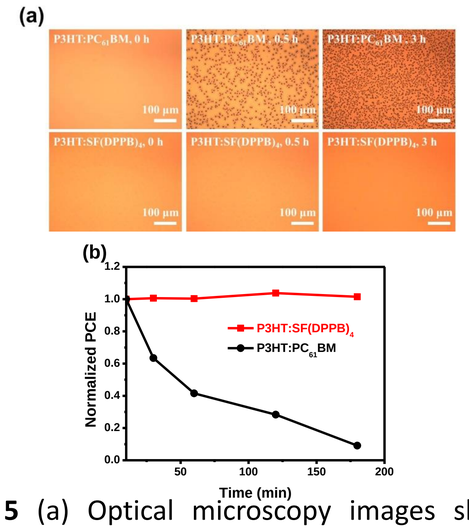


**Fig. 5** (a) Optical microscopy images showing morphological stability of P3HT:$PC_{61}BM$ (1:0.8, by wt.) and P3HT:$SF(DPPB)_4$ (2:1, by wt.) blended films after thermal treatment at 150 °C for various time; (b) graph showing the stability of the PCEs for the devices based on P3HT:$SF(DPPB)_4$ (2:1, by wt.) and P3HT:$PC_{61}BM$ (1:0.8, by wt.) blended films after thermal treatment at 150 °C for various time.

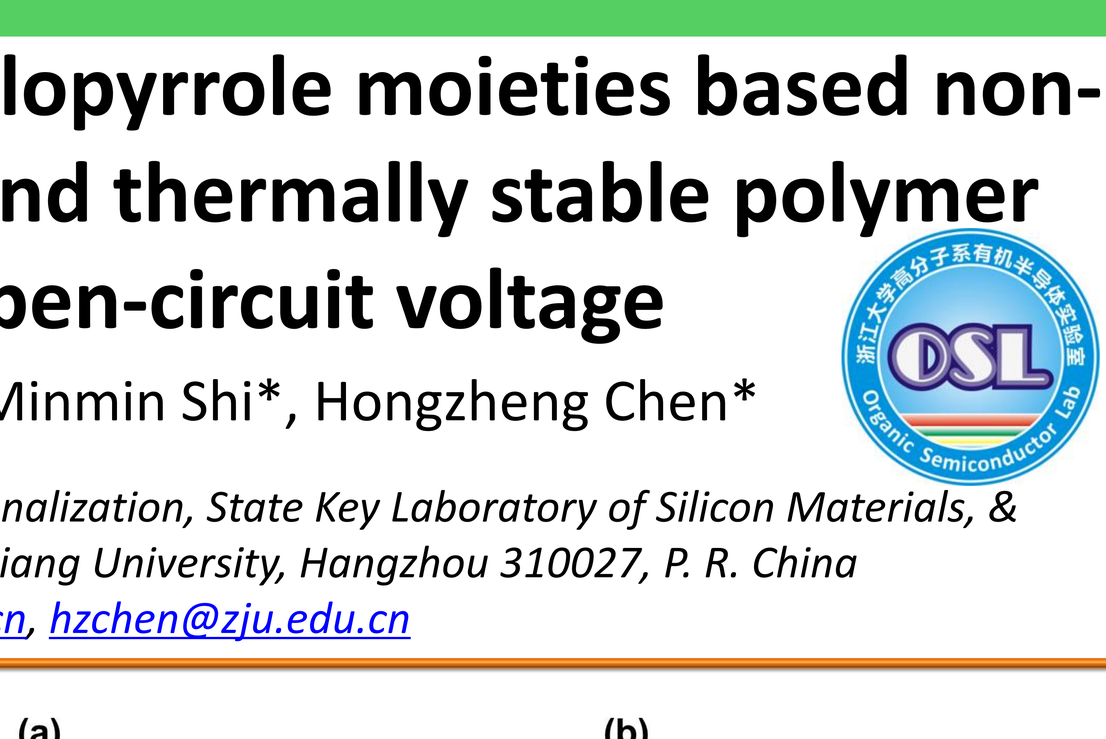


**Fig. 2** (a) Energy levels of P3HT, $SF(DPPB)_4$ and $PC_{61}BM$; (b) the diagram of device structure; (c) *J-V* curves of PSCs with the structure of ITO/PEDOT:PSS/P3HT:$SF(DPPB)_4$/PFN/Al; (d) EQE spectra of P3HT:$SF(DPPB)_4$ based PSCs.

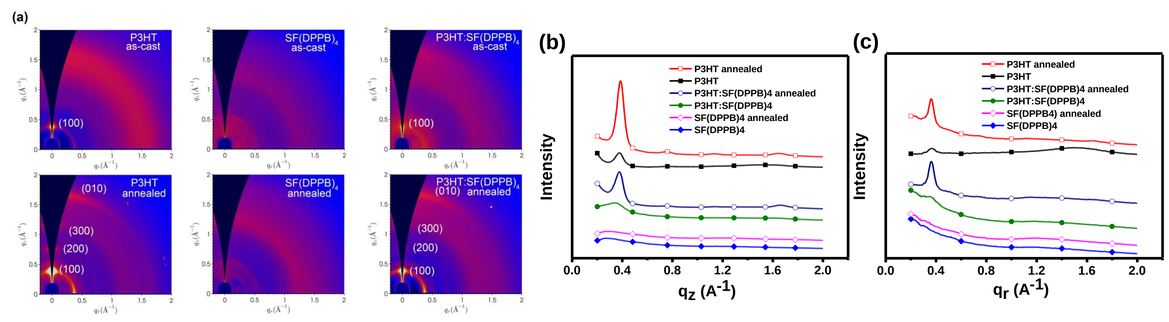


**Fig. 3** (a) 2D GIWAXS images of P3HT, $SF(DPPB)_4$ and 2:1 P3HT:$SF(DPPB)_4$ thin films with or without the thermal annealing at 120 °C for 10 min; (b) intensity profiles along $q_z$ axis of P3HT, $SF(DPPB)_4$ and 2:1 P3HT:$SF(DPPB)_4$ thin films; (c) corresponding intensity profiles along $q_r$ axis.

## Conclusions

In summary, a spirobifluorene core based non-fullerene electron acceptor, $SF(DPPB)_4$, was designed and synthesized. $SF(DPPB)_4$ possesses a cruciform molecular configuration, which assures fine phase separation in the active layer of corresponding PSCs. In addition, $SF(DPPB)_4$ exhibits appropriate absorption bands and matching energy levels for P3HT. Owing to the good morphology and an outstandingly high $V_{oc}$ of 1.14 V, the PSCs based on the P3HT:$SF(DPPB)_4$ blended films provided the best PCE of 5.16%. To the best of our knowledge, this PCE is one of the highest values reported in the literature to date for P3HT-based fullerene-free PSCs. The P3HT:$SF(DPPB)_4$ based devices also show excellent thermal stability upon thermal treatment at 150 °C for up to 3 h, demonstrating that $SF(DPPB)_4$ is a promising non-fullerene acceptor for future practical application of PSCs.

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## Notes and references

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