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

Hangqi Shi(21129043), Minmin Shi*, Hongzheng Chen

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

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. 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.

Result & Discussion

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.

<table>
<thead>
<tr>
<th>Donor Material</th>
<th>D:A ratio</th>
<th>$J_{sc}$ (mA/cm²)</th>
<th>$V_{oc}$ (V)</th>
<th>FF</th>
<th>PCE (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>PDPPP</td>
<td>1:1</td>
<td>1.94</td>
<td>0.74</td>
<td>0.32</td>
<td>0.46</td>
</tr>
<tr>
<td>FPDPFFF</td>
<td>1:2</td>
<td>2.19</td>
<td>0.89</td>
<td>0.28</td>
<td>0.55</td>
</tr>
<tr>
<td>RPDPPP</td>
<td>1:1</td>
<td>4.05</td>
<td>0.88</td>
<td>0.45</td>
<td>1.59</td>
</tr>
</tbody>
</table>

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.

Table 1 shows the photovoltaic parameters of the devices based on DPP molecules.

Conclusion

Terminal alkyl chains in RPDPPP 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, RPDPPP provides the best photovoltaic property among three DPP molecules.

Reference