テトラベンゾポルフィリンを基本骨格とする熱前駆体法で成膜可能な非フラーレンアクセプター分子の開発

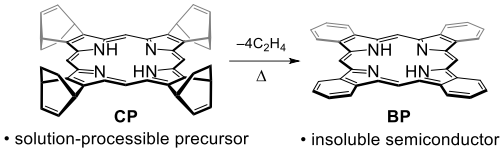
Development of Tetrabenzoporphyrin-Based Non-Fullerene Acceptor Molecules That Can Be Processed via a Thermal-Precursor Approach

奈良先端大物質[1]，阪大院工[2] ○ジョン ウンジョン[1]，鈴木 充朗[2]，荒谷 直樹[1]，山田 容子[1]

NAIST[1], Osaka Univ.[2] ○Eunjeong Jeong[1], Mitsuharu Suzuki[2], Naoki Aratani[1], Hiroko Yamada[1]

E-mail: jeong.eunjeong.jb2@ms.naist.jp

Tetrabenzoporphyrin (BP) holds attractive characteristics for optoelectronics applications, such as the large, rigid π-conjugated framework and high photoabsorption capability. Although BP has poor solubility in any solvents, thin films of BP can be prepared by depositing soluble precursor CP as a solution and then heating it to induce the *retro*-Diels–Alder reaction in situ (Scheme 1).[1] This "thermal precursor approach" would enable straightforward molecular design and clearer understanding of the structure–property relationship because it largely reduces the need for solubilizing groups that often obscure electronic properties of semiconducting molecules in the thin-film state.



Scheme 1. Thermal conversion of CP to BP.

In this work, $2CF_3BP$, $4CF_3BP$ and pCNBP equipped with multiple strongly electron-withdrawing groups have been designed (Fig. 1a), and evaluated as non-fullerene acceptors in organic solar cells (OSCs).[2] These compounds are deposited via the thermal precursor approach together with a common donor polymer, either P3HT or PTB7, to form bulk-heterojunction (BHJ)-type active layers. The resulting devices show clear photovoltaic response, proving that the new BP derivatives serve as acceptor in OSCs (Fig. 1b and Table 1). Although the power conversion efficiencies (PCEs) are rather limited (2.04% at best), this result is an important step in developing a novel class of non-fullerene acceptors for OSCs. Further, this is the first example wherein the thermal precursor approach is successfully employed for the preparation of polymer–small molecule blend films, thereby extending its scope of applicability. In this presentation, we will discuss in detail the relationship among the molecular structure, electronic properties, and thin-film morphology.

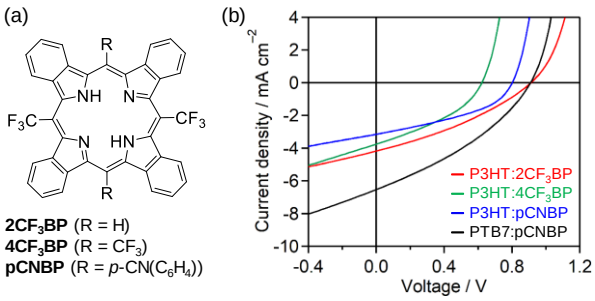


Fig. 1 (a) Chemical structures of $2CF_3BP$, $4CF_3BP$ and pCNBP; (b) *J*–*V* curves of OSCs.

Table 1. Photovoltaic parameters of the BHJ OSCs.[a,b]

Entry	Active layer	J_{SC} / mA cm^{-2}	V_{OC} / V	FF / %	PCE / %
1	P3HT:$2CF_3BP$	4.18	0.912	33.1	1.26
2	P3HT:$4CF_3BP$	3.75	0.623	36.6	0.857
3	P3HT:pCNBP	3.15	0.802	40.5	1.02
4	PTB7:pCNBP	6.53	0.910	34.4	2.04

[a]Data of the best-performing devices. [b]Measured under simulated AM1.5G illumination at 100 mW cm^{-2}.

(1) Ito, S. et al. *Chem. Commun.* **1998**, 1661–1662. (2) Jeong, E. et al. *J. Org. Chem.* **2019**, DOI: 10.1021/acs.joc.9b02386.