Modulation of Orbital Energy Levels of Tetrabenzoporphyrin toward Increased Open-Circuit Voltage and Possibility as n-Type Material in Organic Solar Cells

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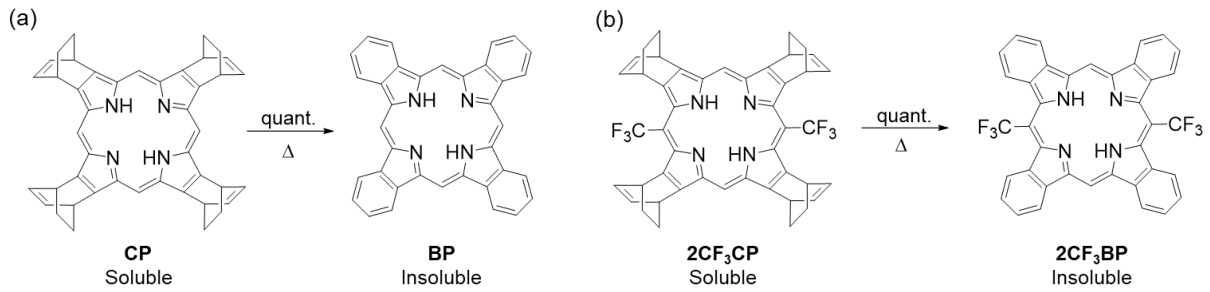
Tetrabenzoporphyrin (BP) is an organic p-type molecular semiconductor having a large π-conjugated system which can form effective charge-carrier paths in the solid state. However, BP has a poor solubility in any solvents, making its processing by cost-effective solution-based techniques quite difficult. This problem has been evaded via a "thermal precursor approach" in which a soluble precursor 1,4:8,11:15,18:22,25-tetraethano-29*H*,31*H*-tetrabenzo[*b*,*g*,*l*,*q*]porphyrin (CP) is solution-deposited then thermally converted to BP by in situ retro-Diels–Alder reaction (Scheme 1a) [1]. By taking advantage of this approach, power conversion efficiencies (PCEs) of over 5% have been achieved with BP or its derivatives[2–3]. However, the open-circuit voltage (V_{OC}) in these devices is relatively low because of the high energy level of the highest occupied molecular orbital (HOMO) of BP.

In this work, a new derivative named $2CF_3BP$ has been designed and evaluated as active-layer material in organic solar cells (OSCs). As $2CF_3BP$ is poor in solubility, it is solution-deposited via the thermal precursor approach from its soluble precursor $2CF_3CP$ (Scheme 1b). A lower HOMO level than that of BP is achieved owing to the strongly electron-withdrawing trifluoromethyl groups. Consequently, $2CF_3BP$ based OSCs show high V_{OC} values of up to 0.96 V, which is the highest obtained so far with BP or its derivative. In addition, the introduction of two trifluoromethyl groups effectively reduced the energy level of the lowest unoccupied molecular orbital (LUMO), allowing $2CF_3BP$ to serve as n-type material in OSCs. The thin-film characteristics and device performance will be discussed in detail in the presentation.



Scheme 1. Thermal conversion of CP to BP (a) and $2CF_3CP$ to $2CF_3BP$ (b)

1. Ito, S. et al. *Chem. Commun.* **1998,** 1661–1662.

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