# An ester-functionalized diketopyrrolopyrrole molecule for solution-processed organic solar cells with the enhanced open-circuit voltage

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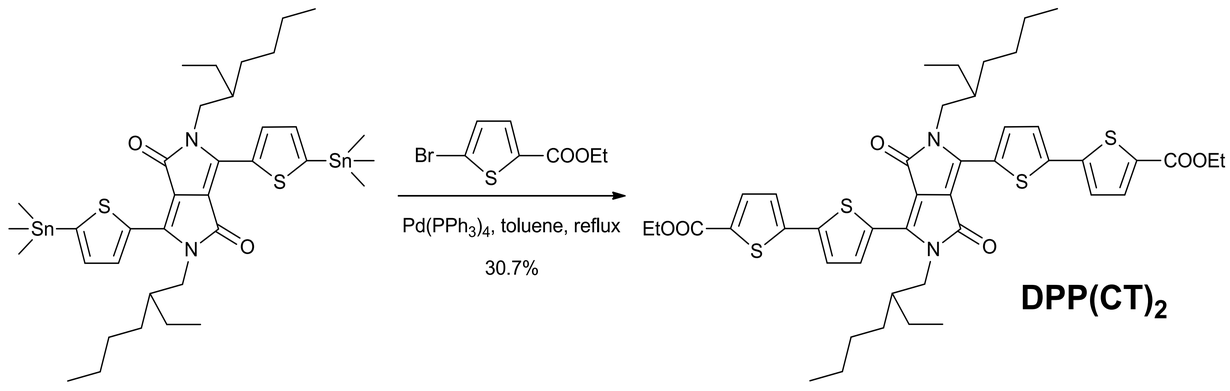
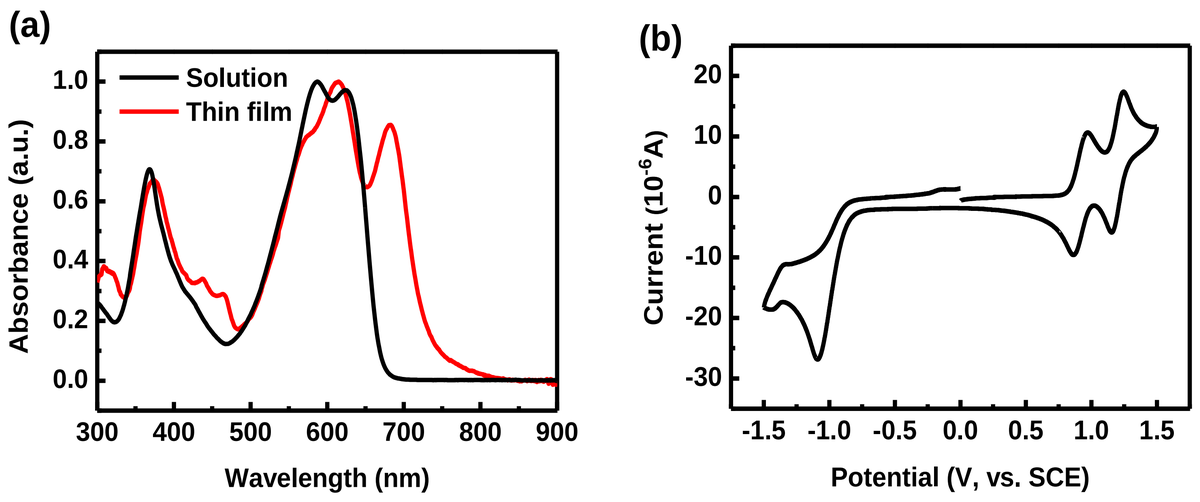
**Introduction:** For highly efficient organic solar cells (OSCs), electron donor should possess not only narrow band gap ($E_g$) but also low highest occupied molecular orbital (HOMO) energy level. To achieve it, here we designed and synthesized a diketopyrrolopyrrole (DPP) derivative end capped with ethyl thiophene-2-carboxylate moiety, DPP(CT)$_2$. When DPP(CT)$_2$ is blended with [6,6]-phenyl-C$_{71}$-butyric acid methyl ester (PC$_{71}$BM) for solution processable OSCs, a power conversion efficiency (PCE) of 4.02% combined with an open-circuit voltage ($V_{OC}$) as high as 0.94 V and a broad photovoltaic response range extending to around 750 nm, is gotten.




**Scheme 1** Synthetic route to **DPP(CT)$_2$**.




**Optical band-gap ($E_g^{opt}$) = 1.65 eV**

**HOMO=-5.33 eV**
**LUMO=-3.60 eV**

**Fig. 1** Energy level structure of **DPP(CT)$_2$**. (a) UV-vis absorption spectra of **DPP(CT)$_2$** in $CH_2Cl_2$ solution and thin film. (b) Cyclic voltammogram of **DPP(CT)$_2$** in $CH_2Cl_2$ solution.

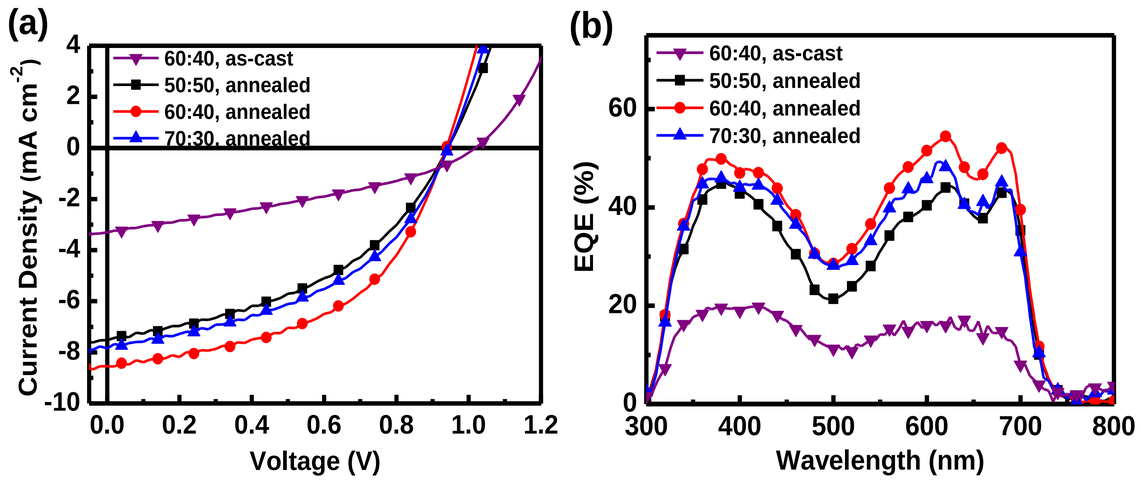



**Fig. 2** (a) *J-V* characteristics and (b) external quantum efficiency spectra of **DPP(CT)$_2$**:PC$_{71}$BM based OSCs under illumination of AM 1.5G, 100 mW cm$^{-2}$.

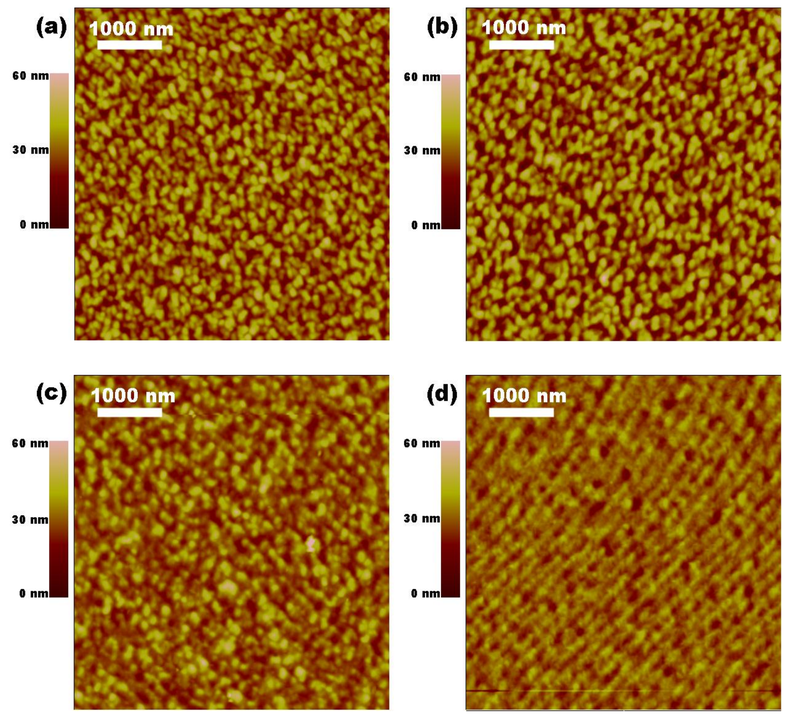



**Fig. 3** AFM images of **DPP(CT)$_2$:PC$_{71}$BM** blended films. (a) As-cast 60:40 film, (b) annealed 50:50 film, (c) annealed 60:40 film, and (d) annealed 70:30 film.

**Table 1.** Photovoltaic Performances of OSCs

| Active layer | Blend ratio | $V_{OC}$ (V) | $J_{SC}$ (mA cm$^{-2}$) | FF | PCE (%) | $\mu_h$ (cm$^2$V$^{-1}$s$^{-1}$) | $\mu_e$ (cm$^2$V$^{-1}$s$^{-1}$) |
|---|---|---|---|---|---|---|---|
| DPP(CT)$_2$:PC$_{71}$BM[a] | 50:50 | 0.94 | 7.53 | 0.44 | 3.11 | $8.68\times10^{-6}$ | $1.91\times10^{-5}$ |
| DPP(CT)$_2$:PC$_{71}$BM[a] | 60:40 | 0.94 | 8.55 | 0.50 | 4.02 | $9.64\times10^{-6}$ | $2.19\times10^{-6}$ |
| DPP(CT)$_2$:PC$_{71}$BM[a] | 70:30 | 0.94 | 7.84 | 0.46 | 3.36 | $9.57\times10^{-6}$ | $1.69\times10^{-6}$ |
| DPP(CT)$_2$:PC$_{71}$BM[b] | 60:40 | 1.02 | 3.31 | 0.34 | 1.14 | $7.44\times10^{-6}$ | $1.66\times10^{-7}$ |

[a] These devices are annealed at 90 $^o$C for 10 min; [b] as-cast.

## References

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