Electronic Supporting Information

Small-molecule semiconductors containing dithienylacrylonitrile for highperformance organic field-effect transistors

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1. Device fabrications and performances of the organic field-effect transistors (OFETs).

The OFET devices based on the small-molecular compounds were fabricated with bottom gate bottom contact (BGBC) configurations. The n⁺⁺-Si/SiO₂ (300 nm) substrates were used as the gate electrode/dielectric. The gold/titanium (30 nm/5 nm) was fabricated as source/drain electrodes. The silica substrates were modified with octadecyltrichlorosilane (OTS) to form an OTS self-assembled monolayer on their surfaces. A small-molecule semiconducting thin film layer was fabricated on the OTS-treated substrate by spin-coating. The device performance was evaluated by employed a Keithley 4200 SCS semiconductor parameter analyzer on a probe stage in ambient air. The charge carrier mobility (μ) was calculated from the data in the saturated regime according to the following equation,

$$I_{\rm DS} = \left(\frac{W}{2L}\right) C_{\rm i} \mu (V_{\rm G} - V_{\rm T})^2$$

In the above equation, I_{DS} , W/L, C_i , V_G and V_T are the saturation drain current, the channel width/length, the capacitance per unit area of the gate dielectric layer, the gate voltage and threshold voltage, respectively.

2. TGA curves of the DPP-DTE-based compounds



Fig. S1 TGA curves of the DPP-DTE-based compounds.



3. Absorption spectra of the DPP-DTE-based compounds

Fig. S2 UV-Vis-NIR absorption spectra of the DPP-DTE-based compounds in (a) chloroform solutions and (b) thin films.



4. Theoretical calculation results of the DPP-DTE-based compounds

Fig. S3 Optimized molecular geometries and frontier molecular orbital distributions of the model compounds DPP-CN-DTE and DPP-DTE-CN.

5. NMR spectra of the DPP-DTE-based compounds



Fig. S4 ¹H NMR spectrum of DPP-CN-DTE-1.



Fig. S5 ¹³C NMR spectrum of DPP-CN-DTE-1.



Fig. S6 HRMS (MALDI) spectrum of DPP-CN-DTE-1.





Fig. S8 ¹³C NMR spectrum of DPP-CN-DTE-2.



Fig. S9 HRMS (MALDI) spectrum of DPP-CN-DTE-2.



Fig. S10 ¹H NMR spectrum of DPP-DTE-CN-1.



Fig. S11 ¹³C NMR spectrum of DPP-DTE-CN-1.

Fig. S12 HRMS (MALDI) spectrum of DPP-DTE-CN-1.

Fig. S13 ¹H NMR spectrum of DPP-DTE-CN-2.

Fig. S14 ¹³C NMR spectrum of DPP-DTE-CN-2.

Fig. S15 HRMS (MALDI) spectrum of DPP-DTE-CN-2.