New thiophene-based C\textsubscript{60} fullerene derivatives as efficient electron transporting materials for perovskite solar cells

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Device Characterization

Current-Voltage ($J-V$) characteristics of photovoltaic cells were tested using a Keithley 2420 source meter under a Photo Emission Tech SS100 Solar Simulator, and the light intensity was calibrated by a standard Si solar cell. External quantum efficiency (EQE) was measured using a Bentham (from Bentham Instruments Ltd) measurement system. The light intensity was calibrated using a single-crystal Si photovoltaic cell as reference. The $J-V$ and EQE measurements were obtained in air. The scanning electron microscopy (SEM) images were collected using a ZEISS Sigma FE-SEM, where the electron beam was accelerated in the range of 500 V to 30 kV. Film thicknesses were measured using a KLA Tencor profilometer. The steady-state PL spectra were recorded on a Horiba Yvon Nanolog spectrometer coupled with a time-correlated single photon counting (TCSPC) with nanoLED excitation sources for time-resolved emission measurements.
Figure S1: a) $^1$H and b) $^{13}$C NMR spectra of compound 6.

$^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 7.18 (dd, 1H), 6.97 (dd, 1H), 6.89-6.88 (m, 1H), 4.39 (t, 2H), 4.22 (q, 2H), 3.41 (s, 2H), 3.20 (t, 2H), 1.29 (t, 3H) ppm.

$^{13}$C NMR (100 MHz, CDCl$_3$) $\delta$ 166.5, 166.4, 139.5, 126.9, 125.7, 124.1, 65.6, 61.6, 41.6, 29.1, 14.1 ppm.
Figure S2: a) $^1$H and b) $^{13}$C NMR spectra of compound 7.

$^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 7.19 (d, 2H), 6.97 (t, 2H), 6.89 (d, 2H), 4.38 (t, 4H), 3.44 (s, 2H), 3.18 (t, 4H) ppm.

$^{13}$C NMR (100 MHz, CDCl$_3$) $\delta$ 166.4, 139.5, 127.3, 125.7, 124.1, 65.7, 41.5, 29.1 ppm.
Figure S3: a) $^1$H and b) $^{13}$C NMR spectra of compound 8.

$^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 7.62-7.61 (m, 2H), 7.38 (d, 2H), 7.18 (dd, 1H), 6.95 (dd, 1H), 6.81- 6.80 (m, 1H), 4.36 (t, 2H), 3.71 (s, 1H), 3.17 (t, 1H) ppm.

$^{13}$C NMR (100 MHz, CDCl$_3$) $\delta$ 170.1, 139.6, 139.2, 132.3, 130.2, 126.9, 125.6, 124.1, 118.7, 111.2, 65.4, 41.3, 29.2 ppm.
**Figure S4**: a) $^1$H and b) $^{13}$C NMR spectra of compound 9.

$^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 7.46 (d, 2H), 7.19 (dd, 1H), 7.16 (d, 2H), 6.95 (dd, 1H), 6.81 (dd, 1H), 4.34 (t, 2H), 3.61 (s, 2H), 3.16 (t, 2H) ppm.

$^{13}$C NMR (100 MHz, CDCl$_3$) $\delta$ 170.9, 139.7, 132.8, 131.7, 126.9, 124.1, 121.2, 65.2, 40.7, 29.2 ppm.
Figure S5: MALDI-TOF-MS spectrum of compound 10.

Figure S6: a) $^1$H and b) $^{13}$C NMR spectra of compound 10.

$^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 7.20 (dd, 1H), 6.98-6.96 (m, 2H), 4.76 (t, 2H), 4.54 (q, 2H), 3.40 (t, 2H), 1.46 (t, 3H) ppm.

$^{13}$C NMR (100 MHz, CDCl$_3$) $\delta$ 163.6, 163.4, 145.4, 145.3, 145.2, 144.9, 144.7, 144.6, 144.6, 143.9, 143.2, 143.1, 143.0, 143.0, 142.2, 142.0, 141.9, 141.0, 139.1, 139.1, 138.9, 130.6, 127.7, 127.1, 125.9, 124.4, 77.2, 71.5, 67.3, 63.5, 52.1, 29.2, 14.2 ppm.
Figure S7: MALDI-TOF-MS spectrum of compound 11.

Figure S8: a) $^1$H and b) $^{13}$C NMR spectra of compound 11.

$^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 7.20- 7.19 (m, 2H), 6.97 (d, 4H), 4.70 (t, 4H), 3.34 (t, 4H) ppm.

$^{13}$C NMR (100 MHz, CDCl$_3$) $\delta$ 163.3, 145.3, 145.2, 145.1, 145.0, 144.9, 144.7, 144.5, 143.9, 143.1, 143.0, 142.9, 142.2, 141.9, 140.9, 139.1, 139.0, 127.2, 125.9, 124.4, 71.4, 67.3, 51.9, 29.2 ppm.
Figure S9: MALDI-TOF-MS spectrum of compound 11.

Figure S10: a) $^1$H and b) $^{13}$C NMR spectra of compound 12.

$^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 8.22 (dd, 2H), 7.86 (dd, 2H), 7.18 (dd, 1H), 6.92 (dd, 1H), 6.81 (dd, 1H), 4.65 (t, 2H), 3.30 (t, 2H) ppm.

$^{13}$C NMR (100 MHz, CDCl$_3$) $\delta$ 165.6, 146.4, 145.4, 145.3, 145.2, 144.9, 144.8, 144.7, 144.6, 144.5, 144.4, 143.9, 143.7, 143.2, 143.1, 143.0, 142.9, 142.3, 142.2, 142.1, 141.9, 141.1, 141.0, 139.1, 138.3, 138.1, 137.4, 133.2, 132.5, 129.1, 128.2, 127.1, 125.8, 125.31, 124.4, 118.3, 113.3, 77.2, 74.6, 67.1, 54.4, 29.2, 21.5 ppm.
Figure S11: MALDI-TOF-MS spectrum of compound 13.

Figure S12: a) $^1$H and b) $^{13}$C NMR spectra of compound 13.

$^1$H NMR (400 MHz, CDCl$_3$) $\delta$ 7.97 (d, 2H) 7.70 (d, 2H), 7.17 (dd, 1H) 6.92 (dd, 1H) 6.81 (d, 1H) 4.63 (t, 2H), 3.29 (t, 2H) ppm.

$^{13}$C NMR (100 MHz, CDCl$_3$) $\delta$ 166.1, 146.9, 145.8, 145.4, 145.3, 145.2, 145.2, 145.1, 144.8, 144.7, 144.6, 144.5, 144.4, 144.3, 143.9, 143.7, 143.1, 143.0, 142.9, 142.9, 142.3, 142.2, 142.1, 142.0, 141.0, 141.0, 139.2, 138.3, 138.0, 134.0, 132.0, 131.4, 127.0, 125.8, 124.3, 123.8, 77.2, 75.1, 66.9, 54.7, 29.3 ppm.
**Figure S13:** Cyclic voltammetry of compounds 10-13.

**Figure S14:** UV-Vis spectra of compounds 10-13.
Figure S15: Forward and reverse scans for a) PC₆₁BM, b) compound 10, c) compound 11, d) compound 12, e) compound 13.
Figure S16: FTIR spectrum of compound 10.

Figure S17: FTIR spectrum of compound 11.
Dielectric constant measurement

We followed the method reported by Hummelen et al.1 Dielectric constants were obtained by spectral impedance measurements using the following architecture: ITO/PEDOT:PSS/fullerene/Al. The capacitance was determined by filling the data to the equivalent circuit (Figure S19) for fabricated capacitors.

![Figure S19. Equivalent circuit to fit the data, with capacitance (C), parallel resistance (Rp) and serial resistance (Rs).]

The dielectric constant was determined using the equation S1:

$$C = \varepsilon_0 \varepsilon_r \frac{A}{d} \quad \text{(S1)}$$

where A is the capacitor’s area (m²), d is the thickness of the fullerene film (m) and \(\varepsilon_0\) is the permittivity of vacuum \((8.85 \times 10^{-12} \text{ F/m})\).
Figure S20. XRD of the perovskite film.

References