Electronic Supplementary Material (ESI) for Materials Chemistry Frontiers.

Electronic Supplementary Information

Supporting Figures

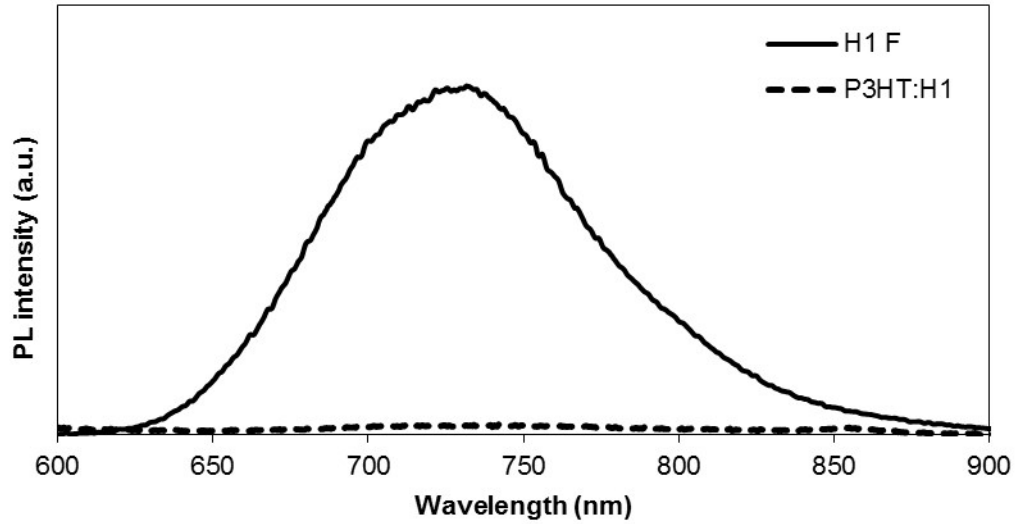

Fig. S1 Photoluminescence quenching measurement of blend film of P3HT: **H1** (1: 1 w/w); excitation at 590 nm.

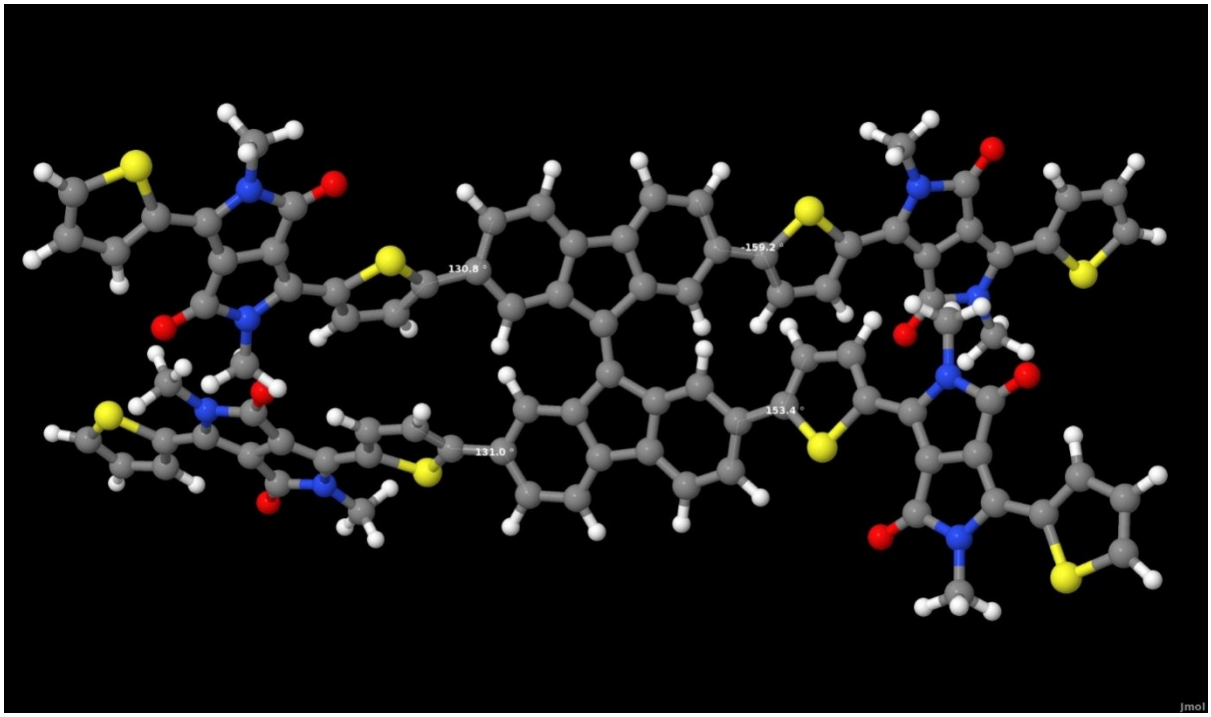

Fig. S2 Torsional angles of ~20° and 50° between the thiophene ring planes (of DPP) and phenyl ring planes (of BF) of **H1** from the minimum energy conformations calculated using the Gaussian 09 suite of programs and the B3LYP/6-311+G(d,p)//B3LYP/6-31G(d) level of theory.

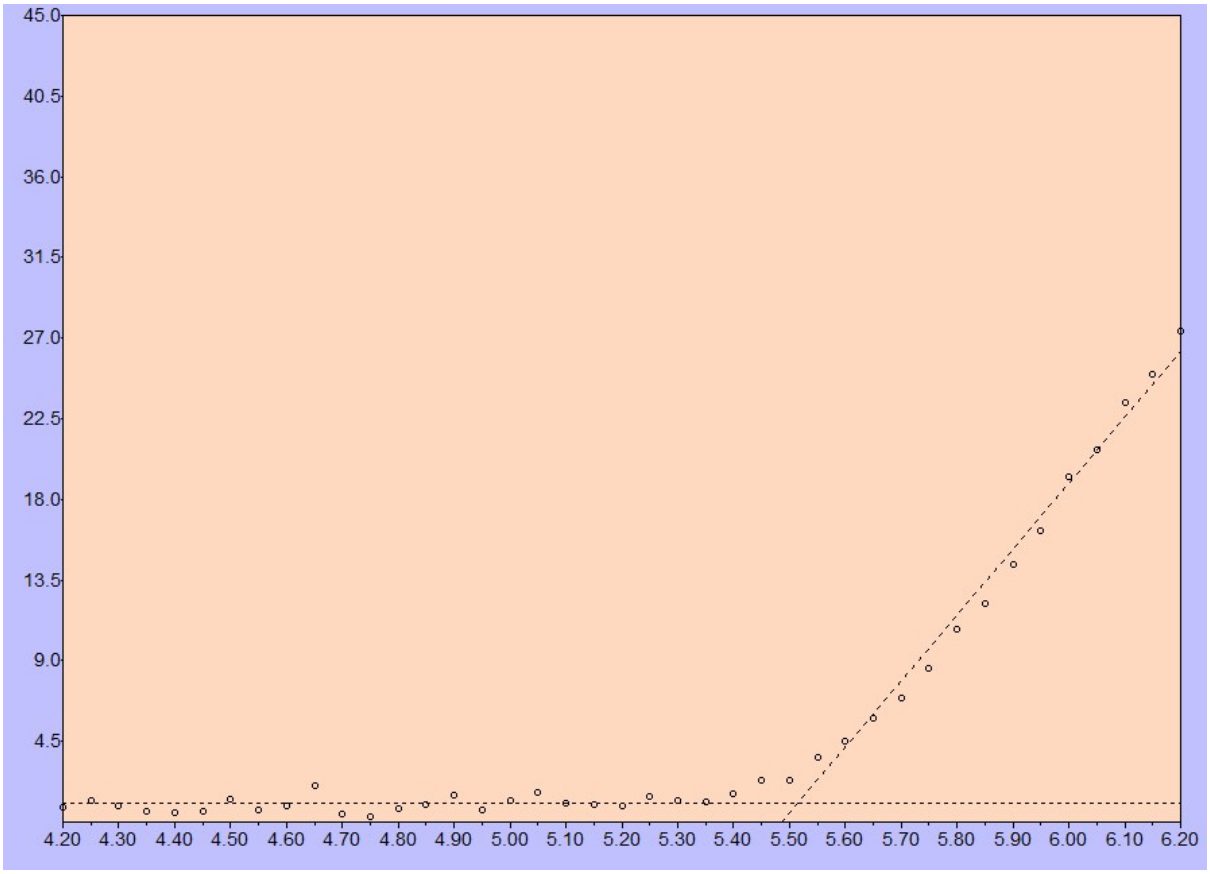

Fig. S3 PESA spectrum of thin film of **H1**. The dashed-lines show the fits to extract ionisation potential (-5.51 eV) which corresponds to the HOMO energy level.

Excited State	1:	Singlet-A	1.5071 eV	822.65 nm	f=0.0775	<S**2>=0.000
Excited State	2:	Singlet-A	1.5533 eV	798.17 nm	f=0.0931	<S**2>=0.000
Excited State	3:	Singlet-A	1.6462 eV	753.15 nm	f=0.0514	<S**2>=0.000
Excited State	4:	Singlet-A	1.7681 eV	701.25 nm	f=0.0160	<S**2>=0.000
Excited State	5:	Singlet-A	1.8385 eV	674.38 nm	f=0.0059	<S**2>=0.000
Excited State	6:	Singlet-A	1.9695 eV	629.51 nm	f=0.1098	<S**2>=0.000
Excited State	7:	Singlet-A	2.0060 eV	618.06 nm	f=0.2198	<S**2>=0.000
Excited State	8:	Singlet-A	2.0190 eV	614.08 nm	f=0.7730	<S**2>=0.000
Excited State	9:	Singlet-A	2.0394 eV	607.94 nm	f=0.0118	<S**2>=0.000
Excited State	10:	Singlet-A	2.1027 eV	589.64 nm	f=0.0102	<S**2>=0.000

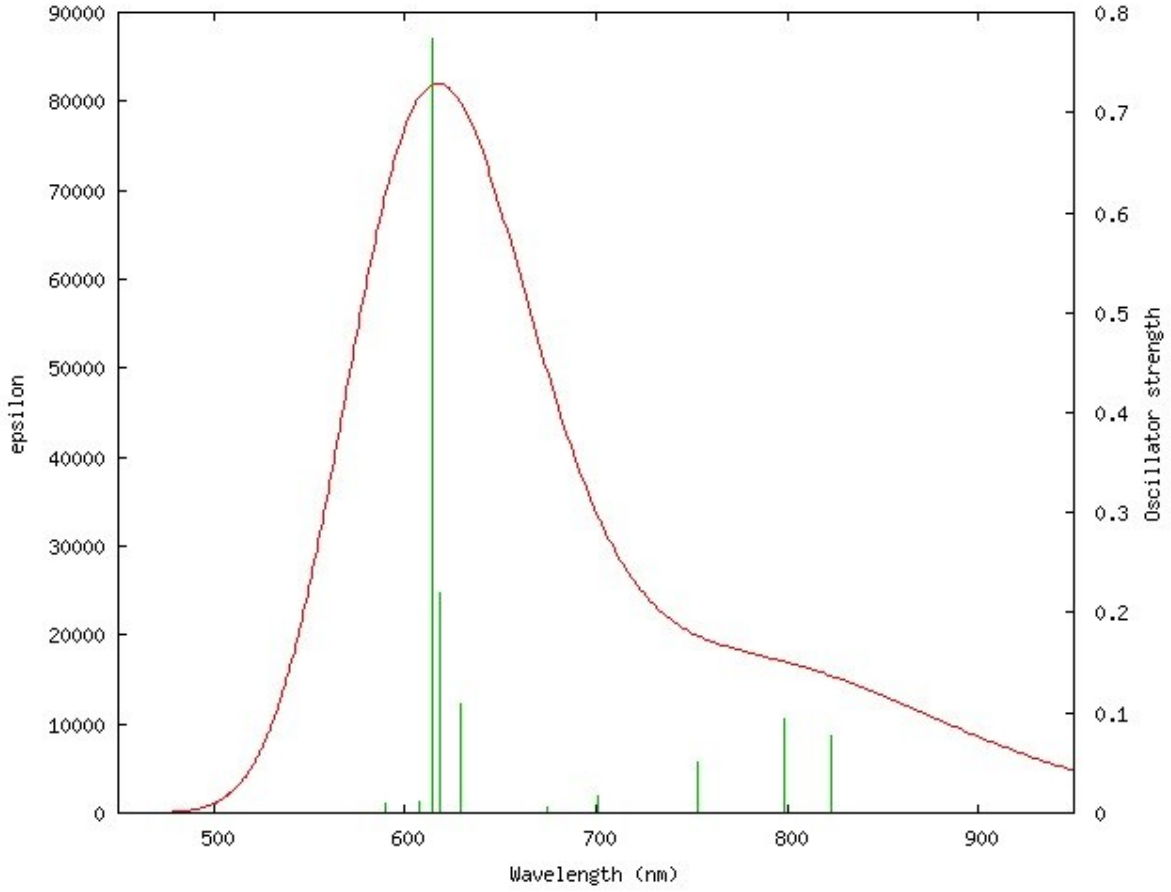

Fig. S4 Theoretical optical absorption transitions and spectrum of **H1**.

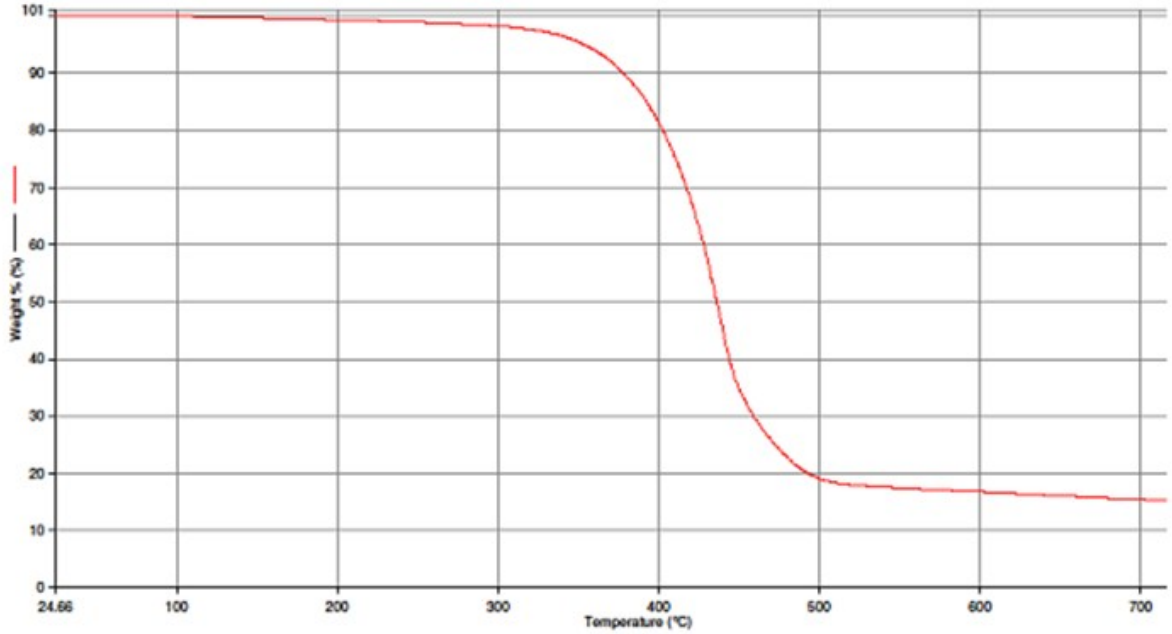

Fig. S5 TGA curve showing thermal stability of **H1**.

Table S1

BHJ solar cell parameters for P3HT: **H1** blends

Dye	**Testing conditions (withP3HT)**	**Blend film thickness**	V_{oc} **(V)**	J_{sc} **(mA/cm^2)**	***FF***	**PCE (%) (Best)**
H1	1: 1[a]	67	1.17±0.02	7.74 ±0.15	0.60 ±0.02	5.26 ±0.20 (5.42)
H1	1: 1[b]	69	0.90±0.02	5.09 ±0.20	0.51 ±0.03	2.10 ±0.30 (2.32)
$PC_{61}BM$	1: 1	64	0.57±0.03	8.28 ±0.15	0.64 ±0.02	2.88 ±0.15 (3.01)
H1	1: 1.5[a]	71	1.06±0.01	2.16±0.10	0.45±0.02	1.01±0.18 (1.03)

[a] As-cast blend (P3HT: **H1**, no annealing); [b] BHJ devices with annealing at 100 °C for 10 min. Device structure is ITO/PEDOT:PSS (38 nm)/active layer/Ca (20 nm)/Al (100 nm) with an active layer thickness of around 68 nm; device area ~0.1 cm^2.

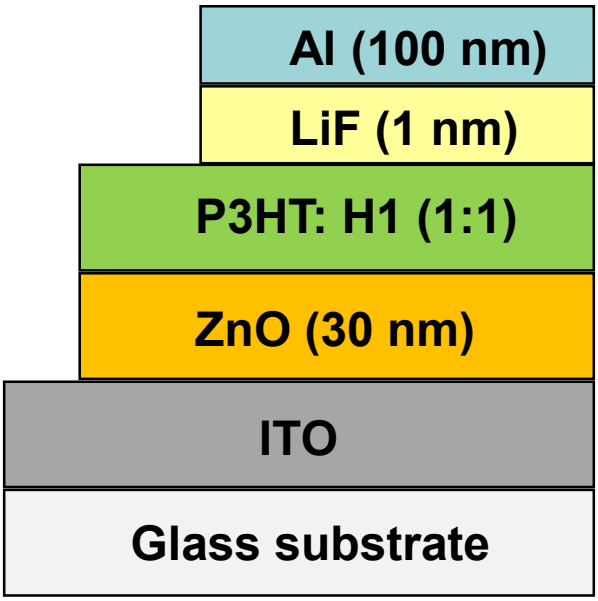

Fig. S6 Device sketch of the electron-only devices that was used to study SCLC method.

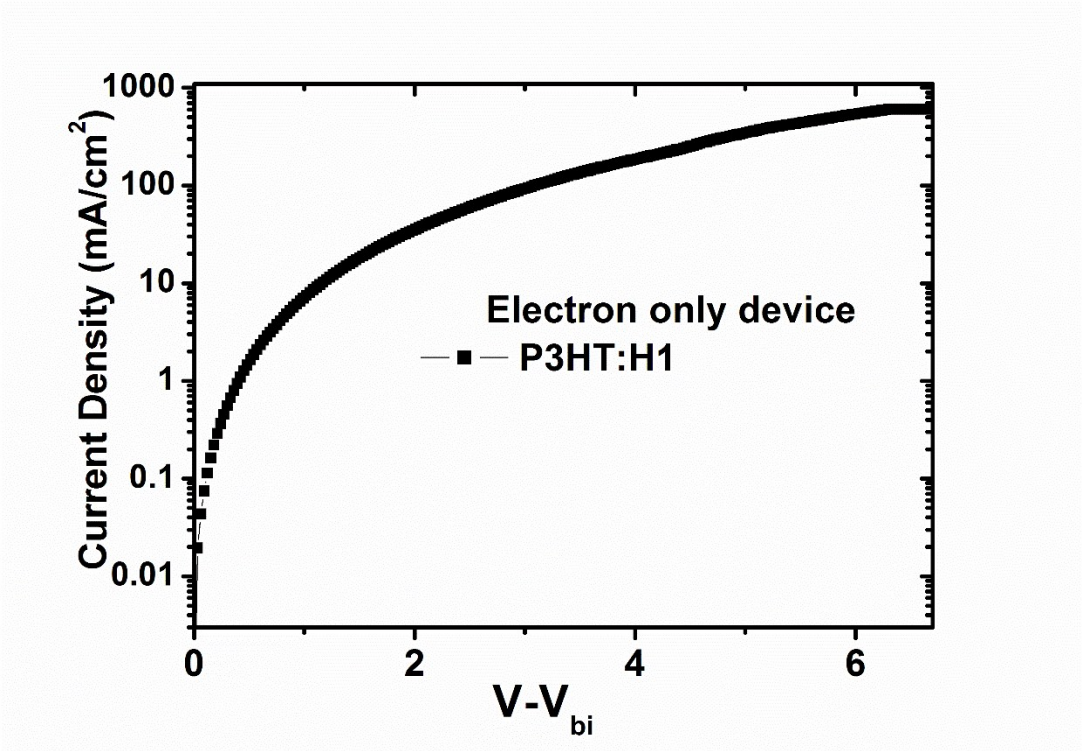

Fig. S7 Current–voltage characteristics of electron only devices which were applied to Mott-Gurney equation to calculate electron mobility of **H1**.

Experimental spectra