Supplementary Information

Synthesis, optical and electrochemical properties of small molecules DMM-TPA[DTS(FBTTh$_3$)$_3$] and TPA[DTS(FBTTh$_3$)$_3$] and their application as donors for bulk heterojunction solar cells

Nara Cho, [a] Sanhhyun Paek, [a] Jihye Jeon, [b] Kihyung Song, [b] G. D. Sharma,*[c] and Jaejung Ko*[a]

[a]Department of Materials Chemistry, Korea University, Chungnam 330-700, Republic of Korea. Fax: +82- 44-860-1331; Tel: +82-44-860-1337; E-mail: jko@korea.ac.kr

[b]Department of Chemical Education, Korea National University of Education, Chungbuk, 363-791, Republic of Korea

[c]R & D center for Engineering and Science, JEC group of colleges, Jaipur Engineering College campus, Kukas, Jaipur (Raj.), India; E-mail: gdsharma273@gmail.com

*Corresponding authors

Content

S1. Isodensity surface plots of **DMM-TPA[DTS(FBTTh$_3$)$_3$]** (**1**) and **TPA[DTS(FBTTh$_3$)$_3$]** (**2**) calculated by the time dependent-density functional theory (TD-DFT) using the B3LYP functional/6-31G* basis set.

Table S1. Calculated excitation energy characteristics of the **DMM-TPA[DTS(FBTTh$_3$)$_3$]** (**1**) and **TPA[DTS(FBTTh$_3$)$_3$]** (**2**)

Table S2. Photovoltaic parameters of devices with different weight ratio of small molecules and PC$_{71}$BM

Table S3. Photovoltaic parameters of the devices based on 1:PC$_{71}$BM processed with different concentration of DIO in CB

Reference

S1. Isodensity surface plots of **DMM-TPA[DTS(FBTTh₃)₃]** (**1**) and **TPA[DTS(FBTTh₃)₃]** (**2**) calculated by the time dependent-density functional theory (TD-DFT) using the B3LYP functional/6-31G* basis set.
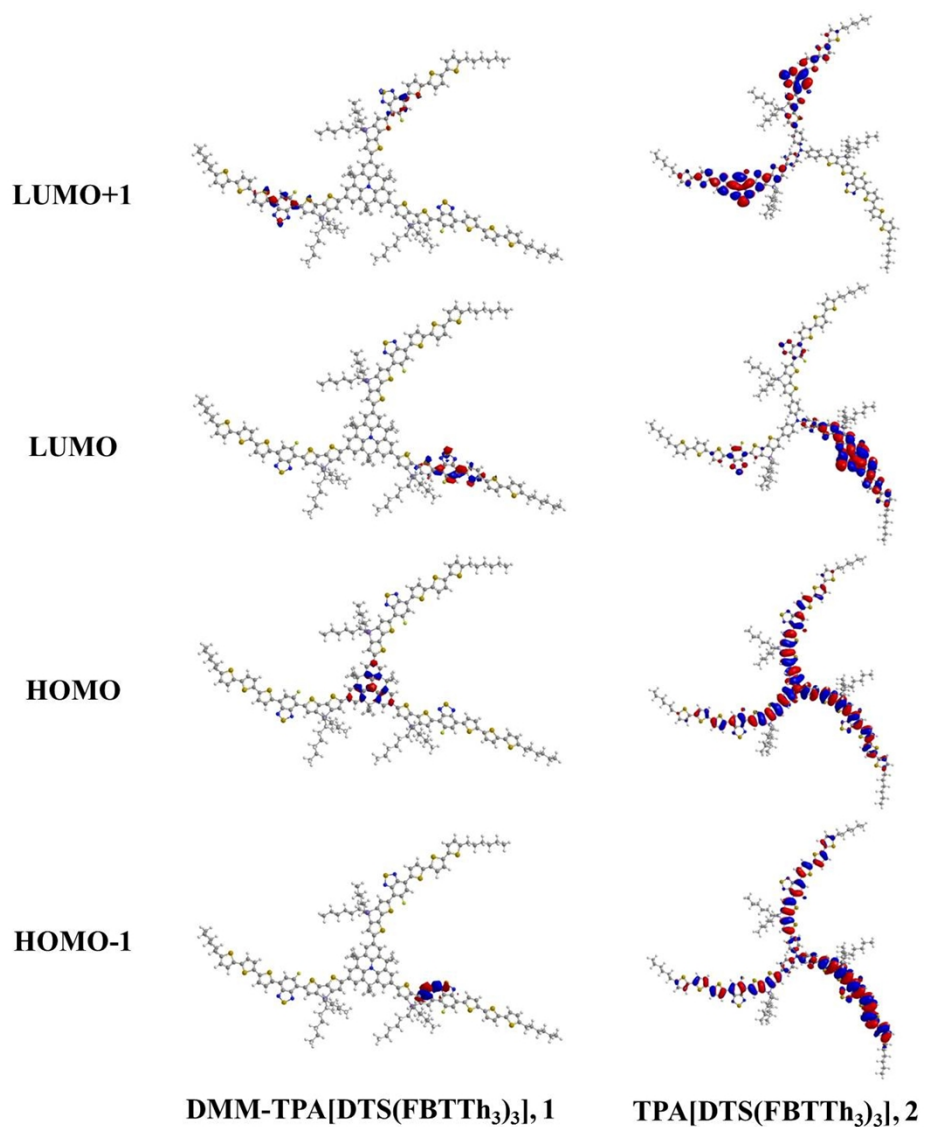

LUMO+1

LUMO

HOMO

HOMO-1

DMM-TPA[DTS(FBTTh₃)₃], **1**   TPA[DTS(FBTTh₃)₃], **2**

Table S1. Calculated excitation energy characteristics of the **DMM-TPA[DTS(FBTTh$_3$)$_3$] (1)** and **TPA[DTS(FBTTh$_3$)$_3$] (2)** [a]

Compounds	E(eV)/nm	f[b]	Composition (%)[c]
1	1.525/812.8	1.511	64 (HOMO → LUMO)
			11 (HOMO-2 → LUMO)
	1.535/807.8	0.548	18 (HOMO → LUMO)
			62 (HOMO → LUMO+1)
	1.810/684.8	1.272	52 (HOMO-2 → LUMO)
			15 (HOMO-2 → LUMO+1)
			15 (HOMO-2 → LUMO+2)
			35 (HOMO-1 → LUMO+1)
	1.832/677.0	0.536	12 (HOMO-3 → LUMO+2)
			22 (HOMO-2 → LUMO+1)
			46 (HOMO-1 → LUMO+1)
2	1.557/796.1	1.361	67 (HOMO → LUMO)
			14 (HOMO-1 → LUMO)
	1.580/784.7	1.272	16 (HOMO-2 → LUMO+2)
			66 (HOMO → LUMO+1)
	1.803/687.7	0.545	66 (HOMO-1 → LUMO)
			14 (HOMO-1 → LUMO+2)
	1.829/677.8	0.656	22 (HOMO-2 → LUMO)
			39 (HOMO-1 → LUMO+1)
			21 (HOMO → LUMO+1)
	1.838/674.4	0.314	50 (HOMO-2 → LUMO+1)
			11 (HOMO-1 → LUMO)
			12 (HOMO-1 → LUMO+1)

[a] The characteristics were calculated by the time dependent-density functional theory (TD-DFT) using the B3LYP functional/6-31G* basis set
[b] The oscillator strength (f) of a transition is a measure of its intensity and is related to the molar absorption coefficient
[c] The composition means contribution of each transition for excitation energies.

Table S2

Photovoltaic parameters of devices based 1: PC$_{71}$BM and 2:PC$_{71}$BM with different weight ratio

	w/w ratio	J$_{sc}$ (mA/cm^2)	V$_{oc}$ (V)	FF	PCE (%)
1:PC$_{71}$BM					
	1:1	8.45	0.67	0.42	2.38
	1:2	9.18	0.68	0.46	2.87
	1:3	8.94	0.66	0.44	2.60
	1:4	8.46	0.66	0.40	2.23
2:PC$_{71}$BM	**1:1**	7.86	0.68	0.38	2.03
	1:2	8.54	0.70	0.42	2.51
	1:3	8.23	0.70	0.40	2.30
	1:4	7.96	0.68	0.36	1.95

Table S3. Photovoltaic parameters of the devices based on 1:PC$_{71}$BM processed with different concentration of DIO in CB

Concentration by volume %	J$_{sc}$ (mA/cm^2)	V$_{oc}$ (V)	FF	PCE (%)
1%	9.67	0.68	0.48	3.16
2%	9.92	0.68	0.50	3.37
3%	10.78	0.66	0.54	3.84
4%	12.62	0.66	0.62	5.16
5%	10.46	0.64	0.53	3.54

Reference

1. Cho, N.; Song, K.; Lee, J. K.; Ko, J. *Chem. Eur. J.* **2012**, *18*, 11433-11439
2. Paek, S.; Cho, N; Cho, S.; Lee, J. K; Ko, J. *Org. Lett*., **2012**, *14*, 6326-6329