Supporting Information

Effects of Fused Thiophene Bridges in Organic Semiconductors for Solution-Processed Small-Molecule Organic Solar Cells

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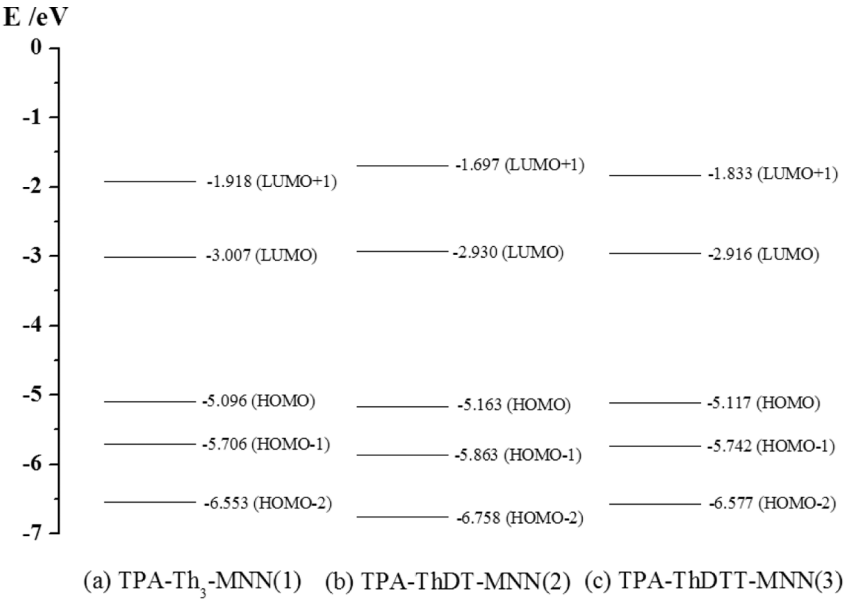

(a) TPA-Th_3-MNN(1) (b) TPA-ThDT-MNN(2) (c) TPA-ThDTT-MNN(3)

Figure S1. Molecular orbital surfaces from HOMO-2 to LUMO+2 of **TPA-[π-bridges]-MMN [1, 2, and 3]** obtained at B3LYP/6-31G* level.

Table S1. Caculated excitation energy characteristics of the **1**, **2**, and **3**[a]

Compound	E(eV)/nm	f [b]	Composition (%) [c]
	1.903/651.2	0.7977	HOMO→LUMO (70.54)
1	2.545/487.1	1.0485	HOMO-1→LUMO (68.38)
	3.317/373.7	0.0999	HOMO-2→LUMO (52.78)
	2.043/606.6	0.8173	HOMO→LUMO (70.44)
2	2.795/443.5	1.1405	HOMO-1→LUMO (67.04)
	3.169/391.2	0.1766	HOMO-2→LUMO (18.78)
	1.974/627.8	0.8414	HOMO→LUMO (70.44)
3	2.639/469.8	1.111	HOMO-1→LUMO (67.63)
	2.994/414.0	0.2453	HOMO-2→LUMO (19.64)

[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.