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Supporting Information

for

Charge-transfer interactions between fullerenes and a mesoporous tetrathiafulvalene-based metal–organic framework

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Additional figures and tables

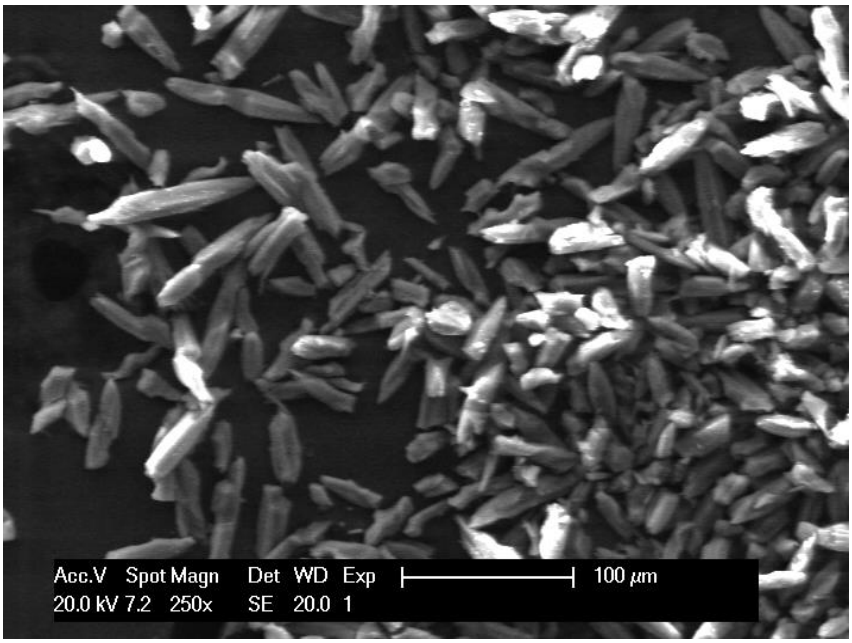


Figure S1: SEM image of **C_{60}@MUV-2**.

a b

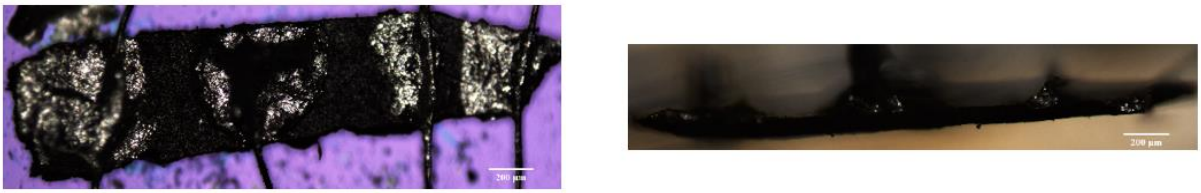


Figure S2: Top view (a) and lateral view (b) for **MUV-2** electrical measurements**.**

a b

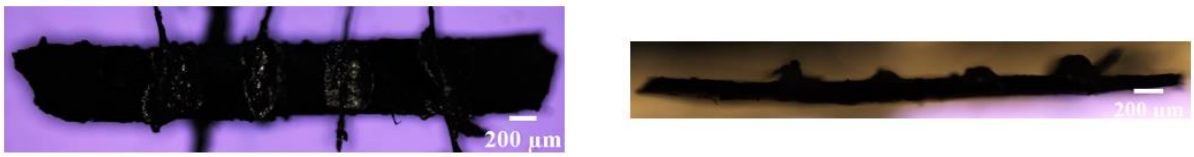
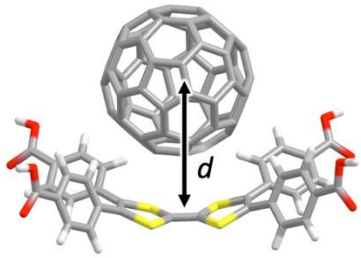


Figure S3: Top view (a) and lateral view (b) for **C_{60}@MUV-2** electrical measurements**.**

Table S1: Interaction energy (in kcal/mol) of the two conformations A and B of the host-guest **C_{60}@MUV-2** complex at the B3LYP level using different basis sets and including or not the counterpoise (CP) correction.

	Conformation A		**Conformation B**	
	6-31G**	6-31+G*	6-31G**	6-31+G*
No CP	-23.00	-22.10	-26.85	-24.96
½ CP	-20.01	-19.99	-23.72	-22.86
Full CP	-17.02	-17.88	-20.59	-20.75

Table S2: Charge transfer (in electron charge units, e) from the electron-donor TTFTB ligand to the electron-acceptor C_{60} guest in the ground state (GS) and the charge-transfer S_1 state (CT) of **C_{60}@TTFTB** as a function of the distance between centroids (*d*). Data corresponding to the minimum-energy geometry is in bold.



***d* (Å)**	**GS**	**CT**
6.61	0.05	0.92
6.86	**0.02**	**0.94**
7.11	0.01	0.96
7.36	0.00	0.97
7.61	0.00	0.98
7.86	0.00	0.99
8.11	0.00	0.99

Table S3: Intense lowest-lying singlet excited states of TTFTB ligand and C_{60} guest, calculated at the CAM-B3LYP/6-31G** level of theory. The energy (*E*), oscillator strength (*f*), major monoexcitation, and description of each state are included.

State	*E* (eV)	*E* (nm)	*f*	Monoexcitation	Description
			TTFTB		
S_1	2.907	426.4	0.0760	H → L (68%)	TTF → peripheral
S_3	3.486	355.7	0.1043	H → L+4 (58%)	TTF
S_6	4.261	291.0	0.4840	H → L+3 (52%)	TTF → peripheral
S_8	4.430	279.9	0.5490	H-1 → L+1 (51%)	TTF → peripheral
S_{21}	5.217	237.7	0.4389	H-3 → L (15%)	TTF → peripheral
S_{54}	6.623	187.2	0.7300	H-4 → L+5 (13%)	TTF + peripheral
			C_{60}		
S_{37}	4.309	287.7	0.2196	H-2 → L+3 (18%)	-
S_{38}	4.312	287.6	0.2196	H-3 → L+5 (21%)	-
S_{39}	4.315	287.3	0.2206	H-4 → L+5 (31%)	-
S_{52}	4.703	263.7	0.1192	H-6 → L+2 (19%)	-
S_{53}	4.704	263.6	0.1181	H-6 → L+1 (21%)	-
S_{54}	4.706	263.5	0.1133	H-8 → L (17%)	-

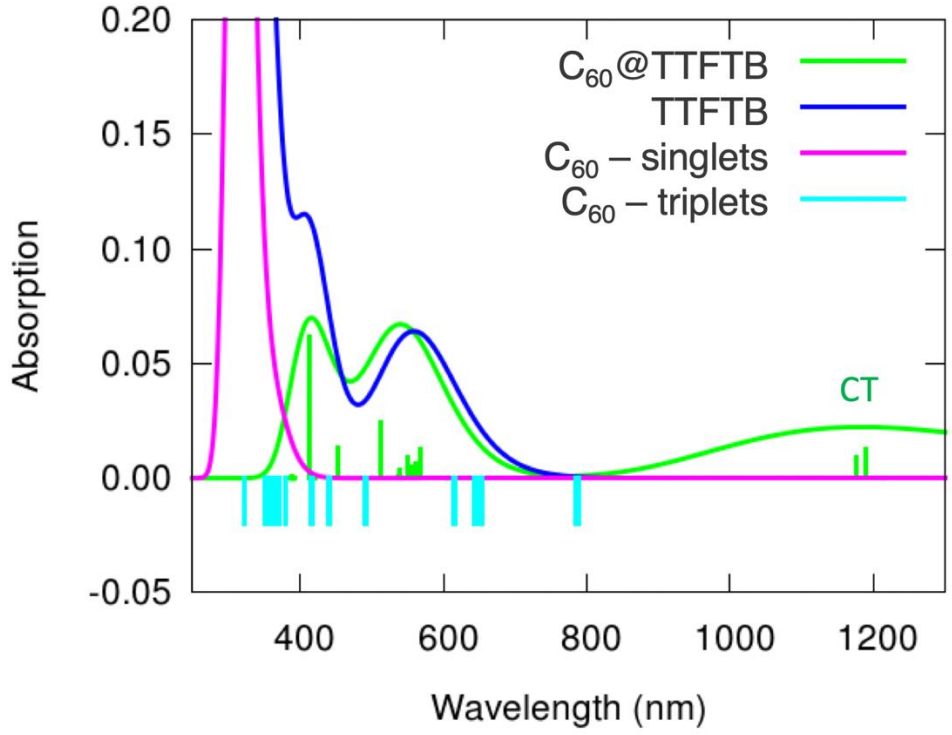
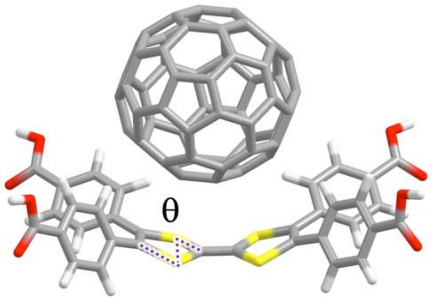


Figure S4: TDDFT absorption spectra calculated at the B3LYP/6-31G** for host-guest **C_{60}@TTFTB (**including vertical excitation energies), TTFTB ligand, and fullerene C_{60} (singlets and triplet energies).

Table S4: Evolution of S_1 CT excitation for **C_{60}@TTFTB** as a function of distance *d* (as defined in Table S1) and the TTF boat dihedral angle (θ). Data corresponding to the minimum-energy geometry is in bold.



d **(Å)**	***E*** **(eV)**	***E*** **(nm)**	***f***
6.61	2.146	577.8	0.0284
6.86	**2.143**	**578.6**	**0.0178**
7.11	2.167	572.1	0.0103
7.36	2.209	561.3	0.0054
7.61	2.258	549.0	0.0027
7.86	2.310	536.8	0.0012
8.11	2.360	525.4	0.0005
θ (º)	***E*** **(eV)**	***E*** **(nm)**	***f***
162	**2.143**	**578.6**	**0.0178**
171	2.044	606.7	0.0131
180	2.025	612.3	0.0079