Electronic Supplementary Information (ESI)

Park et al.

## Variation of Excited-State Dynamics in Trifluoromethyl Functionalized C<sub>60</sub> Fullerenes

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**Fig. S1** Gaussian deconvolution fitting for ground-state electronic absorption spectra of a) **C60/4-1** and b) **C60/10-1** measured in toluene. The FWHM noted in the figure shows the FWHM results for the lowest-energy absorption peak.



**Fig. S2** Photoluminescence excitation spectra of **C60/4-1** and **C60/6-2** in toluene. (a,c) Photoluminescence excitation spectra of **C60/4-1** and **C60/6-2** (blue, right y-axis), monitored at the emission wavelengths noted, are overlaid with electronic absorption spectra (black, left y-axis). (b,d) Photoluminescence excitation spectra of **C60/4-1** and **C60/6-2** in toluene monitored at the multiple emission wavelengths are normalized.



Fig. S3 Representative femtosecond pump/probe transient absorption spectra of a)  $PC_{61}BM$  and b) bis- $PC_{61}BM$  in toluene obtained at the time delays noted. Experimental conditions:  $\lambda_{ex} = 400$  nm, pulse energy = 300 nJ/pulse, room temperature.



Fig. S4 Representative femtosecond pump-probe transient absorption spectra of C60/10-1 in toluene, obtained at the time delays noted. Experimental conditions:  $\lambda_{ex} = 400$  nm, pulse energy = 450 nJ/pulse, room temperature.



**Fig. S5** Exponential fitting results of the transient decay signals for a) C60/4-1, b) C60/6-2, c) C60/10-1. Experimental conditions:  $\lambda_{pr} = a$ ) 902 nm, b) 935 nm, and c) 1001 nm;  $\lambda_{ex} = a$ ,b) 400 nm and c) 550 nm, pulse energy = 300 nJ/pulse, room temperature.



Fig. S6 Single-exponential fitting results of the transient signal rise for a) C60/4-1 and b) C60/6-2 using the method described earlier to determine the rise time constant of the  $T_1 \rightarrow T_n$  transition (see the earlier section for the method). Experimental conditions:  $\lambda_{ex} = 400$  nm, pulse energy = 300 nJ/pulse, room temperature.



Fig. S7 Comparative femtosecond pump-probe transient absorption spectrum (solid black) of C60/10-1 in toluene obtained at the time delay noted. Inversed electronic absorption spectrum (dashed blue) of C60/10-1 in toluene is displayed for comparison. Experimental conditions:  $\lambda_{ex} =$  400 nm, pulse energy = 300 nJ/pulse, room temperature.



Fig. S8 Exponential fitting results of the transient decay signals for a) C60/4-1 and b) C60/6-2, dispersed in a polystyrene matrix. Experimental conditions:  $\lambda_{pr} = a$ ) 901 nm and b) 941 nm;  $\lambda_{ex} = 400$  nm, pulse energy = 500 nJ/pulse, room temperature.