

Supporting Information for

“Effects of Supramolecular Encapsulation on Photophysics and Photostability of a 9,10-Bis(arylethynyl)anthracene-Based Chromophore Revealed by Single-Molecule Fluorescence Spectroscopy”

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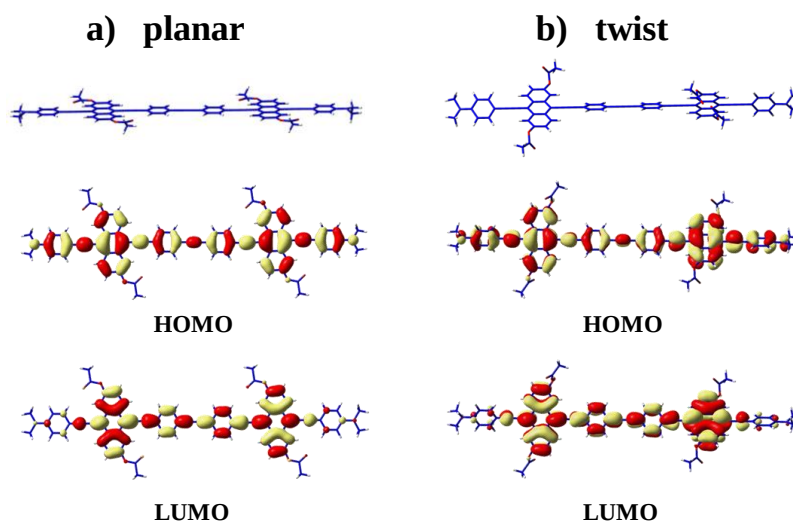


Figure S1. a) Planar and b) twist structures of bare G2, together with their HOMO and LUMO, obtained at HF/6-31G(d).

Table S1 Total electronic energies and zero point vibrational energies obtained at the HF/6-31G(*d*) and HF/6-31G(*d,p*)

G2	HF/6-31G(<i>d</i>)		HF/6-31G(<i>d,p</i>)	
	E_e	ZPVE	E_e	ZPVE
	hartree	hartree	hartree	hartree
planar	−3540.196814	+1.135226	−3540.286033	+1.131172
twist	−3540.196550	+1.134372	−3540.285511	+1.130325