Supporting Information for

The Role of Singlet Diradical Character in Carbon Nanomaterials: a Novel Hot Spot for Efficient Nonlinear Optical Materials

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Table S1. Calculated orbital energies for single trannulene [5]cyclacene and single trannulene [5]cyclacene at MP2 and LC-BLYP with 6-311G* basis set.

Orbitals	Single Trannulene [5]cyclacene Energies (eV)		Single Trannulene [6]cyclacene Energies (eV)	
	LC-BLYP	**MP2**	**LC-BLYP**	**MP2**
LUMO+4	**3.553**	**5.115**	3.760	5.186
LUMO+3	**3.553**	**5.115**	**2.903**	**4.457**
LUMO+2	1.941	3.385	**2.903**	**4.457**
LUMO+1	**1.703**	**2.926**	2.699	3.917
LUMO	**1.703**	**2.926**	-0.556	1.586
ΔE = H–L	**8.980**	**9.508**	**4.682**	**7.013**
HOMO	**-7.277**	**-6.582**	-5.238	-5.428
HOMO-1	**-7.277**	**-6.582**	**-9.133**	**-8.892**
HOMO-2	**-11.503**	**-11.364**	**-9.133**	**-8.892**
HOMO-3	**-11.503**	**-11.364**	**-11.983**	**-12.098**
HOMO-4	-12.864	-13.053	**-11.983**	**-12.098**