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Physical Mechanism of One-Photon Absorption, Two-Photon Absorption, and Electron Circular Dichroism of 1,3,5 Triazine Derivatives Based on Molecular Planarity

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1. MO transition

Table S1. Major orbital transition contributions in OPA excited states.

Excited energy, Wavelength, Oscillator strength, Spin multiplicity and percentage contribution of orbital transition (>5%)

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o-Br-TRZ

Excited states: S_1 Excited energy :4.081eV Wavelength:281.26nm Oscillator strength :1.3162 Spin multiplicity=1

MO transitions:H→L 27.2%, H-2→L 24.6%, H-1→L+1 20%, H→L+2 6.8%

Excited states: S_2 Excited energy :4.415eV Wavelength:280.80nm Oscillator strength :1.3588 Spin multiplicity=1

MO transitions:H-2→L+1 27.2%, H-1→L 22.9%, H→L+1 19.8%, H-1→L+2 6.9%

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m-Br-TRZ

Excited states: S_1 Excited energy :4.288eV Wavelength:289.12nm Oscillator strength :1.6480 Spin multiplicity=1

MO transitions:H-1→L+1 24.8%, H→L 15.8%, H-2→L+1 13.5%, H-2→L 10.1%, H→L+2 8.3%, H-1→L 8.2%, H→L+1 6.5%

Excited states: S_2 Excited energy :4.293eV Wavelength:288.82nm Oscillator strength :1.7098 Spin multiplicity=1

MO transitions:H-2→L 30.4%, H→L+1 20.8%, H-1→L 10.8%, H-2→L+1 10.7%, H-1→L+2 7.9%

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p-Br-TRZ

Excited states: S_1 Excited energy :4.215eV Wavelength:294.16nm Oscillator strength :1.8720 Spin multiplicity=1

MO transitions:H-2→L 23.4%, H→L+1 15.2%, H-1→L 15%, H→L+2 10.4%, H-2→L+1 8.5%, H→L 8.1%, H-1→L+1 7.2%

Excited states: S_2 Excited energy :4.216eV Wavelength:294.07nm Oscillator strength :1.8768 Spin multiplicity=1

MO transitions:H-2→L+1 25.4%, H-1→L+1 14.3%, H→L 14.1%, H-1→L+2 10.4%, H-2→L+2 9.4%, H-1→L 7.6%

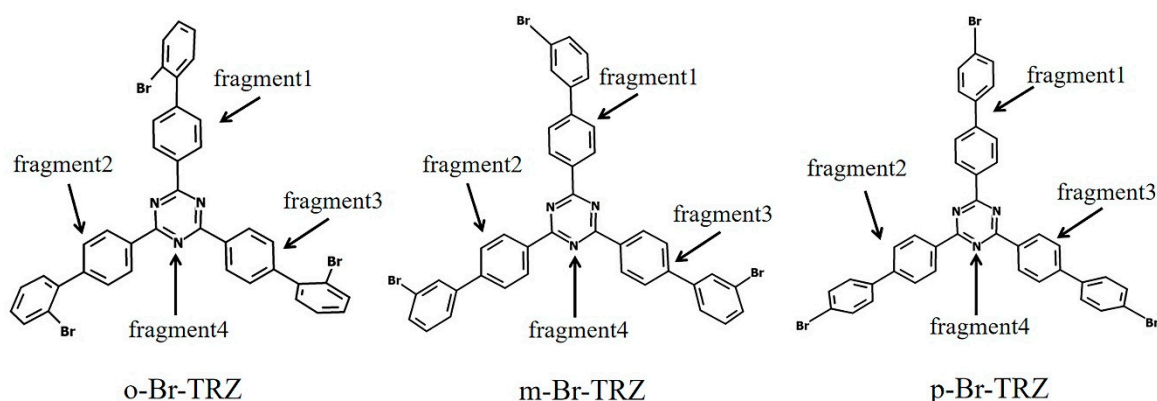## 2. Interfragment charge transfer (IFCT) analysis

Figure S1. 1,3,5 Triazine derivative molecules with three branched fragments and triazine cores.

Table S2. Interfragment charge transfer and net CT of 1,3,5 triazine derivatives during electron excitation were calculated by IFCT method.

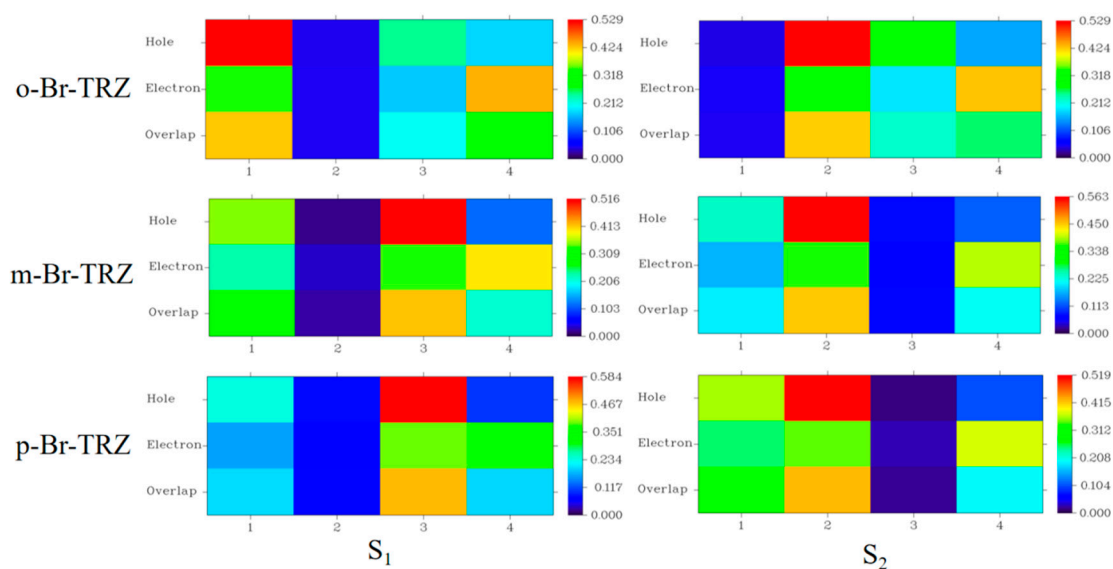| Molecule	states	Variation of population number of fragment				Net charge transfer between segments		
		f1	f2	f3	f4	Net f1→f4	Net f2→f4	Net f3→f4
o-Br-TRZ	S1	-0.1861	0.0011	-0.0756	0.2605	0.1712	0.0116	0.0777
	S2	0.0050	-0.1801	-0.0919	0.2670	0.0111	0.1667	0.0891
m-Br-TRZ	S1	-0.1171	0.0152	-0.1789	0.2808	0.1118	0.0032	0.1658
	S2	-0.0718	-0.1978	-0.0075	0.2772	0.0757	0.1798	0.0217
p-Br-TRZ	S1	-0.0705	-0.0083	-0.1956	0.0386	0.0721	0.0219	0.1803
	S2	-0.1121	-0.1743	0.0129	0.2734	0.1106	0.1601	0.0027

Figure S2. Heat map of the contribution of molecular fragment in 1,3,5 triazine derivatives to electron and hole contribution of electrons, holes, and electron hole overlap.
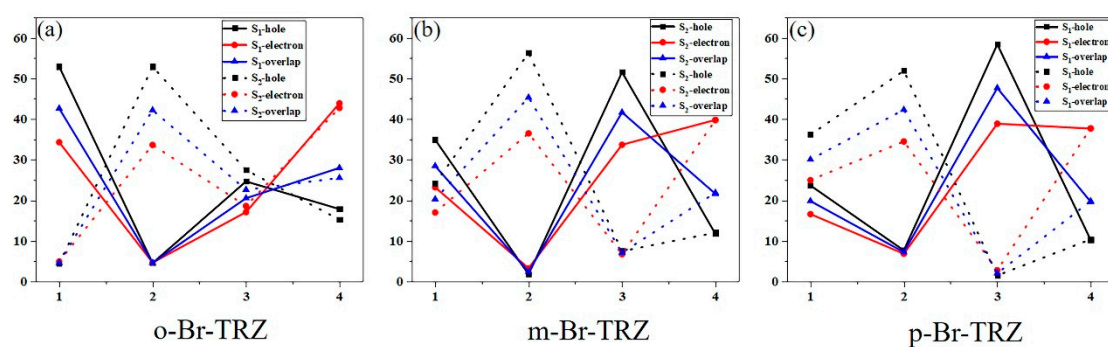
Figure S3. Scatter plot of the percentage contribution of different fragments of 1,3,5 triazine derivatives to electron excitation, hole and hole overlap.
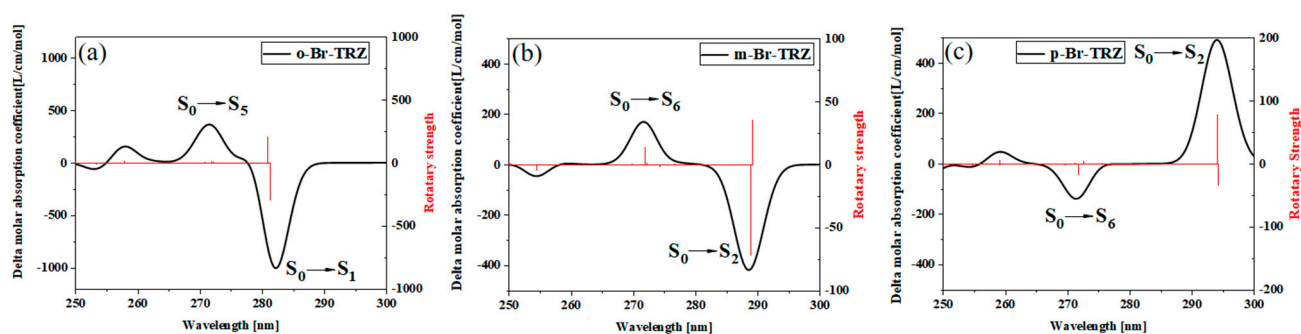

Figure S4. (Electron Circular Dichroism) ECD spectrum of o-Br-TRZ, m-Br-TR and p-Br-TRZ.