Electronic Supplementary Information (ESI)

Revealing the Synergetic Interaction between Amino and Carbonyl Functional Groups on the Electronic and Optical Properties of Carbon Dots

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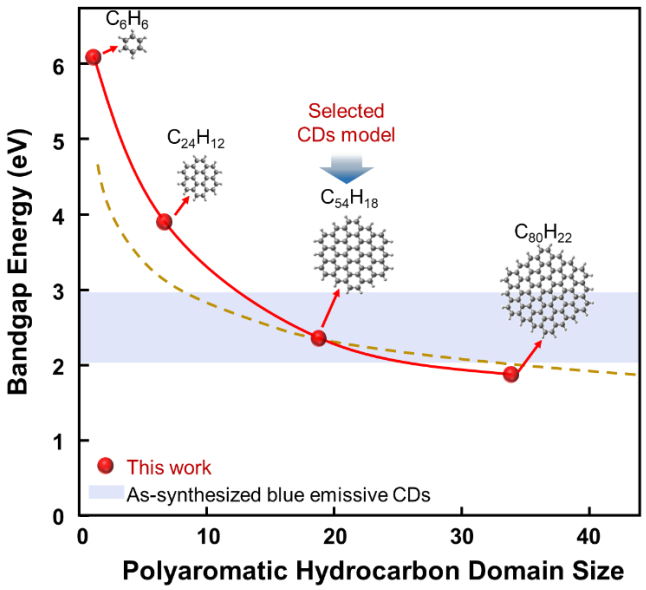

Figure S1. Bandgap energy relation with the polyaromatic hydrocarbon size.

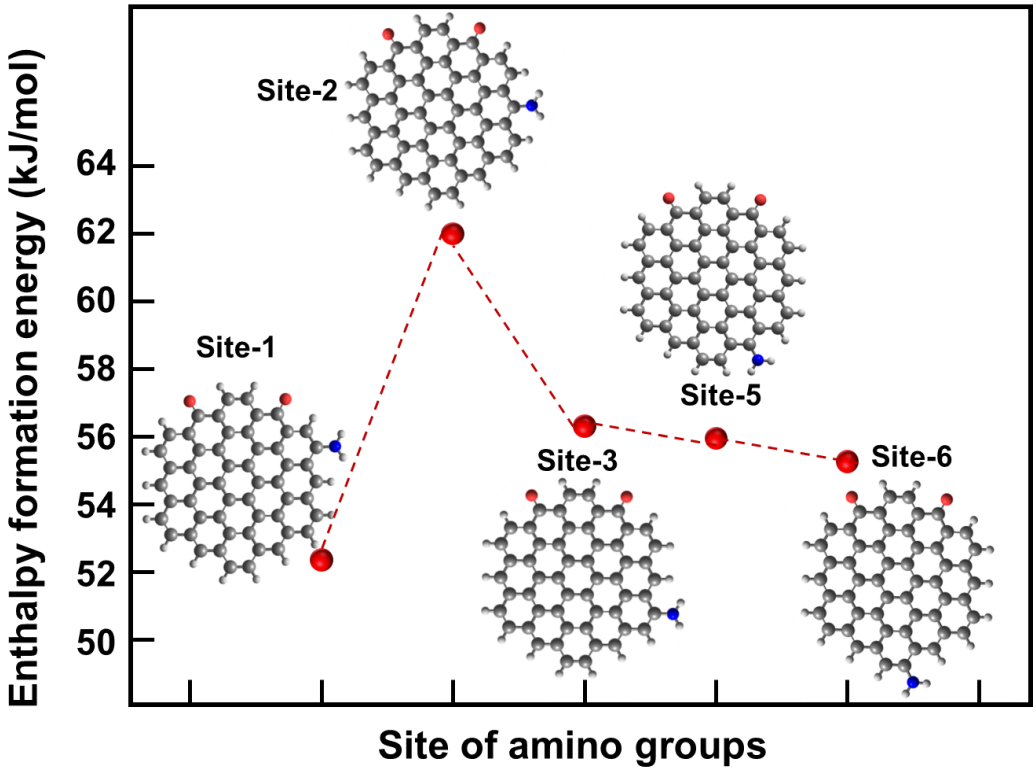

Figure S2. Enthalpy formation energy of amino CDs carbonyl models in various functional groups position.

Table S1 Excitation energies, wavelengths, oscillator strengths, transition coefficients and percentage transition contribution of excited states in Carbonyl CDs.

CDs carbonyl	Sn	Exc. energy (eV)	Wavelength absorbance (nm)	Oscillator (a.u.)	Transition	Contribution (%)	Carbon		Oxygen	
							Occ.	Unocc.	Occ.	Unocc.
O/C=0 (Pristine CDs)	S1	2.2346	554.84	0.0000	H-1→L	50	1.00	1.00	-	-
					H→L+1	50	1.00	1.00	-	-
	S3	2.8098	441.26	1.3035	H-1→L+1	39	1.00	1.00	-	-
					H→L	39	1.00	1.00	-	-
O/C=0.04	S1	1.1253	1101.76	0.1418	H→L	100	0.95	0.86	0.05	0.14
	S2	1.9379	639.79	0.2243	H-1→L	90	0.97	0.86	0.03	0.14
O/C=0.07	S1	1.5012	825.89	0.0010	H→L+1	100	0.92	0.80	0.08	0.20
	S2	1.7242	719.07	0.5096	H→ L	100	0.92	0.86	0.08	0.14
O/C=0.11	S1	1.6323	759.58	0.0665	H→L	75	0.88	0.75	0.12	0.25
	S2	1.657	748.24	0.0195	H-1→L	70	0.92	0.75	0.08	0.25

Table S2 Excitation energies, wavelengths, oscillator strengths, transition coefficients and percentage transition contribution of excited states in Amino CDs.

Amino CDs	Sn	Exc. energy (eV)	Wavelength absorption (nm)	Oscillator (a.u.)	Transition	Contribution (%)	Carbon		Nitrogen	
							Occ.	Unocc.	Occ.	Unocc.
N/C=0.02	S1	2.1910	565.86	0.0180	H→L	59%	0.95	1.00	0.05	0.00
					H-1→L+1	35%	1.00	0.99	0.00	0.01
	S3	2.7060	458.15	0.9610	H-1→L	35.%	1.00	1.00	0.00	0.00
					H-1→L+1	26%	1.00	0.99	0.00	0.01
N/C=0.06	S1	2.0758	597.27	0.0000	H→L+1	50%	0.88	0.96	0.12	0.04
					H-1->L	50%	0.89	0.95	0.11	0.05
	S3	2.5696	482.50	1.1984	H-1→L	26%	0.89	0.95	0.11	0.05
					H→L+1	26%	0.88	0.96	0.12	0.04
N/C=0.11	S1	1.9268	589.81	0.0000	H→L+1	34%	0.85	0.95	0.15	0.05
					H-1→L	34%	0.85	0.95	0.15	0.05
	S3	2.3653	483.57	1.1281	H-1→L+1	38%	0.85	0.95	0.15	0.05
					H→L	38%	0.85	0.95	0.15	0.05
N/C=0.22	S1	1.9617	632.04	0.0067	H→L	51%	0.87	0.97	0.13	0.03
					H-1→L+1	37%	0.89	0.98	0.11	0.02
	S3	2.348	528.04	0.8245	H-1→L+1	59%	0.89	0.98	0.11	0.02
					H→L	41%	0.87	0.97	0.13	0.03