Electronic Supplementary Information (ESI)

A rational design of Carbon Dots via the combination of Nitrogen and Oxygen Functional Groups toward the first NIR window Absorption

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

Structure CDs	Sn	λ abs (nm)	Oscillator strength (f)	Transition coefficients	Contribution (%)	Carbon		Nitrogen	
						Occ.	*Unocc.*	*Occ.*	*Unocc.*
Pristine CDs	S3	441	1.303	H-1 → L+1	38.6%	1.00	1.00	-	-
				H → L	38.4%	1.00	1.00	-	-
				H → L+1	11.5%	1.00	1.00	-	-
				H-1 → L	11.5%	1.00	1.00	-	-
Amino CDs	S1	585	0.087	H-1 → L	77.5%	0.91	1.00	0.09	0.00
				H → L+1	22.5%	1.00	0.97	0.00	0.03
N-pyrrolic CDs	S2	525	0.101	H → L	74.7%	1.00	0.99	0.00	0.01
				H-1 → L+1	25.3%	0.93	1.00	0.07	0.00
N-pyridinic CDs	S3	446	1.147	H → L+1	52.3%	1.00	1.00	0.00	0.00
				H-1 → L	44.7%	0.97	0.94	0.03	0.06
				H-2 → L+2	3.0%	0.97	0.94	0.03	0.06
N-graphitic CDs	S2	786	0.215	H → L+1	89.3%	1.00	0.93	0.00	0.07
				H-1 → L	7.3%	1.00	0.90	0.00	0.10
				H-2 → L+2	3.3%	1.00	1.00	0.00	0.00

Table S2. The percentage of N-pyridinic, N-pyrrolic, N-graphitic and amino content in XPS N1s of the as-synthesized CDs

Sample	N-pyridinic	N-pyrrolic	N-Graphitic	Amino groups
N-pyrrolic CDs-C=O	(2.98±3) %	(54.80±3) %	(18.30±3) %	(23.92±3) %
N-graphitic CDs-C=O	(1.25±3) %	(15.82±3) %	(63.43±3) %	(19.50±3) %

Table S3. The percentage of the presence of surface functional O atom bonds in the XPS O1s of the as-synthesized CDs

Sample	C=O	C-O-C, C-O-OH
N-pyrrolic CDs-C=O	(53.80±3) %	(46.20±3) %
N-graphitic CDs-C=O	(55.87±3) %	(44.23±3) %

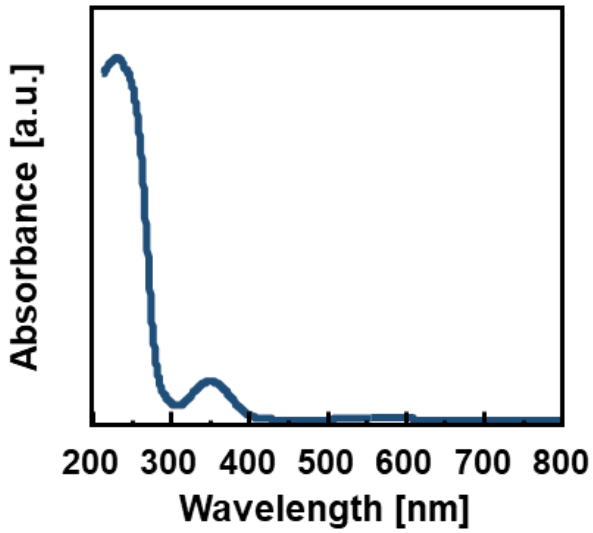

Fig. S1. The absorbance spectra of CDs that was prepared by microwave assisted-hydrothermal for 4h at 140°C.

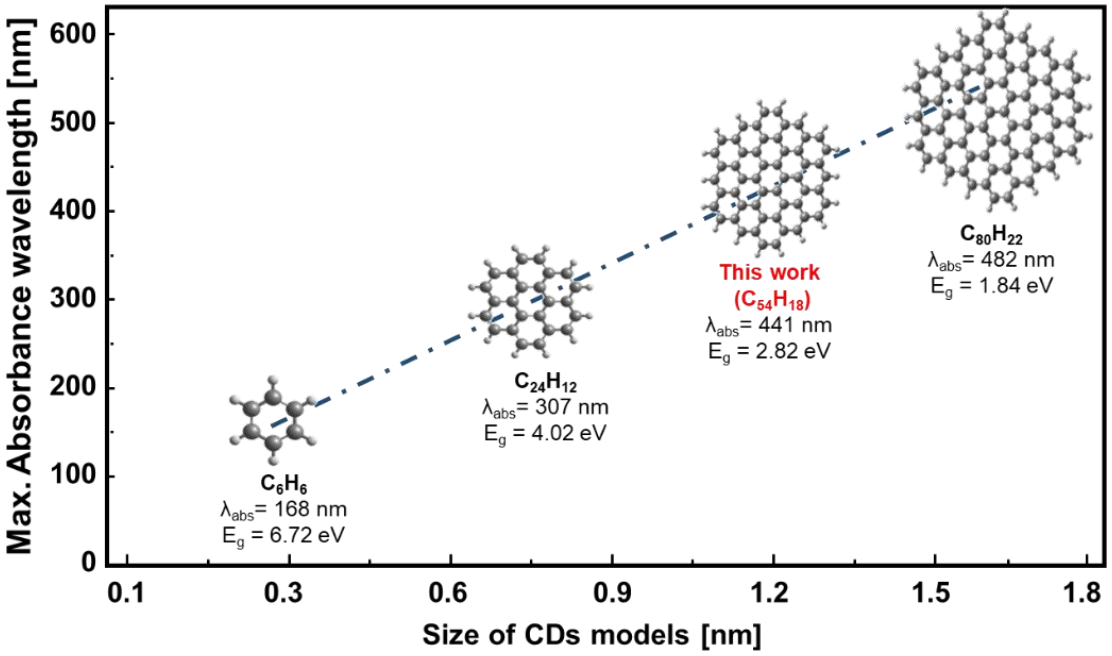

Fig. S2 The Optimized structure and calculated absorption wavelength of PAH with different size as a CDs' model.

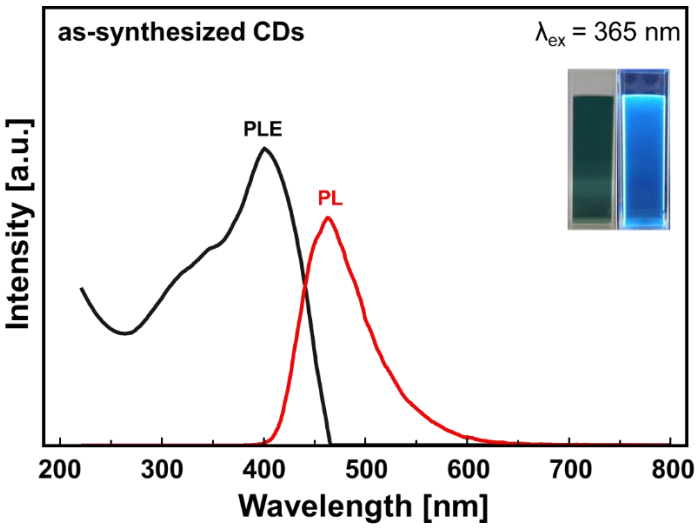

Fig. S3 Photoluminescence (PL) emission and excitation spectra of the as-synthesized CDs. The inset picture is digital photograph of the as-synthesized CDs under Visible light and 365 nm-UV irradiations.

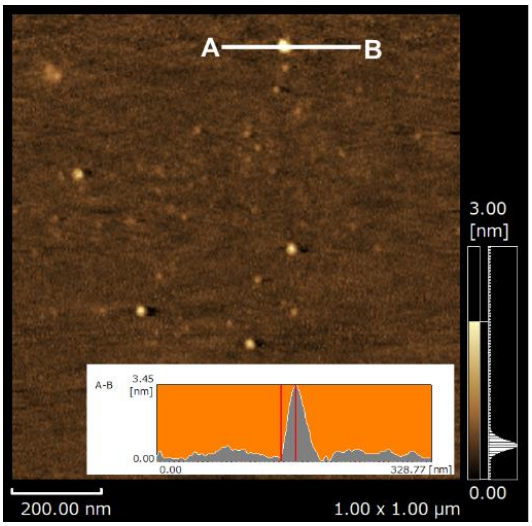

Fig. S4 AFM image of the as-synthesized CDs that exhibit a first NIR window. The inset image is the height profile of the CDs along AB axis. The CDs particle in spherical shape with the height of 3.45 nm.

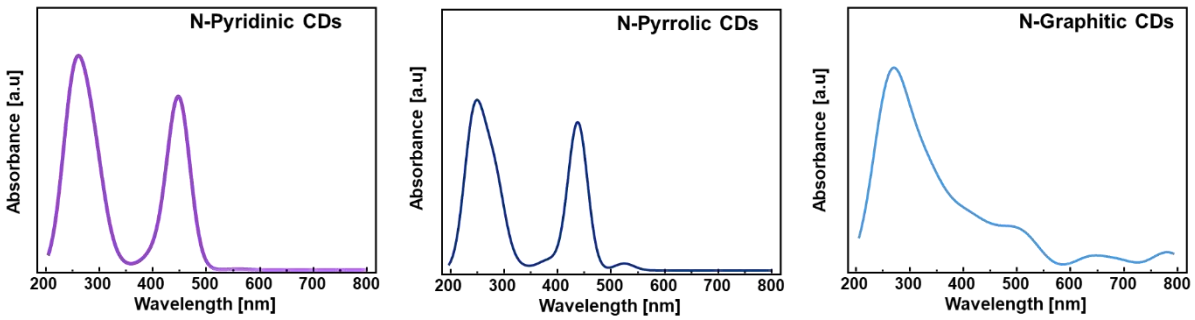

Fig. S5. The calculation of absorbance spectra on CDs doped configuration-N (pyridinic-N, pyrrolic-N and graphitic-N).

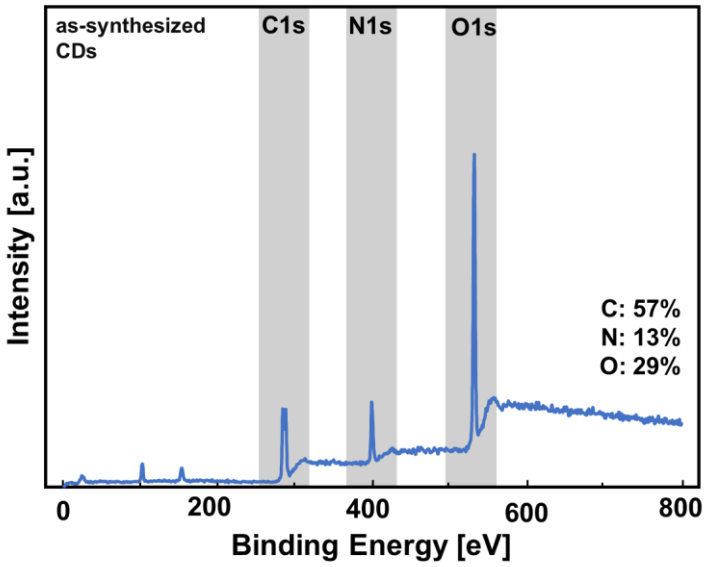

Fig. S6 Full Scan XPS of the as-synthesized Carbon Dots that prepared through a microwave assisted hydrothermal. The chemical composition was calculated based on the Full scan XPS with weighting RSF factor in CasaXPS.

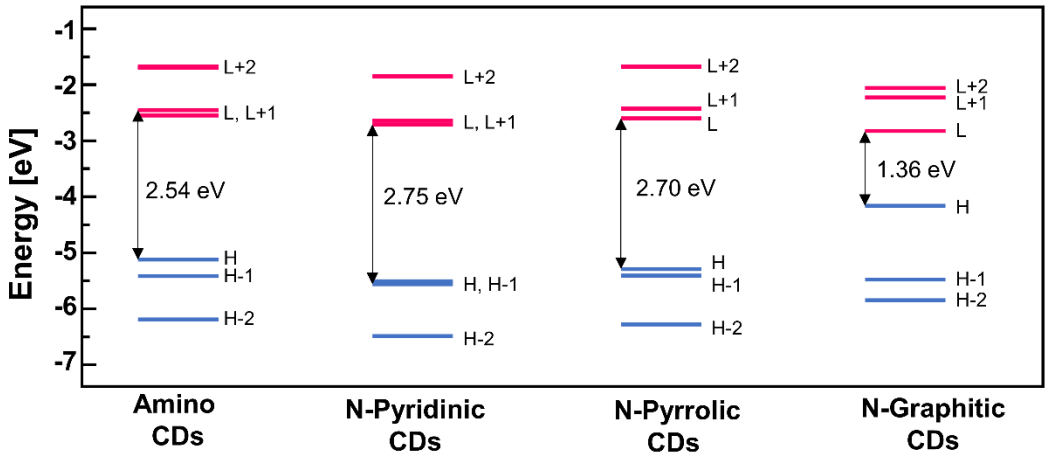

Fig. S7 The bandgap energy levels on CDs doped configuration-N (pyridinic-N, pyrrolic-N and graphitic-N).

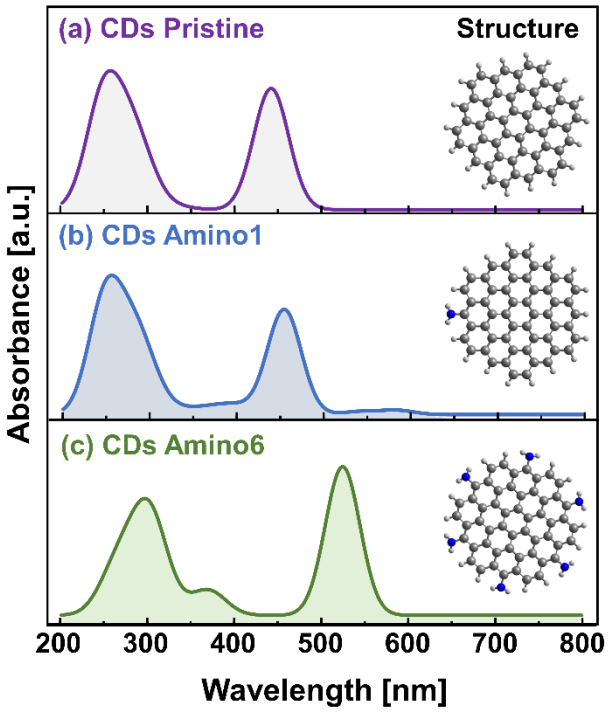

Fig. S8 The calculation of absorbance spectra on CDs with variations in the number of amino.

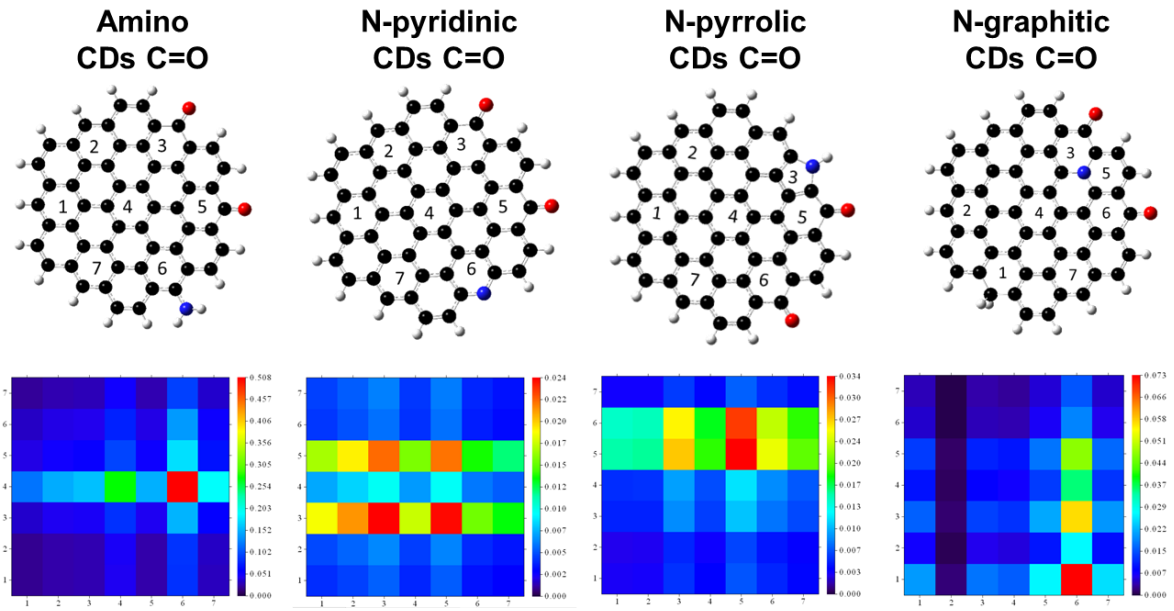

Fig. S9 Transition Density Matrix of the CDs with various combination N and O surface functional groups. Each model was defined as seven fragments that represents the sp^2 carbon structure, N configurations (amino, N-pyridinic, N-pyrrolic and N-Graphitic) and O functional groups (carbonyl).

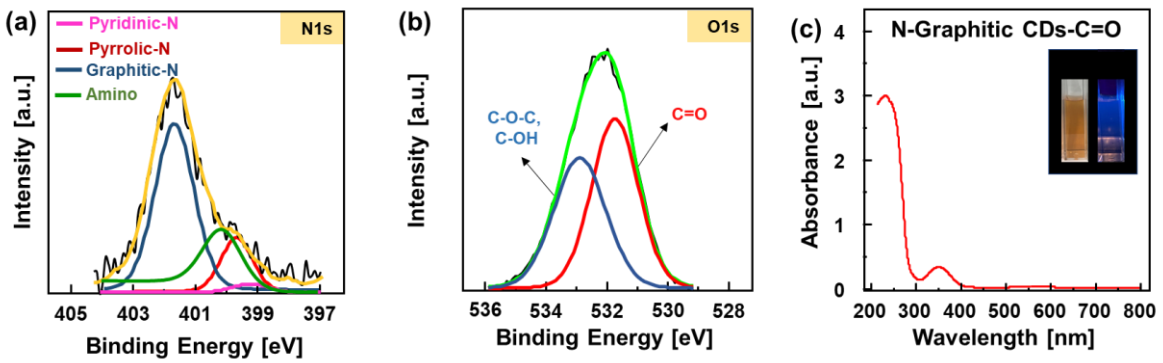

Fig. S10 (a) N1s XPS spectrum of the N-Graphitic CDs-C=O. (b) O1s XPS spectrum of the N-Graphitic-C=O. (c) Absorption spectrum of the N-Graphitic CDs-C=O. The inset picture is the digital image of the samples under visible light and 365 nm UV lamp irradiation.