Electronic Supplementary Information

Energy level engineering of carbon dots based on post-synthetic treatment with acids and amines

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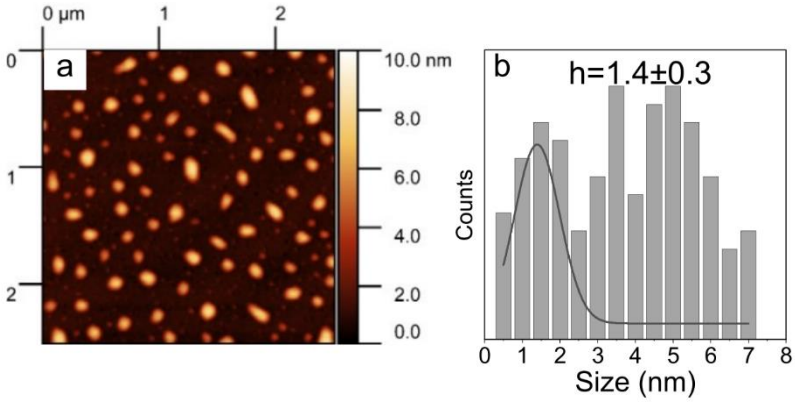

Figure S1. (a) AFM image of CD-s, and (b) their height distribution from AFM measurements. There are two types of particles in the CD-s sample with different lateral sizes, which corresponds to the appearance of two peaks in the height distribution, with average height of 1.4 and 4.6 nm. The larger particles are assumed to be aggregates with lateral sizes of up to 50 nm.

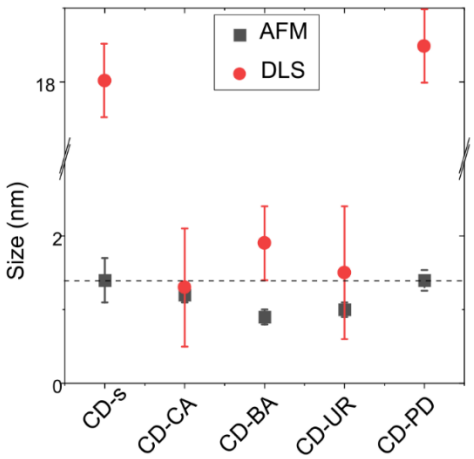

Figure S2. Size of five CD samples estimated from AFM (black squares) and DLS (red circles) measurements.

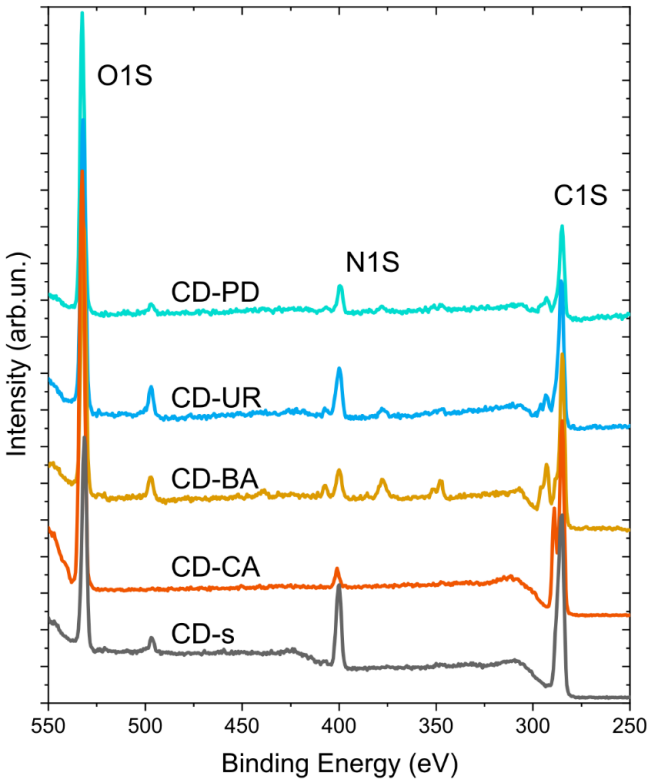

Figure S3. Full survey XPS spectra of five CD samples.

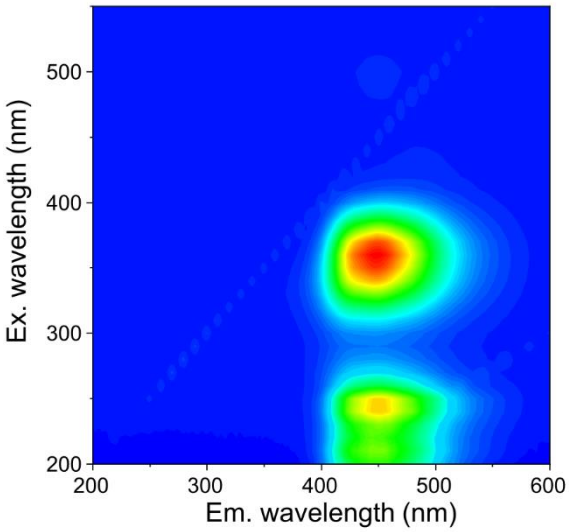

Figure S4. PLE-PL map of CD-s in water.

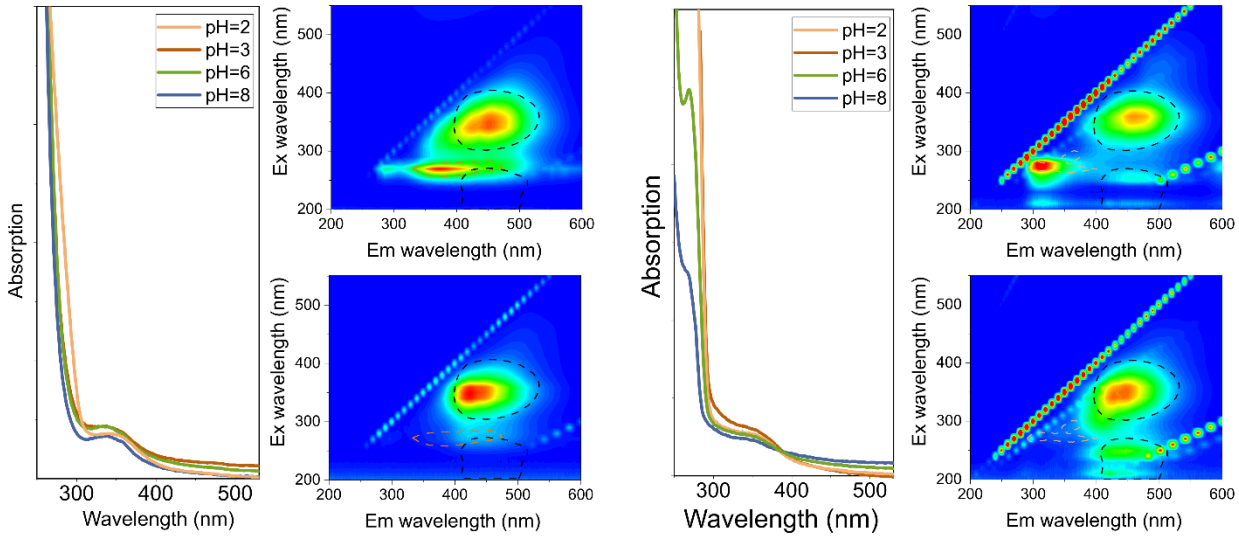

Figure S5. Absorption (a, d) and PLE-PL maps (b, c, e, f) of CD-CA (a-c) and CD-BA (d-f) at different pH shown in the legend. On PLE-PL maps, by orange dashed line the emissive band attributed to the acid-treatment is shown.

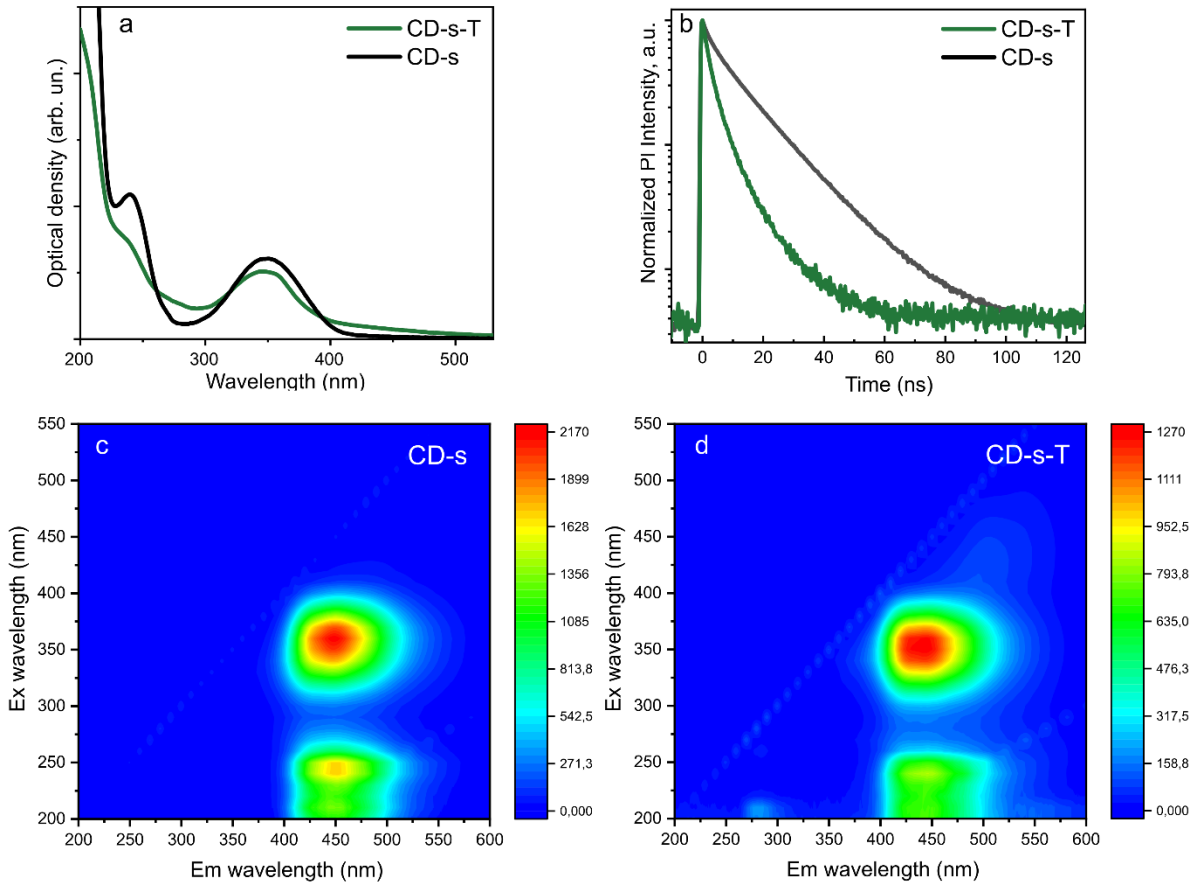

Figure S6. Absorption spectra (a) and PL decay curves of CD-s (black lines) and heated CD-s to 180 ˚C for 6h (CD-s-T, green lines). PLE-PL maps of CD-s (c) and CD-s-T (d).

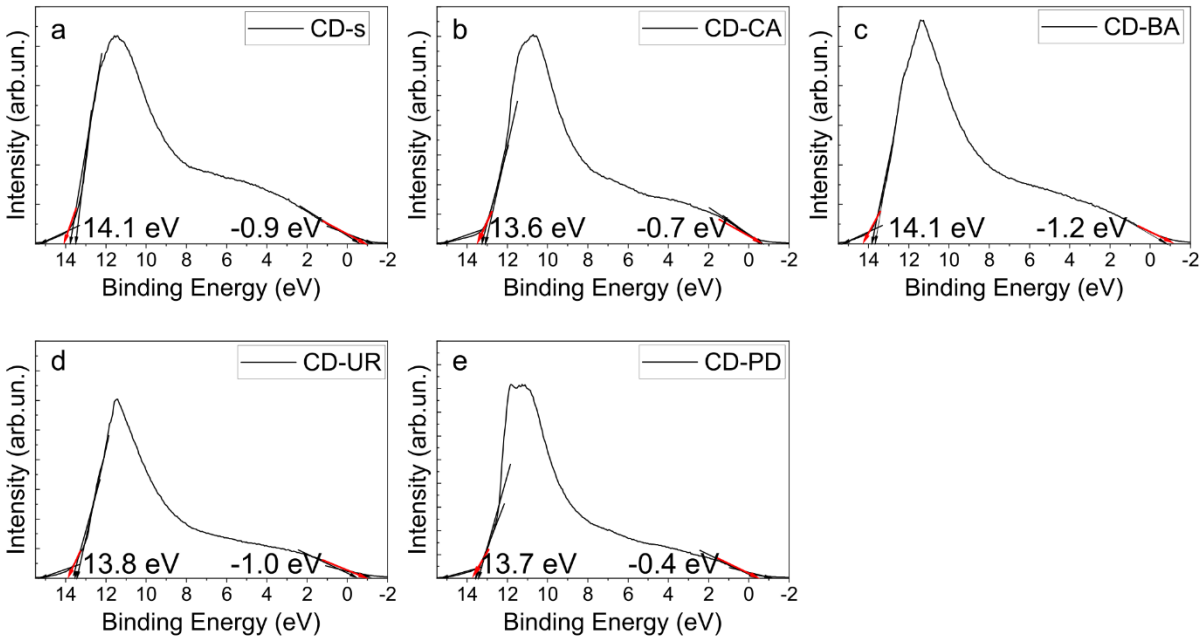

Figure S7. (a-e) UPS spectra of five CD samples. Black arrows show different ways of drawing the spectrum's edges; red arrows mark the average edge of the spectra.

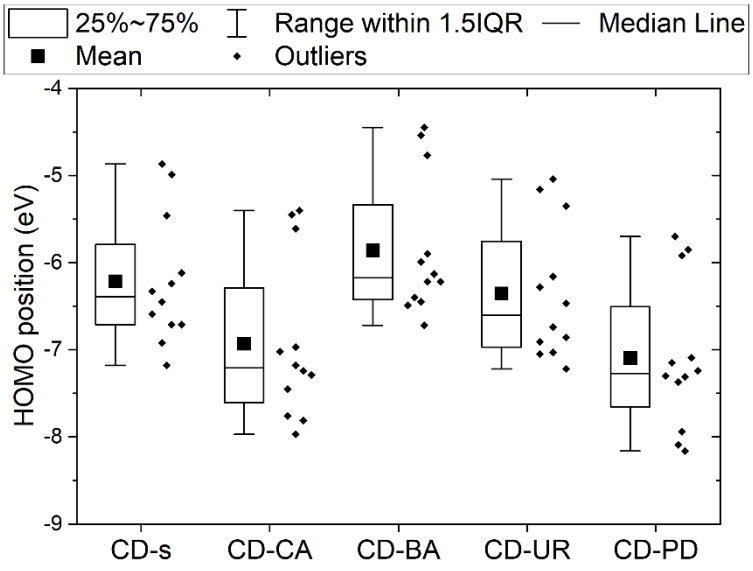

Figure S8. Estimation of the HOMO position from UPS spectra shown in Figure S5.

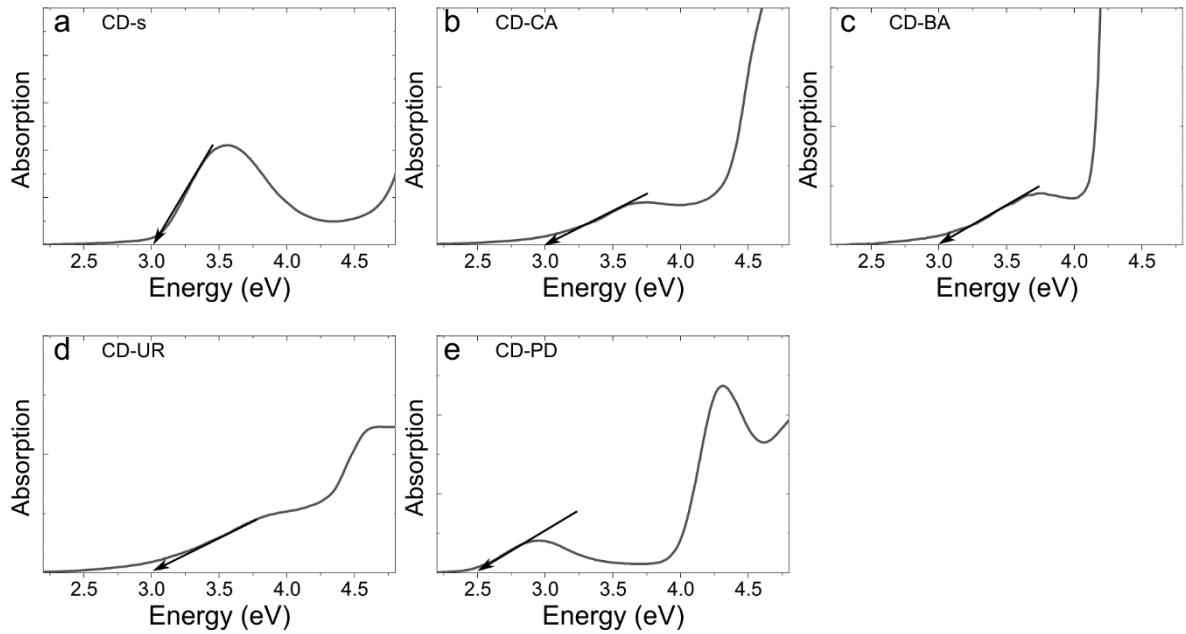

Figure S9. Absorption spectra of five CD samples. The arrows mark the absorption edge, determining the energy gap in eV.

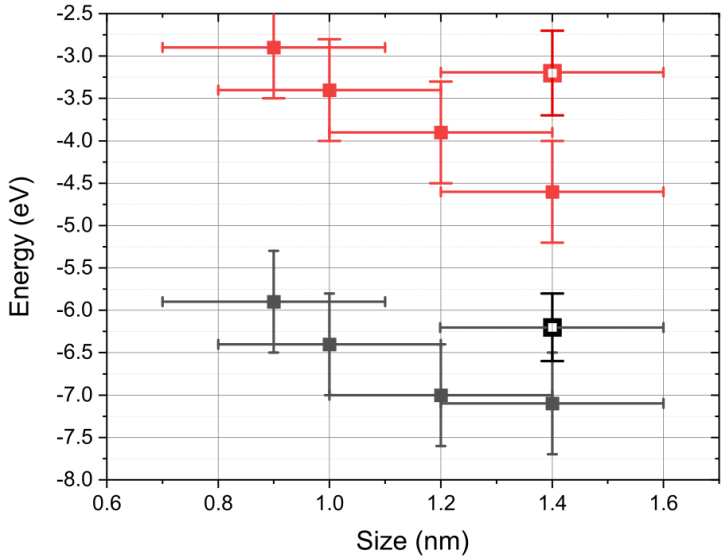

Figure S10. Dependence of the HOMO (black squares) and LUMO (red squares) energy levels of five CDs on their size. The values for CD-s are shown by open squares.

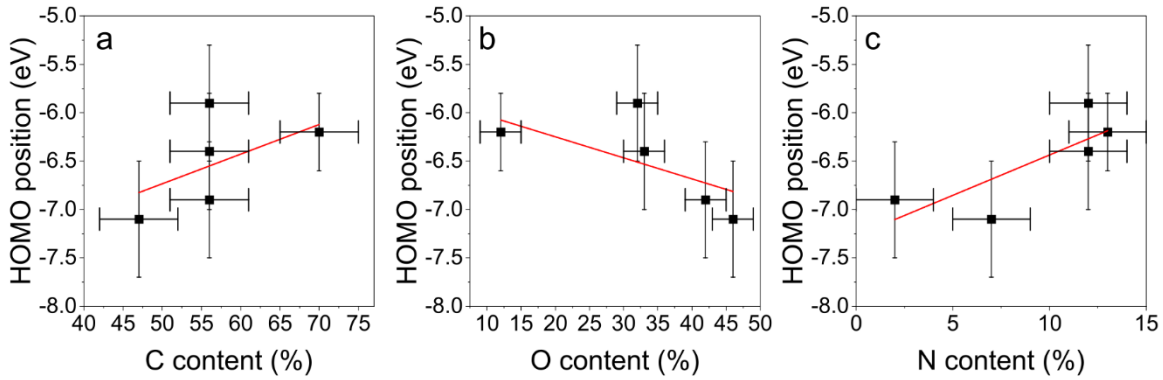

Figure S11. Dependence of the HOMO position on chemical composition of CDs in terms of the C (a), O, (b), and N (c) content (%). Red lines provide linear fits of experimental data.

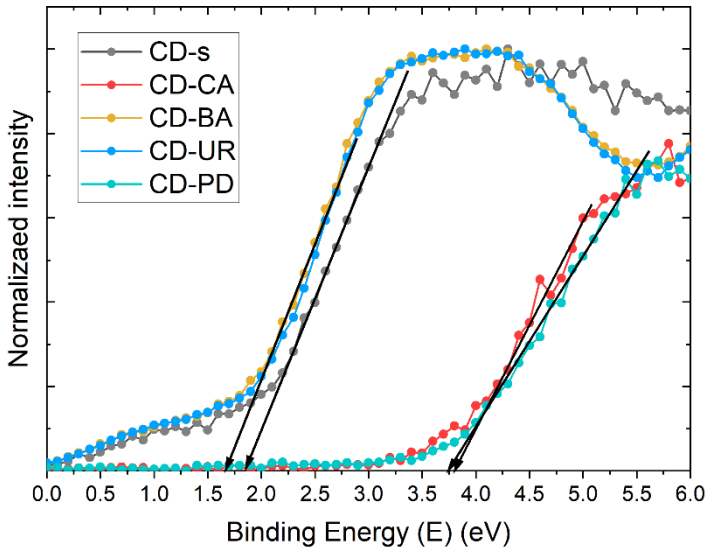

Figure S12. Estimation of the Fermi energies of five CD samples from the valence band spectra (black arrows).

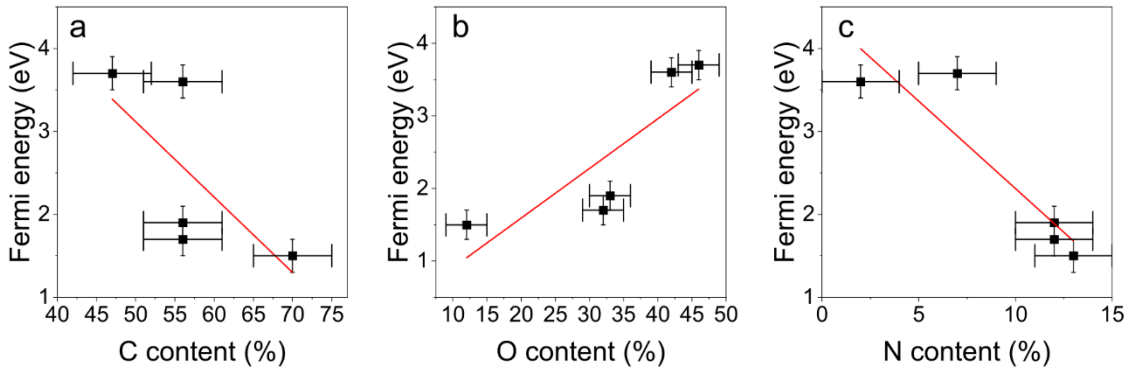

Figure S13. Dependence of the Fermi energy on the chemical composition of CDs in terms of the C (a), O, (b), and N (c) content (%).

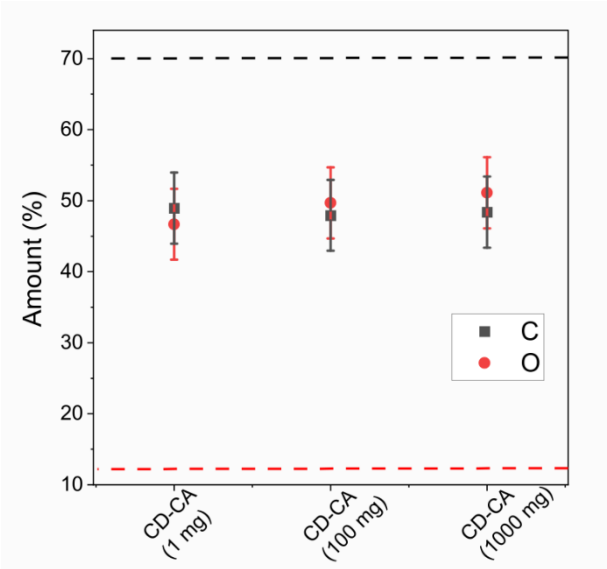

Figure S14. Change in the carbon (black squares) and oxygen (red circles) amount in CD-s treated with different amount of citric acid: 1 mg, 100 mg, and 1000 mg. The amount of carbon and oxygen in CD-s is shown by dashed black and red lines, respectively.

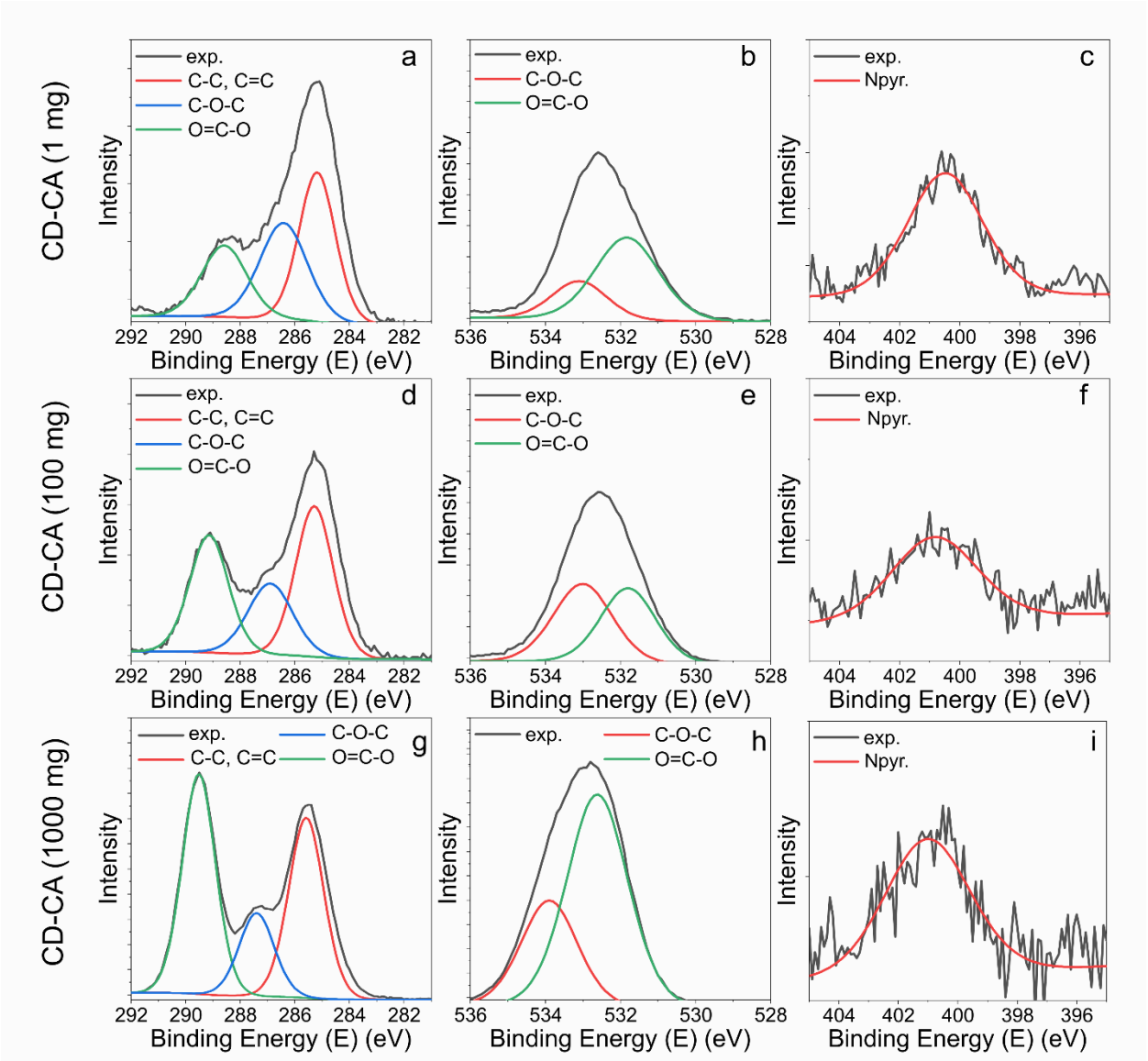

Figure S15. High resolution XPS spectra of C 1S (a, d, g), O 1S (b, e, h), and N 1S (c, f, i) for the CD-CA samples with different amount of CA added: 1 mg (a-c), 100 mg (d-f), and 1000 mg (g-i), with corresponding deconvolution into contributions from different functional surface groups provided in the legend.

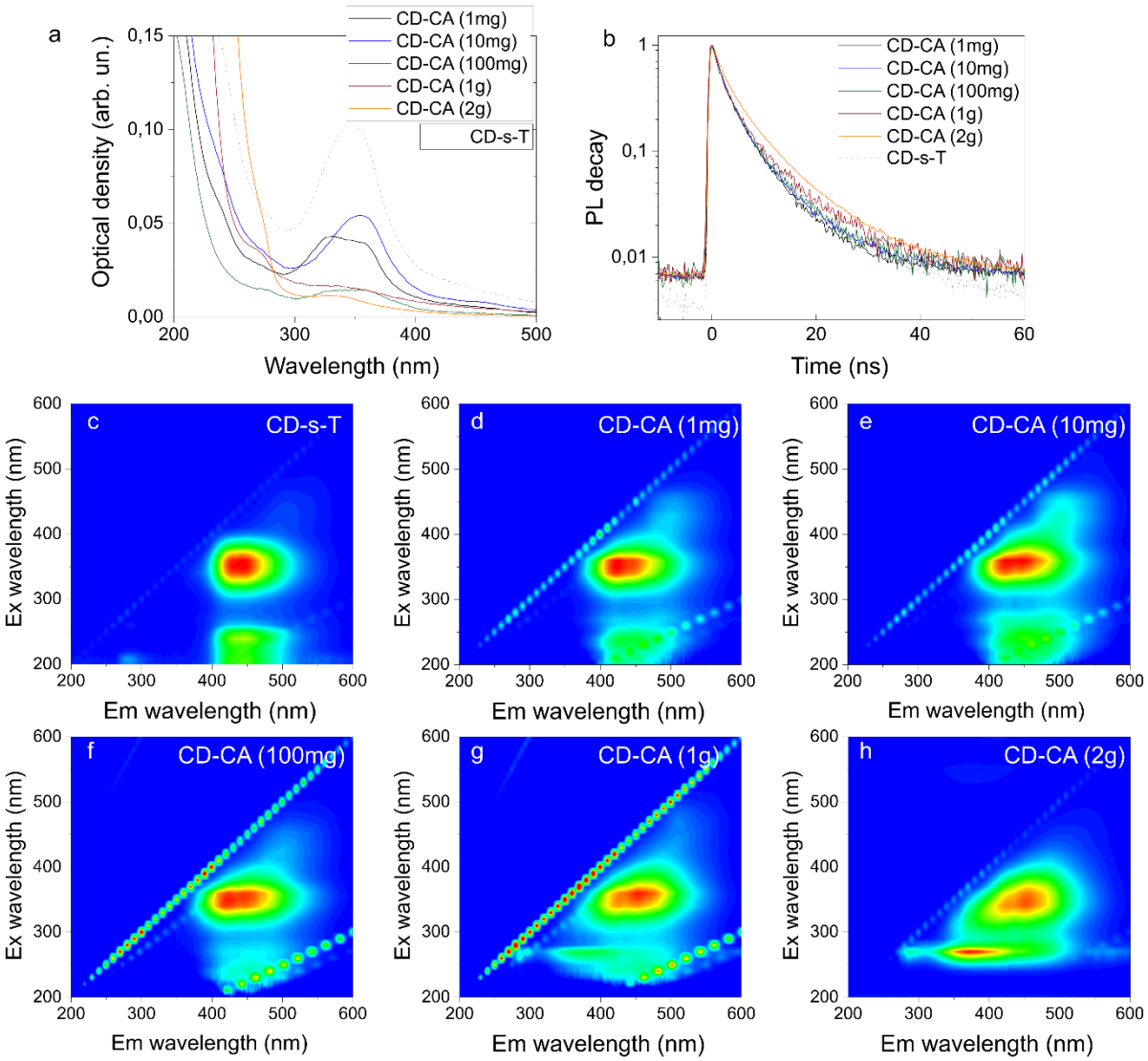

Figure S16. Absorption spectra (a), PL decays (b), and PLE-PL maps (c-h) of CDs treated with different amount of CA compared to the treated CDs without addition of CA (CD-s-T).

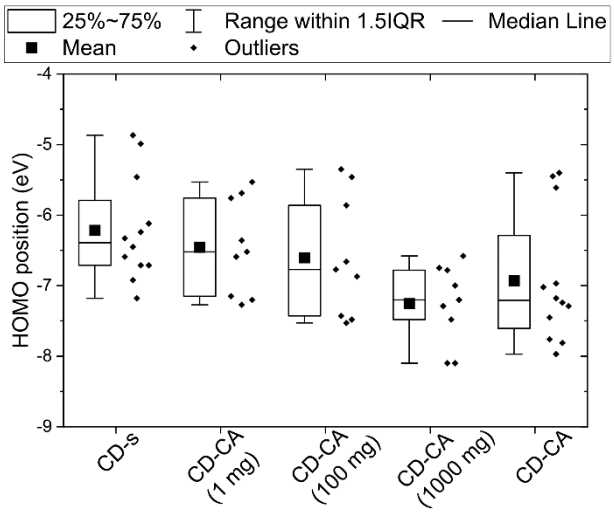

Figure S17. Estimation of the HOMO position from UPS spectra for the CD-s and CD-CA samples with different amount of CA added: 1 mg, 100 mg, 1000 mg, and 2 g (CD-CA).

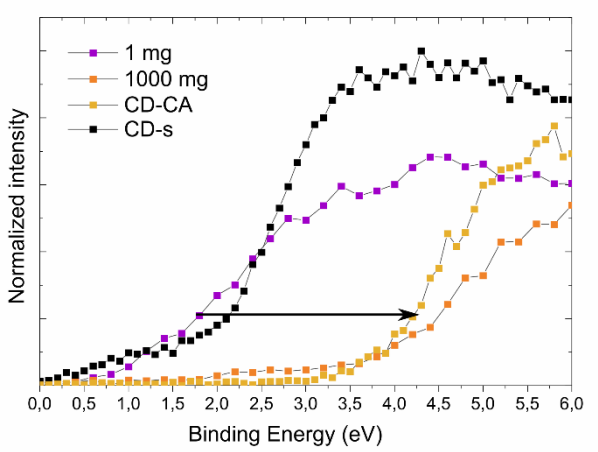

Figure S18. Valence band spectra for CD-s and CD-CA with different amount of CA added: 1 mg, 1000 mg, and 2 g (CD-CA).

Table S1. Summary of absorption (Abs), PLE, and PL peak positions for five CD samples

Sample name	Abs 1, nm	Abs 2, nm	PLE 1, nm	PLE 2, nm	PL 1, nm	PL 2, nm
CD-s	240	350	260	360	-	450
CD-CA	270	330	260	360	380	450
CD-BA	280	340	290	360	380	450
CD-UR	270	320	280	350	300	420
CD-PD*	230	290/420	280	350/420	310	420/550

** for CD-PD in Abs 2, PLE 2, and PL 2 values for both 2nd and 3d peaks are shown divided from each other by a slash*

Table S2. Summary of average PL lifetimes and PL QYs for five CD samples

Sample name	A_1, %	τ_1, ns	A_2, %	τ_2, ns	$\tau_{av.}$, ns	PL QY, %
CD-s	63	15.2	37	2.7	14	69
CD-CA	30	9.1	70	2.5	6.5	29
CD-BA	32	10.6	68	2.7	7.8	35
CD-UR	34	6.8	66	1.8	5.1	16
CD-PD	5	4.3	95	1.7	2	6

Table S3. Summary of absorption (Abs) and PL peak positions for CD samples treated with different amounts of citric acid.

	Abs (S2), nm	Abs (S1), nm	PL peak, nm	PL QY, % $\lambda_{ex} = 350\ nm$	$\boldsymbol{\tau}$, ns
CD-CA (1mg)	-	343	427	16	4.5
CD-CA (10mg)	-	355	434	18	5.1
CD-CA (100mg)	275	346	434	19	5.1
CD-CA (1g)	270	339	447	17	5.8
CD-CA (2g)	270	330	447	29	6.5