

Supporting Information

Elucidating the Quenching Mechanism in Carbon Dot-Metal Interactions–Designing Sensitive and Selective Optical Probes

Farah Noun, Evelyne Anastasia Jury and Rafik Naccache

Table S1: Summary of characterization for FG-CDs showing (A) the functional groups observed from FTIR analysis (B) the functional groups observed from XPS analysis and (C) the elemental composition of the dots.

(A) FTIR Analysis

Wavenumber (cm ⁻¹)	Type of vibration	Type of bond	Functional group
1307 & 1386	Stretch	C-N	amide/amine
1583	Stretch	C=N	-
1583	Stretch	C=C	Aromatic
1645	Stretch	C=O	Amide
3000-3500	Stretch	N-H	amide/amine
3000-3500	Stretch	O-H	hydroxyl/carboxylic acid

(B) XPS Analysis

Peak	Binding energies (eV)	Type of bond	Functional group
C1s	285.58	C=O/C=N	amide/carboxylic
	286.89	C-O	-
	288.68	C-C/C=C	-
N1s	400.58	C=N/C-N	graphitic nitrogen
	402.71	NH ₂	pyrrolic nitrogen
O1s	532.02	C=O	amide/carboxylic
	533.26	C-OH/C-OC	-
S2p	163.38	C ₄ S-H	thiophene
	164.14	C ₄ S-H	thiophene
	165.51	C-S-H	thiol

(C) Elemental Analysis

Element	Percent Composition
Carbon	53.10%
Oxygen	26.10%
Nitrogen	17.40%
Sulfur	3.40%

Table S2: Fluorescence lifetimes of FG-CDs at increasing concentrations of lead (II) ions.

[Pb ²⁺]	Lifetime 1 (ns)	±	Lifetime 2 (ns)	±	χ ²
0 nM	0.8	2.8E-03	5.7	4.5E-03	1.2
400 nM	0.8	4.1E-03	5.9	8.1E-03	1.1
1000 nM	0.8	3.3E-02	5.7	3.5E-02	1.1

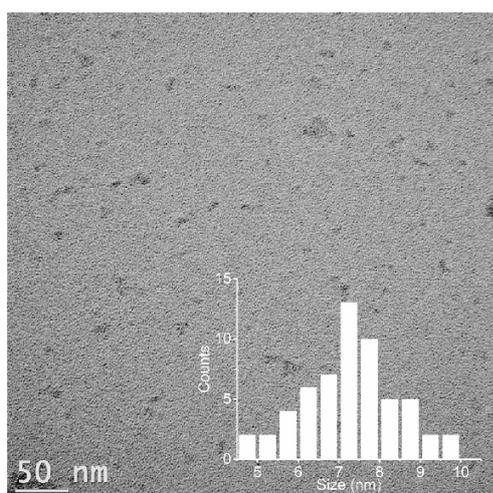


Figure S1: TEM image of FG-CDs with overlaid size distribution plot showing an average size of 7.7 ± 1.5 nm.

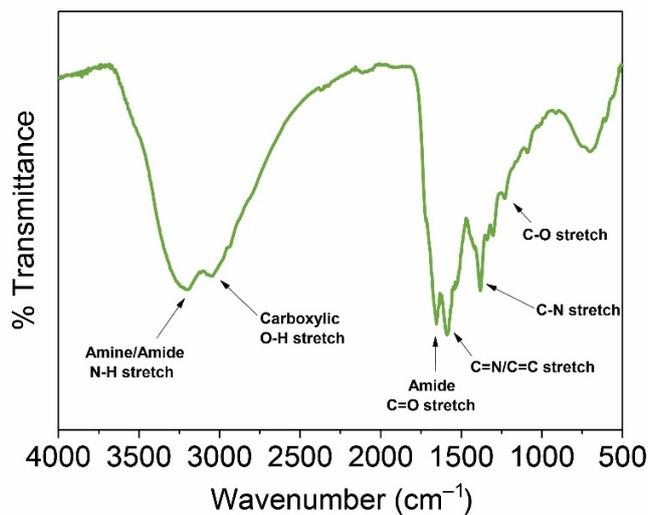


Figure S2: FTIR spectrum of FG-CDs showing the presence of amide and carboxyl stretches as well as N-H and O-H functional groups.

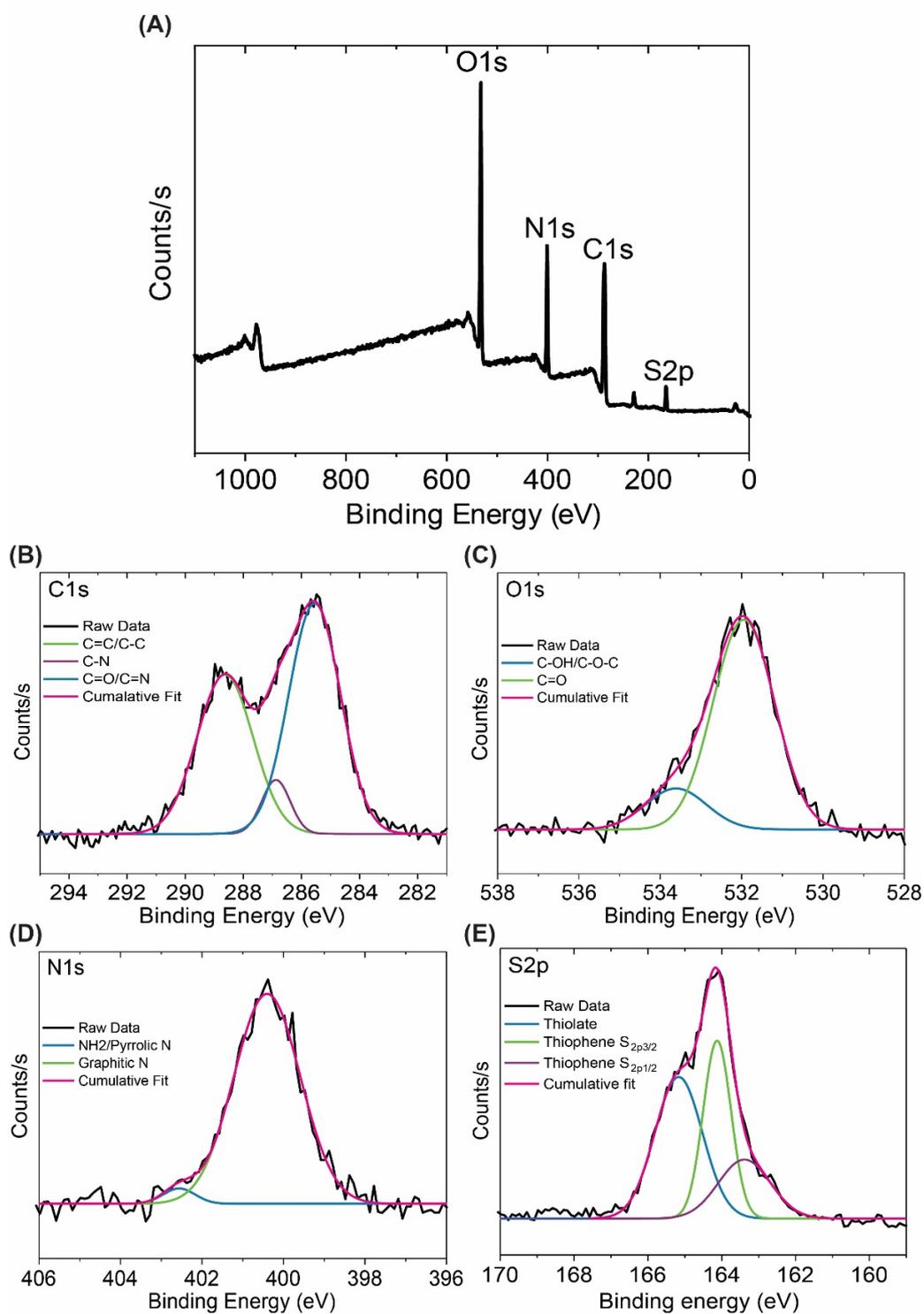


Figure S3: (A) XPS survey spectrum of FG-CDs showing binding energies of C1s, N1s, O1s and S2p. Spectra of deconvoluted binding energies reveal (B) a maximum for C1s at 286.08 eV, (C) a maximum at 400.08 eV for N1s (D) a maximum at 532.08 eV for O1s and (E) for S2p a maximum at 165.08 eV.

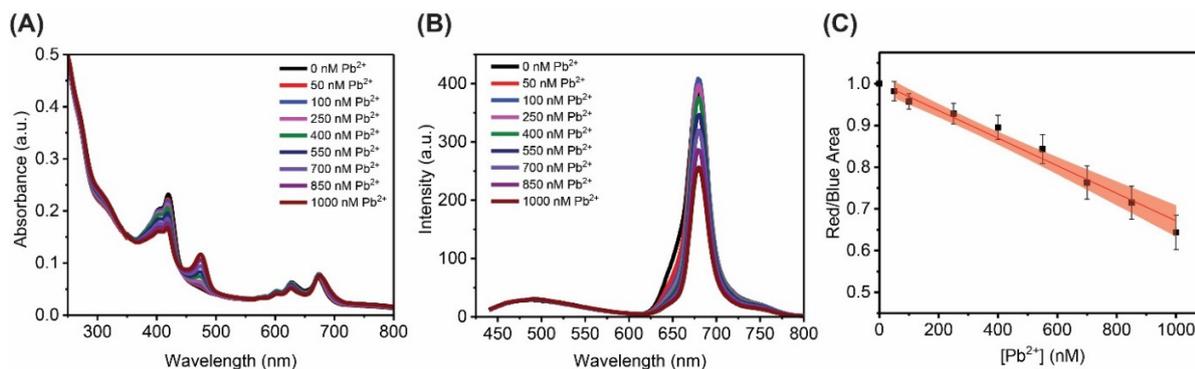


Figure S4: (A) Absorbance spectra for FG-CDs showing a new peak at ~ 475 nm in the presence of Pb^{2+} . (B) Fluorescence spectra for FG-CDs in the presence of Pb^{2+} . (C) The linear plot of the decreasing overall R/B area ratio showing a $\sim 40\%$ in red fluorescence with an $r^2=0.98$.

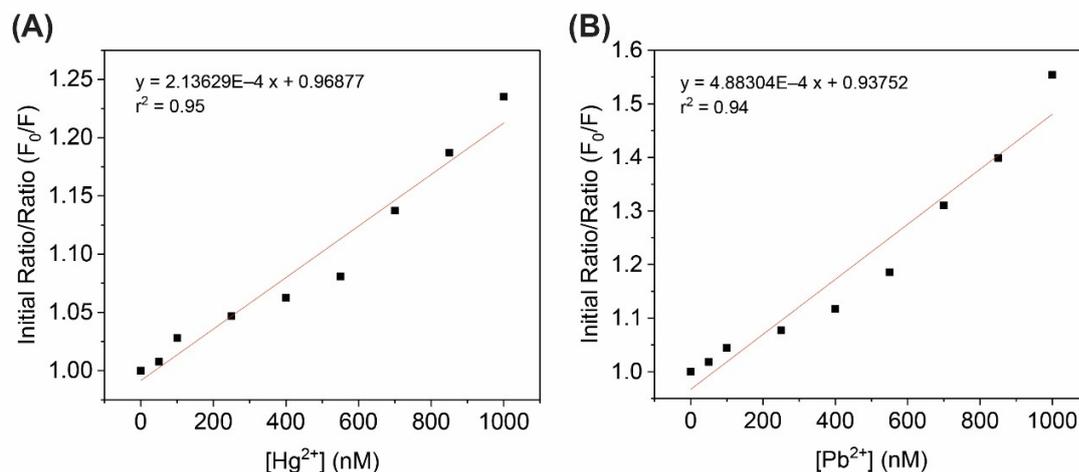


Figure S5: (A) Stern-Volmer plot displaying the linear equation for FG-CDs and Hg^{2+} with $k_{sv} = 2.14 \times 10^{-4}$ and $r^2 = 0.95$ (B) Stern-Volmer plot displaying the linear equation for FG-CDs and Pb^{2+} with $k_{sv} = 4.88 \times 10^{-4}$ and $r^2 = 0.94$.

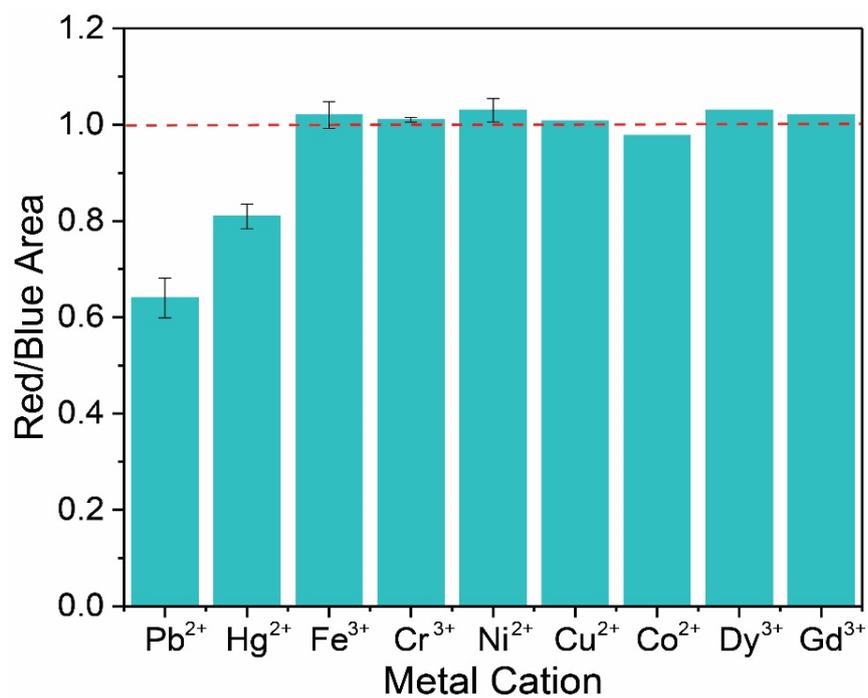


Figure S6: R/B area ratio of FG-CDs with 1000 nM of various metallic cations showing comparison of quenching effectiveness.