

SUPPORTING INFORMATION

Boosting Carbon Quantum Dots/fullerene electron transfer via surface group engineering

Alberto Privitera, Marcello Righetto, Dario Mosconi, Francesca Lorandi, Abdirisak A. Isse, Alessandro Moretto, Renato Bozio, Camilla Ferrante, Lorenzo Franco*

Department of Chemical Sciences, University of Padova, via Marzolo 1, 35131 Padova

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Synthesis of functionalized CQDs

Anhydrous Dimethylformamide (DMF, 2 ml) was poured into a 100 ml flask equipped with a CaCl₂ tube. Thiophene-derived carboxylic acid (2.6 mmol) was dispersed in DMF under vigorous stirring. The mixture was cooled at 0 °C in an ice bath and 1-Hydroxy-7-azabenzotriazole (HOAt, 0.389 g, 2.86 mmol) was added. After 10 minutes that HOAt dissolved, N-(3-Dimethylaminopropyl)-N'-ethylcarbodiimide hydrochloride (EDC, 0.548 g, 2.86 mmol) was poured into the solution. Afterwards, CQDs (0.150 g, corresponding to about 2.6 mmol of -NH₂ reactive sites) were added and the pH was adjusted to 8 using triethylamine (TEA, 0.440 ml). After 10 minutes, the ice bath was removed and the reaction was carried on at r.t. for 8 h. An additional quantity of EDC (0.274 g, 1.43 mmol) and TEA (0.440 ml) was dispersed and stirred overnight. The solvent was removed at 60°C under reduced pressure and the reaction crude was redissolved in dichloromethane. The organic phase was washed with KHSO₄ 10% wt/V (3 x 50 ml), deionized water (2 x 50 ml) and NaHCO₃ 5% wt/V (3 x 50 ml). The solution was dehydrated using Na₂SO₄ and, subsequently, dichloromethane was removed under reduced pressure. The product was dried overnight under vacuo. Elemental analysis: pristine CQD C=71.47%, H=5.05%, N=17.09% and 5.39% for residual elements, CQD-1 C=68.15%, H=3.65%, N=11.13% S=9.06 % and 8.01% for residual elements, CQD-2 C=66.05% H=3.16%, N=10.14%, S=11.47% and 9.18% for residual elements.

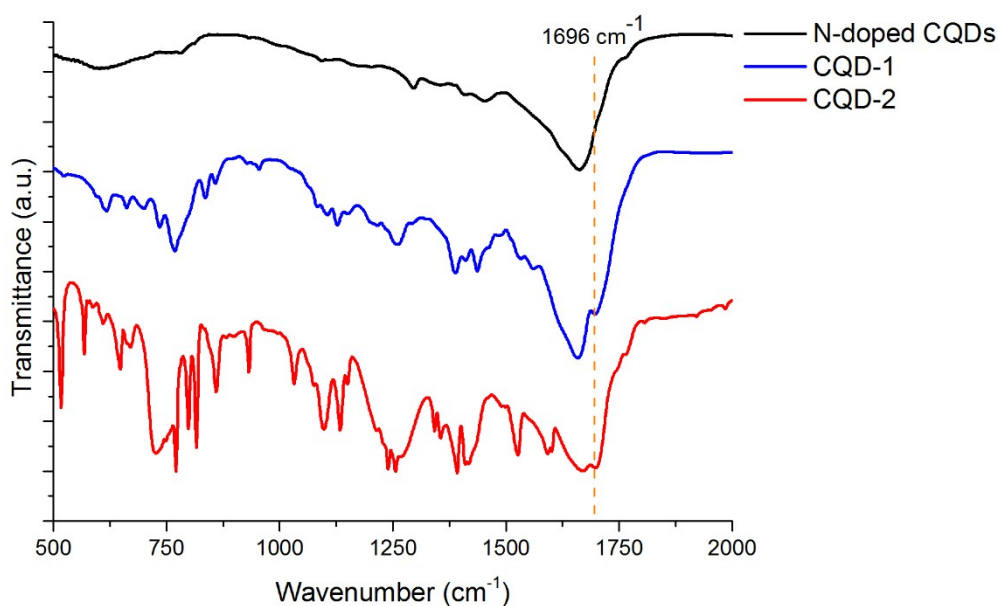


Figure S1. IR spectra of pristine and functionalized CQDs

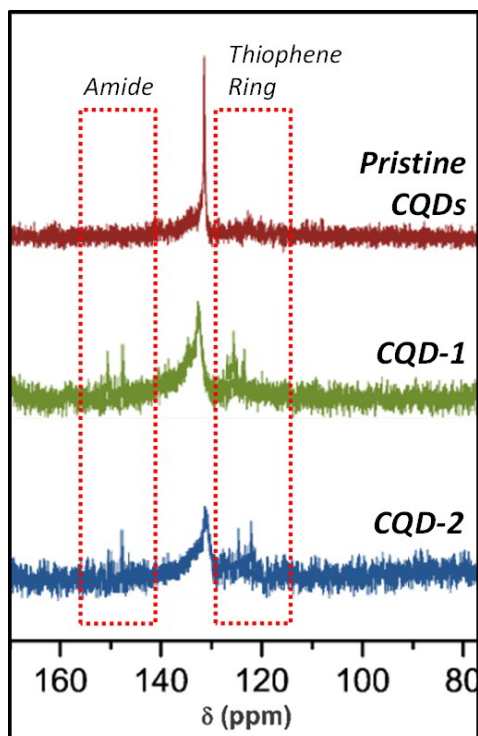


Figure S2: ^{13}C NMR spectra (DMSO d_6) of pristine (red), CQD-1 (green), and CQD-2 (blue). Highlighted regions represent the new amide and aromatic carbons. The main peak at 130 ppm, present in all the NMR traces, is related to sp^2 carbons.

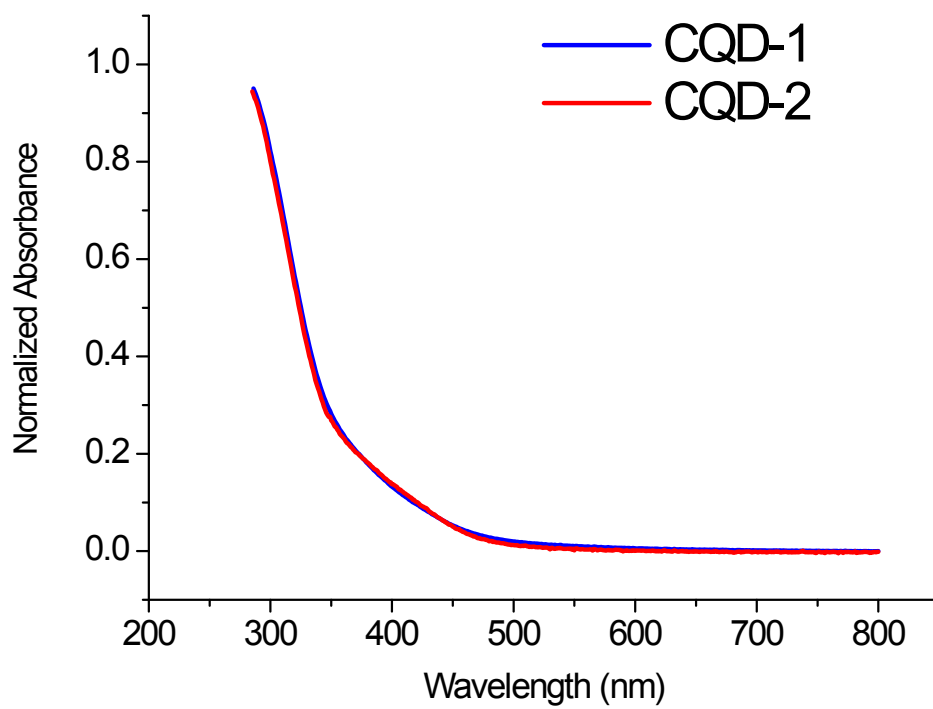


Figure S3: Absorption Spectra of CQD-1 and CQD-2 in DMF.

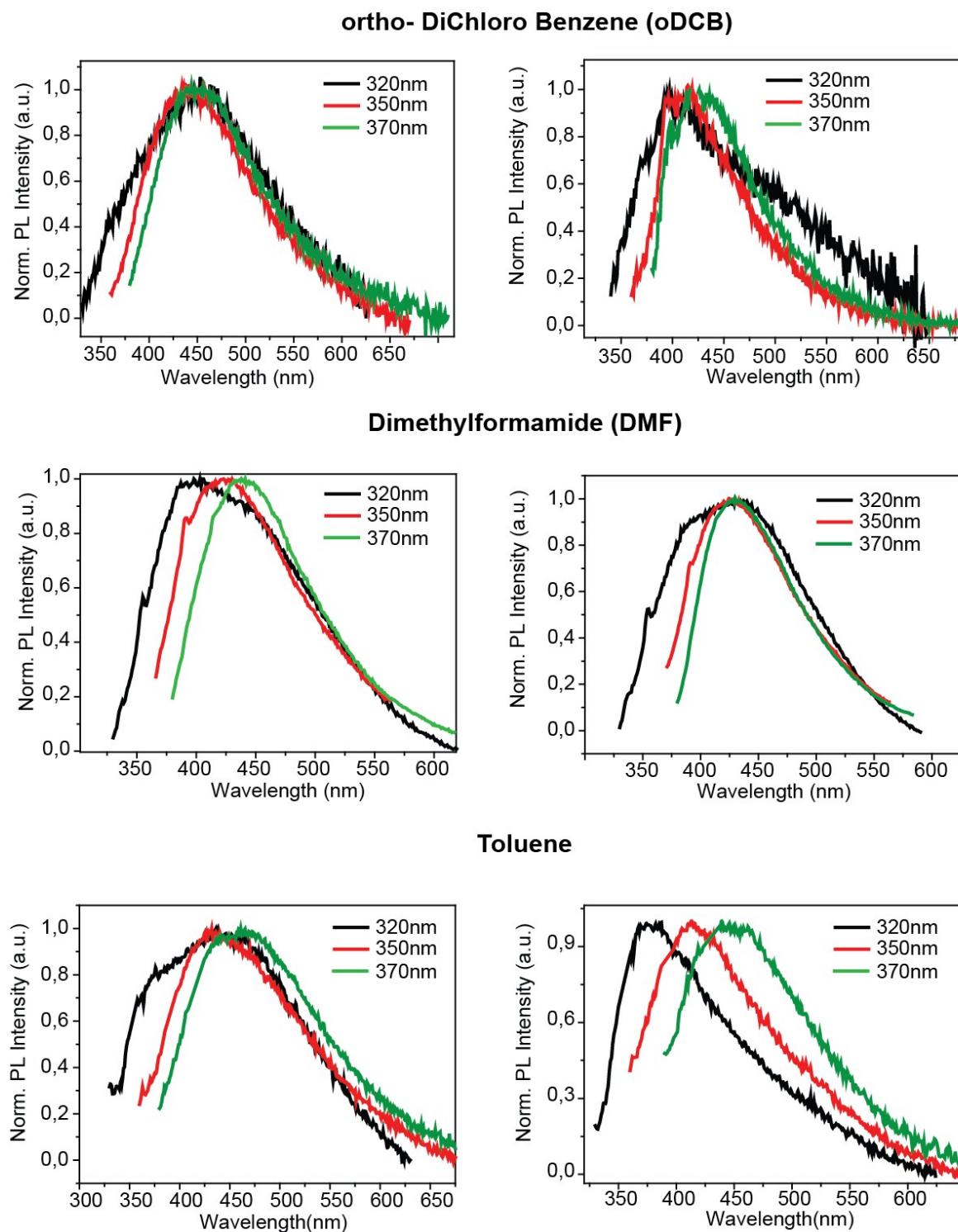


Figure S4. Fluorescence Spectra of CQD-1(left column) and CQD-2 (right column) recorded in different solvent at different excitation wavelength

	Pristine CQDs	CQD-1	CQD-2
PL Peak (nm)	412	424	430
PL FWHM (nm)	93	122	103
Exc. Peak (nm)	352	361	373
Exc. FWHM (nm)	88	79	66
PL Av. Lifetime (ns)	3.1	2.3	2.1

Table S5. Spectroscopic characterization result summary