Electronic Supplementary Material (ESI) for Journal of Materials Chemistry

Supporting information

Facile Synthesis of Water-Soluble, Highly Fluorescent Graphene Quantum Dots as a Robust Biological Label for Stem Cells

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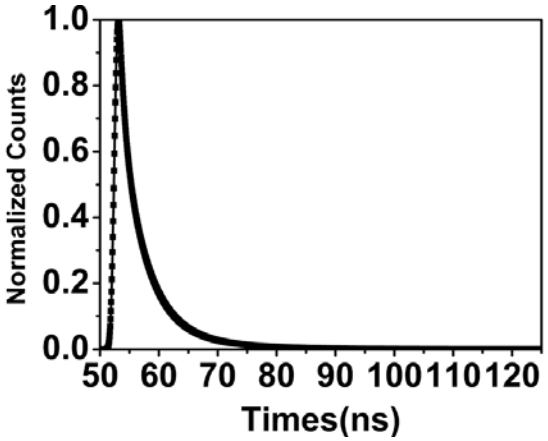

Figure S1 Time-resolved fluorescence decay profile of GQDs aqueous solution.

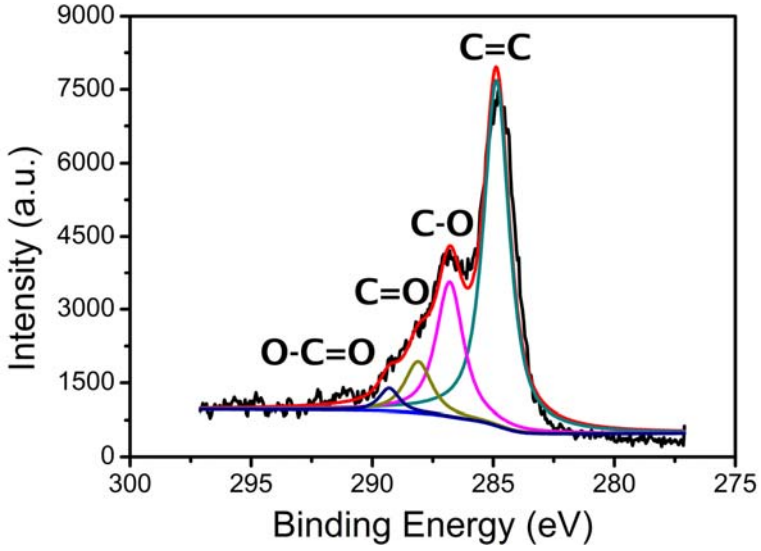

Figure S2 C 1s XPS spectrum of EOGs.

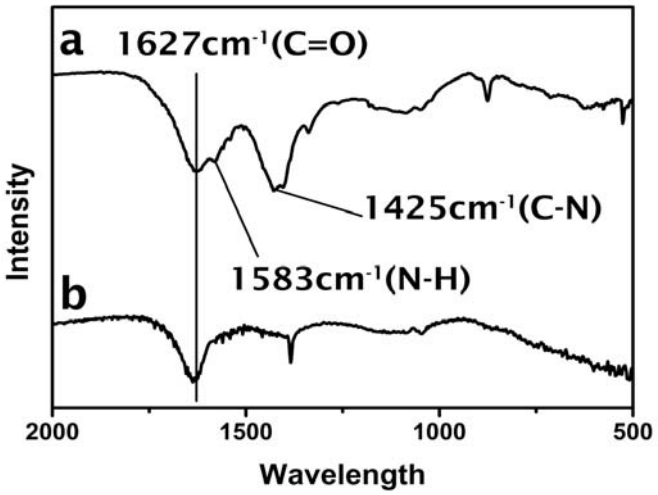

Figure S3 FTIR spectra of GQDs (a) and EOGs (b).

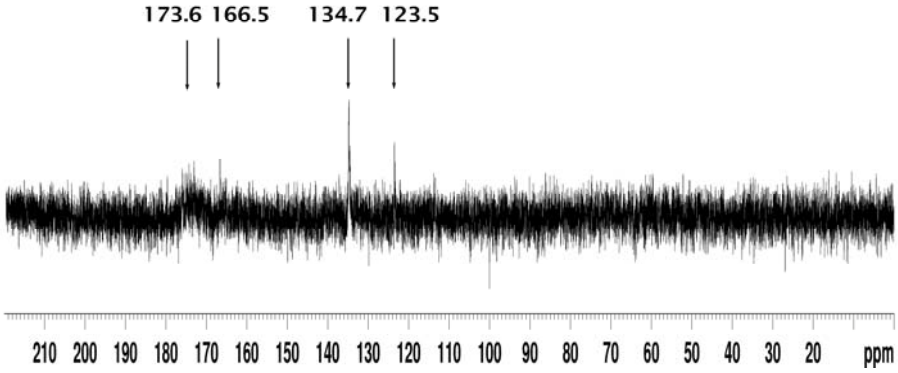

Figure S4 ^{13}C NMR spectrum of GQDs in D_2O.

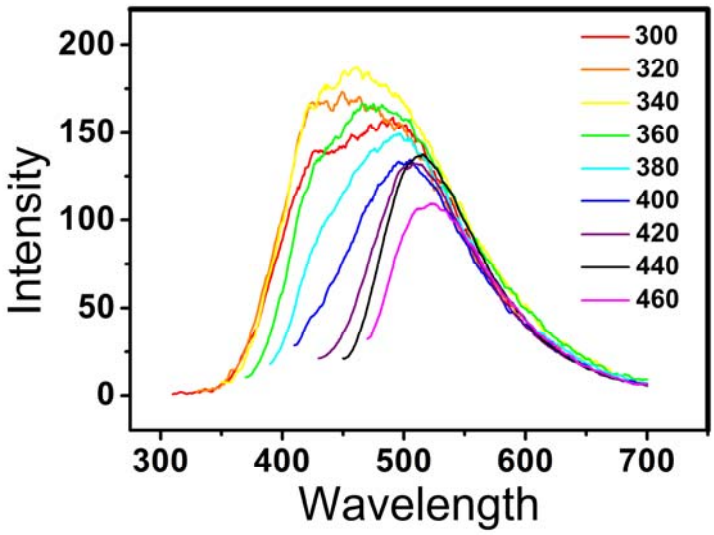

Figure S5 PL spectra of the electrochemically generated aqueous solution reduced by sodium borohydride at different excitation wavelengths.

Table S1 Optimized Cartesian coordinates(Å) of the luminescent unit for ground state and first excited state.

Species	Cartesian coordinates			Species	Cartesian coordinates		
Ground state	C	1.23062	-0.34304 -0.41925	First excited state	C	1.22198	-0.34883 -0.42977
	C	1.07760	1.05461 -0.45959		C	1.09181	1.06608 -0.48424
	C	2.19578	1.97467 -0.52304		C	2.22606	1.96068 -0.53469
	C	-0.24044	1.60060 -0.53659		C	-0.21835	1.60083 -0.54141
	C	1.98745	3.33707 -0.66116		C	2.00666	3.36865 -0.71575
	C	0.66359	3.91169 -0.51798		C	0.67367	3.91333 -0.55273
	C	-0.44730	3.01461 -0.53227		C	-0.42886	3.02748 -0.54408
	C	-1.78002	3.52766 -0.51306		C	-1.76715	3.53530 -0.52050
	C	-1.97373	4.91105 -0.42616		C	-1.99626	4.93529 -0.46670
	C	-0.89311	5.76885 -0.31562		C	-0.92987	5.79300 -0.36779
	C	0.41825	5.29156 -0.34312		C	0.39052	5.30861 -0.36959
	C	-1.36731	0.72365 -0.56794		C	-1.34652	0.72271 -0.54310
	C	-2.68988	1.27760 -0.60319		C	-2.64937	1.26900 -0.56510
	C	-2.88733	2.61877 -0.56872		C	-2.85374	2.63996 -0.55482
	C	3.59391	1.48442 -0.33084		C	3.58235	1.46121 -0.39067
	O	3.89884	0.42421 0.19521		O	3.91654	0.35152 0.03918
	C	1.51174	6.24722 0.04935		C	1.44118	6.27620 0.10355
	O	2.24195	6.01233 1.00009		O	2.02965	6.04720 1.14686
	N	1.58739	7.44478 -0.62116		N	1.56790	7.46007 -0.57437
	H	2.43510	7.95315 -0.38523		H	2.41096	7.96304 -0.31137
	N	1.10851	7.52885 -1.94272		N	1.18170	7.47743 -1.92839
	H	0.87197	8.49059 -2.15214		H	1.00881	8.43209 -2.21601
	H	1.80522	7.17202 -2.59277		H	1.89709	7.02521 -2.49522
	C	-1.16060	-0.66204 -0.54065		C	-1.16440	-0.68001 -0.49951
	C	0.12314	-1.18301 -0.46843		C	0.11594	-1.19738 -0.43959
	O	2.92826	5.18834 -1.86747		O	2.95477	5.31039 -1.74256
	C	3.09571	4.16353 -1.21450		C	3.08357	4.19549 -1.20443
	N	4.36580	3.66582 -1.07939		N	4.36474	3.67084 -1.13013
	H	5.01524	4.01924 -1.77234		H	4.95644	3.97716 -1.89406
	H	5.46745	2.20767 -0.18947		H	5.42375	2.24678 -0.14645
	N	4.60390	2.34709 -0.70036		N	4.61000	2.34218 -0.74289
	H	2.22039	-0.76324 -0.34265		H	2.21918	-0.76012 -0.37391
	H	0.27103	-2.25660 -0.44357		H	0.27180	-2.26915 -0.40126
	H	-3.53236	0.59542 -0.64053		H	-3.50009	0.59626 -0.57670
	H	-1.05800	6.83119 -0.18940		H	-1.08814	6.85816 -0.26077
	H	-2.98411	5.30539 -0.41304		H	-3.01443	5.30752 -0.46880
	H	-2.02021	-1.32347 -0.56556		H	-2.03341	-1.32847 -0.50664
	H	-3.89065	3.03080 -0.57463		H	-3.86265	3.03732 -0.56553

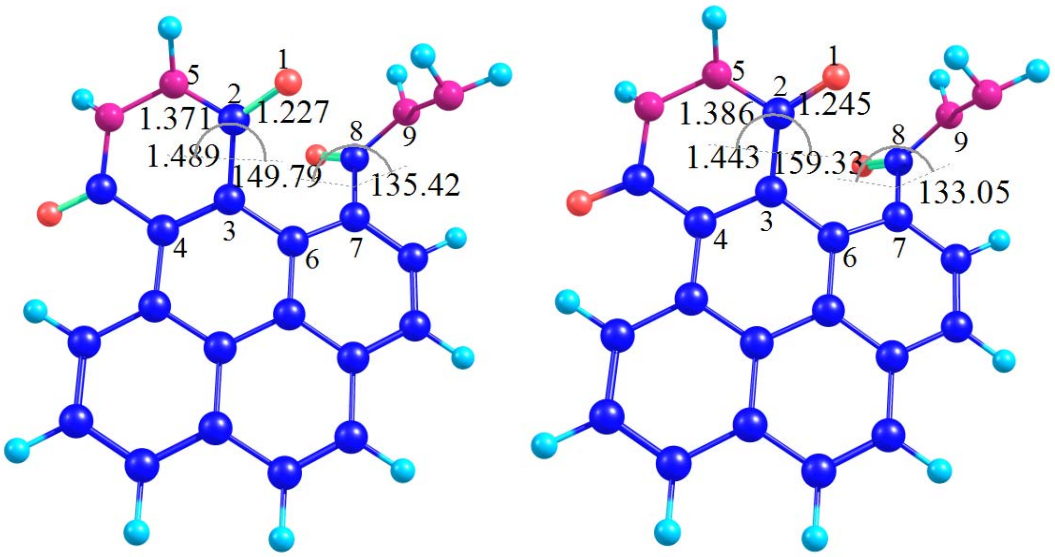

Figure S6 The Ground state (left) and the first excited state (right) of one luminescent unit obtained from theoretical calculation with density function theory (B3LYP/6-311++G(d,p)), in which the geometric parameters of the ground state have been optimized and verified at B3LYP/6-311++G(d,p) level. Based on the optimized geometric parameters, a time-dependent DFT, called TD-B3LYP/ 6-311++G(d,p), has been performed to get the absorption spectra. The absorption wavelength of 390 nm with oscillator strength of 0.1319 is very close to the expeimental one (360 nm). The geometric paprameters of the first excited state have also been optimized with TD-B3LYP/6-311++G(d,p), which indicates that the main differences between excited state and ground state are on the bond-lengths of O1-C2, C2-C3 and C2-N5. The calculated fluorescence wavelength is 532 nm, in good agreement with experimental value of 540 nm.

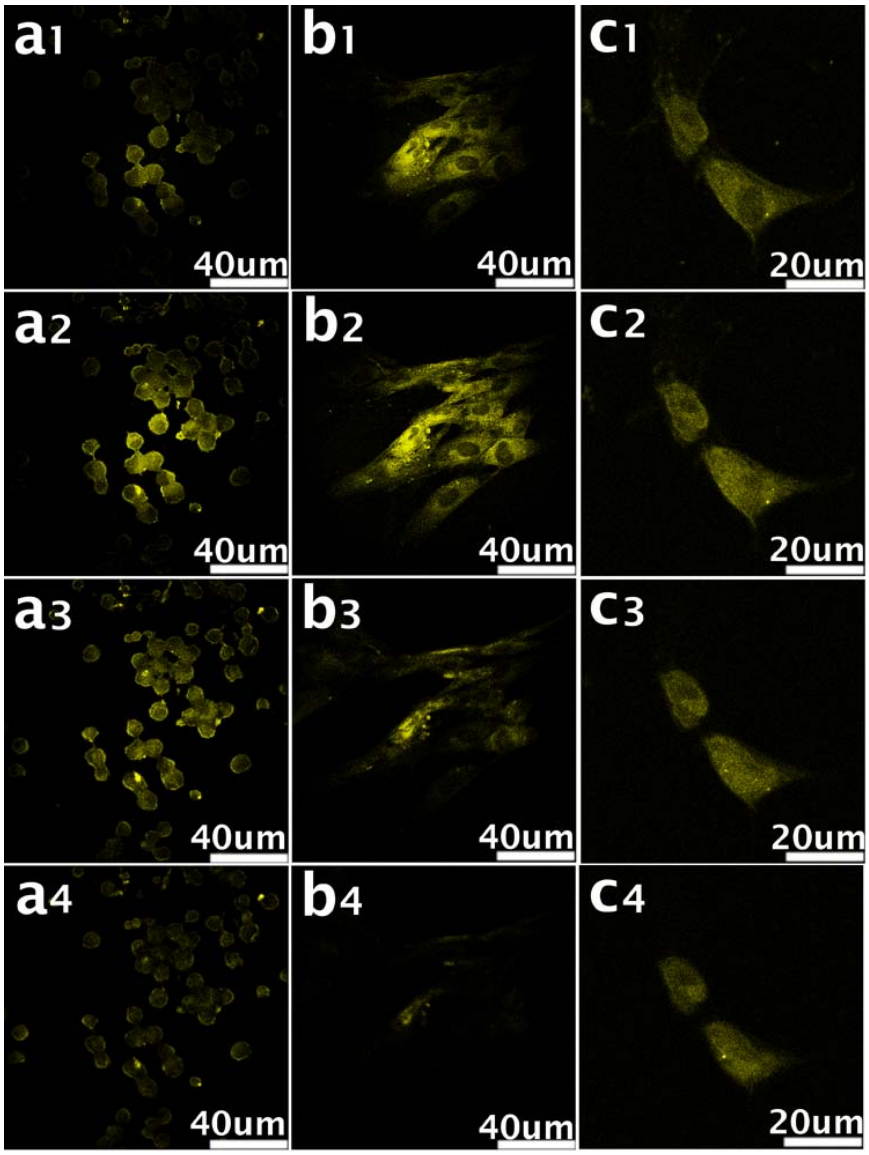

Figure S7 Confocal fluorescence microscopy section images of stem cells of NSCs (a1-a4), PPCs (b1-b4), and CPCs (c1-c4) with the fluorescent GQDs incorporated at excitation wavelength of 405 nm.

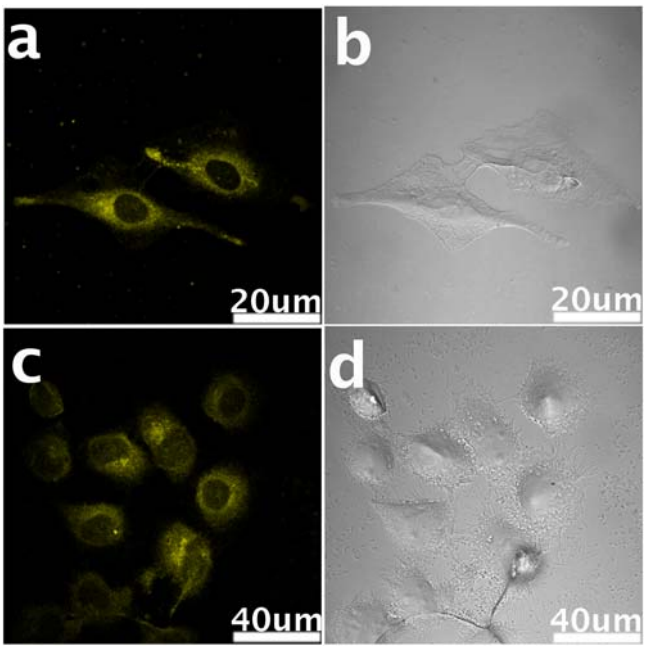

Figure S8 Confocal fluorescence microscopy images of A549 (a) and MCF-7 (c) with the fluorescent GQDs incorporated at excitation wavelength of 405 nm and the corresponding images under bright field (b, d).