Electronic Supporting Information

for

Tailoring Fluorescence Emissions, Quantum Yields, and White Light Emitting from Nitrogen-doped Graphene and Carbon Nitride Quantum Dots

Figure S1. The C 1s peak deconvoluted by a multiple Gaussian function: (a) NCD-1, (b) NCD-2, and (c) NCD-3.
Tauc plot: The absorption coefficient ($\alpha$) is related to photon energy ($h\nu$) by the known equation as [S1,S2]:

$$\alpha = \frac{\beta}{(h\nu - E_g)^n} \quad \text{or} \quad (\alpha h\nu)^{1/n} = \beta (h\nu - E_g)$$

where $\beta$ is a constant called the band tailing parameter, $E_g$ is the energy of the optical band gap and $n$ is the power factor of the transition mode, which is dependent upon the nature of the material, whether it is crystalline or amorphous. According to the Tauc’s relation, the plotting of $(\alpha h\nu)^{1/2}$ versus the photon energy ($h\nu$) gives a straight line in a certain region. The extrapolation of this straight line will intercept the ($h\nu$)-axis to give the value of the indirect optical energy gap ($E_g$).

References:


Figure S3. The Mott-Schottky plots of GQD electrodes: (a) NCD-1 and (b) NCD-3, in 1 M Na$_2$SO$_4$ solution.

**Mott-Schottky (M-S) plot:** The carrier density ($N_D$) of different GQD electrodes can be estimated by the following equation. 

$$N_D = \frac{2}{e\varepsilon_0\varepsilon_r}[d(E - E_{FL})/d(1/C_S^2)]$$

where $C_S$ is the space charge capacitance in the semiconductor, $E_{FL}$ is the potential corresponding to flat band potential, $e$ is the elemental charge constant, $\varepsilon_0$ is the permittivity of free space, $\varepsilon_r$ is the dielectric constant of the semiconductor. According to the M-S plot, the plotting of $(1/C_S)^2$ versus the potential ($E_{FL}$) gives a straight line in a certain region. The extrapolation of this straight line will intercept the ($E_{FL}$)-axis to give the value of the flat.

**References:**


Figure S4. Schematic band structures near surface based on the calculated electronic parameters for (a) NCD-1 and (b) NCD-3 electrodes, based on the flat band potential determined from the intercept of the M-S plots. Here CB and VB represent conduction band and valence band, respectively.

Width of space charge layer: An estimate for the width of the space charge layer, $W_{SC}$, can be determined from the following equation.

$$W_{SC} = \left[2\varepsilon_0\varepsilon_r (E - E_{FL}) / (e N_D)\right]^{1/2}$$

For the similar values of $E_{FL}$, a shorter space charge layer indicates a higher degree of band bending near the GQD surface, leading to more effective collection of charge carriers.

References:

Figure S5. PL emission spectra of different samples in NMP: (a) NCD-1, (b) NCD-2, and (c) NCD-3.
Figure S6. PL emission spectra of different samples in water under 450 nm.
Figure S7. Optical band gap structures on NCD-3 sample under different illuminations: (a) 320 nm UV and (b) 450 nm blue light.
Figure S8. (a) Luminous efficiency, (b) color rendering index, and (c) quantum yield of LED using NCD-1 quantum dots at various working currents. (d) Color coordinates of the white LEDs lamp under 450 nm excitation.