Electronic Supplementary Material (ESI) for Nanoscale.

Electronic Supporting Information

for

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

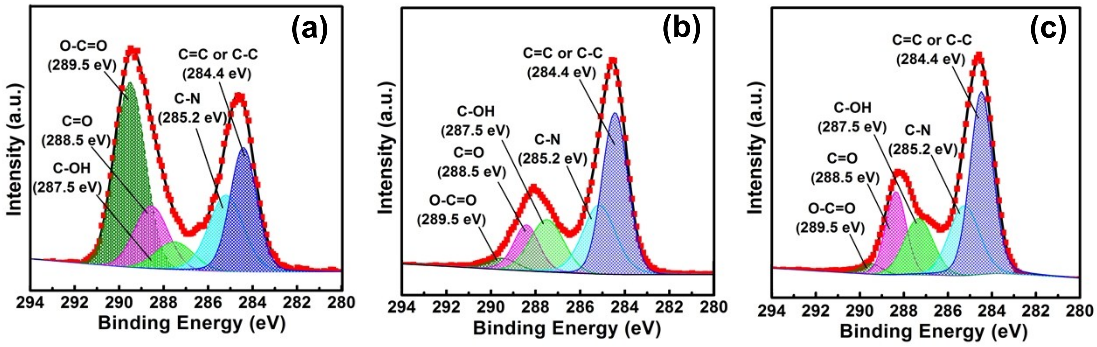

Figure S1. The C 1s peak deconvoluted by a multiple Gaussian function: (a) NCD-1, (b) NCD-2, and (c) NCD-3.

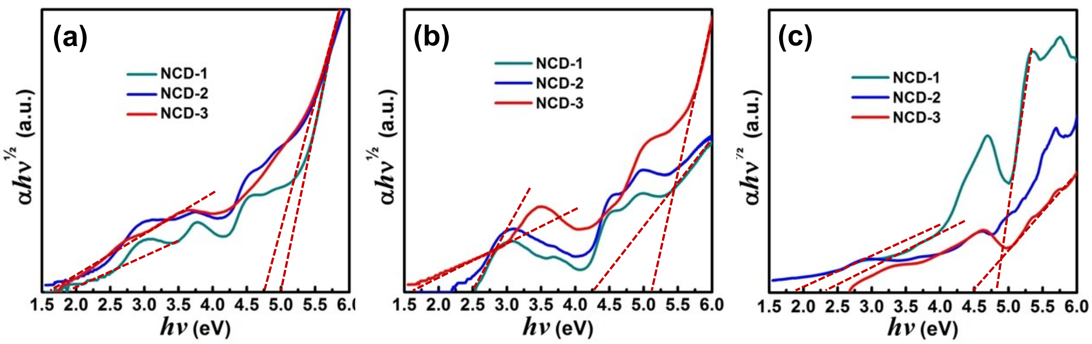

Figure S2. Tacu plots of quantum dots in different solutions: (a) distilled water, (b) ethanol, and (c) NMP.

Tauc plot: The absorption coefficient (α) is related to photon energy ($h\upsilon$) by the known equation as [S1,S2]:

$$\alpha = \beta / (h\upsilon)\,(h\upsilon - E_g)^n \qquad \text{or} \qquad (\alpha\, h\upsilon)^{1/n} = \beta\,(h\upsilon - E_g)$$

where β 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 $(\alpha\, h\upsilon)^{1/2}$ versus the photon energy ($h\upsilon$) gives a straight line in a certain region. The extrapolation of this straight line will intercept the ($h\upsilon$)-axis to give the value of the indirect optical energy gap (E_g).

References:

[S1] P. Kumar, B. Sain and S.L. Jain, *J Mater Chem A* 2014, **2**, 11246-11253.

[S2] M.A. Velasco-Soto, S.A. Pérez-García, J. Alvarez-Quintana, Y. Cao, L. Nyborg and L. Licea-Jiménez, *Carbon* 2015, **93**, 967-973.

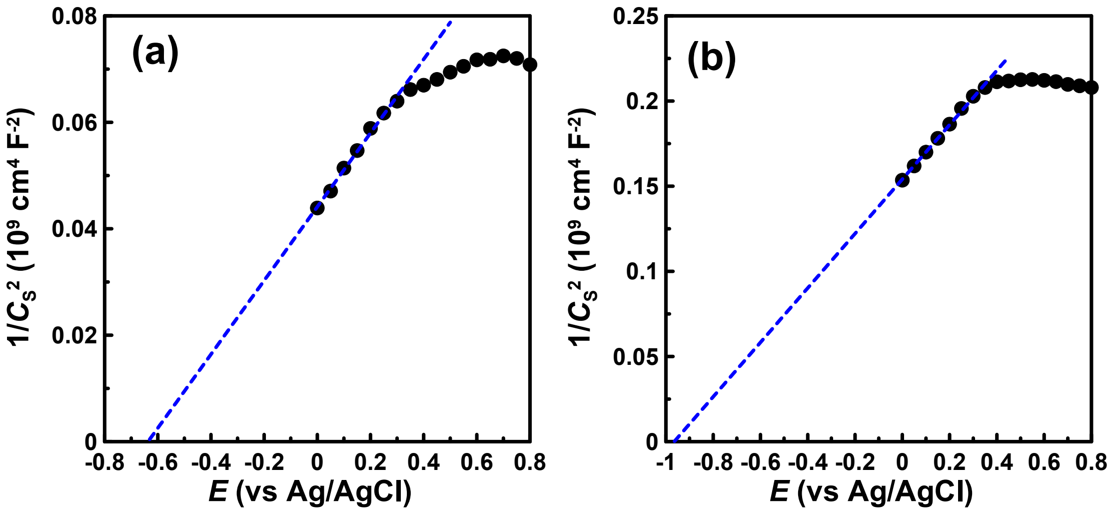

Figure S3. The Mott-Schottky plots of GQD electrodes: (a) NCD-1 and (b) NCD-3, in 1 M Na_2SO_4 solution.

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

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

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, ε_0 is the permittivity of free space, ε_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:

[S3] Z. Zeng, F.-X. Xiao, X. Gui, R. Wang, B. Liu and T.T.Y. Tan, *J. Mater. Chem. A*, 2016, **4**, 16383-16393.

[S4] X. Yang, A. Wolcott, G. Wang, A. Sobo, R. C. Fitzmorris, F. Qian, J. Z. Zhang and Y. Li, *Nano Lett.*, 2009, **9,** 2331-2336.

[S5] J. Qian, C. Shen, J. Yan, F. Xi, X. Dong and J. Liu, *J. Phys. Chem. C* 2018, **122**, 349-358.

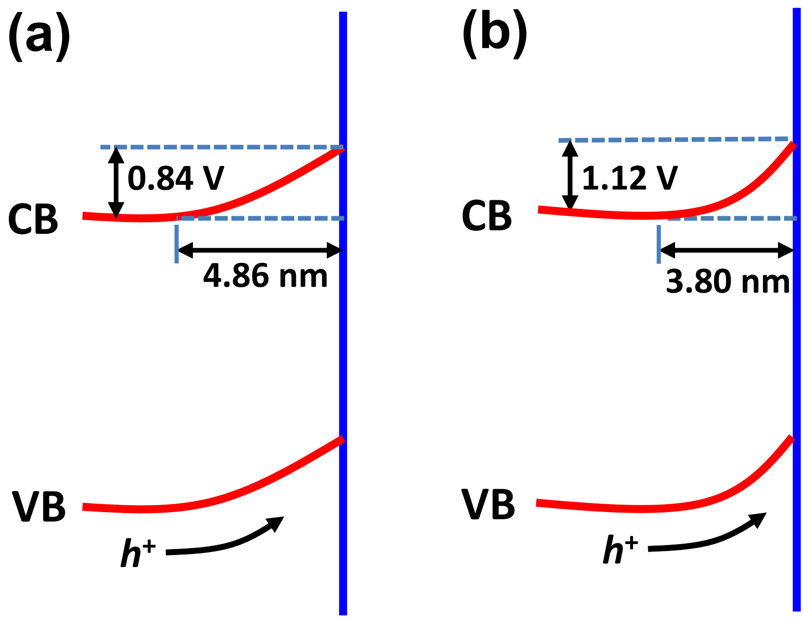

Figure S4. Schematic band structures near surface based on the calculated electronic parameters for (a) NCD-1 and (b) NCD-3 electrodes, based on the flat band potential determined from the intercept of the M-S plots. Here CB and VB represent conduction band and valence band, respectively.

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

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

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:

[S6] M. Zeng, X. Peng, J. Liao, G. Wang, Y. Li, J. Li, Y. Qin, J. Wilson, A. Song and S. Lin, *Phys. Chem. Chem. Phys.,* 2016, **18**, 17404-17413.

[S7] D.W. Kim, S.C. Riha, E.J. DeMarco, A.B. Martinson, O.K. Farha and J.T. Hupp, *ACS Nano*, 2014, **8**, 12199-12207.

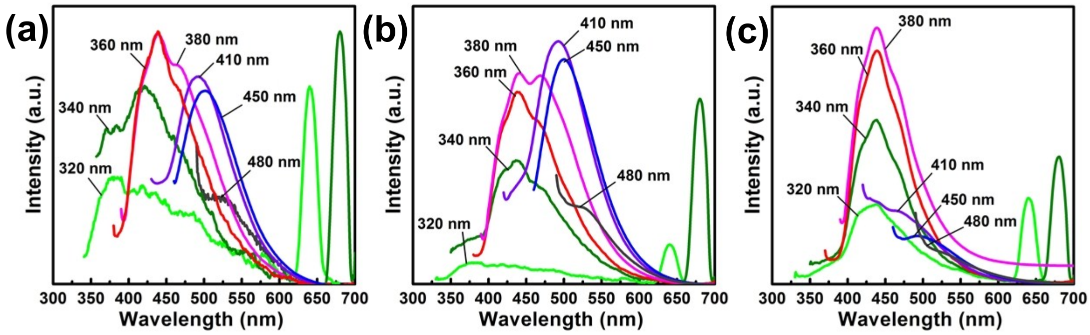

Figure S5. PL emission spectra of different samples in NMP: (a) NCD-1, (b) NCD-2, and (c) NCD-3.

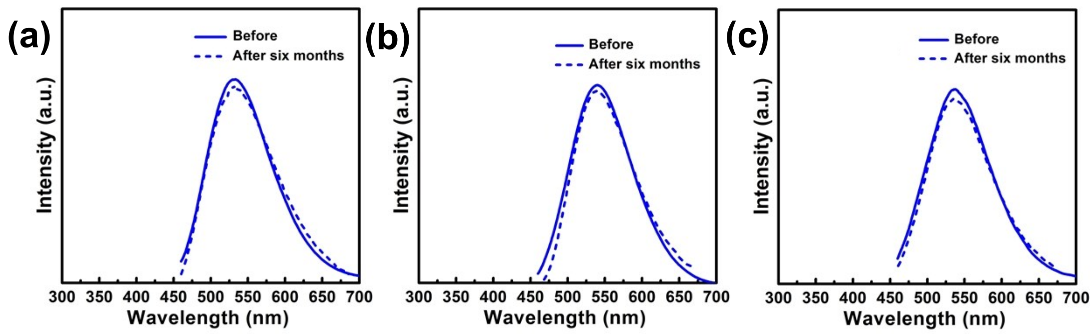

Figure S6. PL emission spectra of different samples in water under 450 nm.

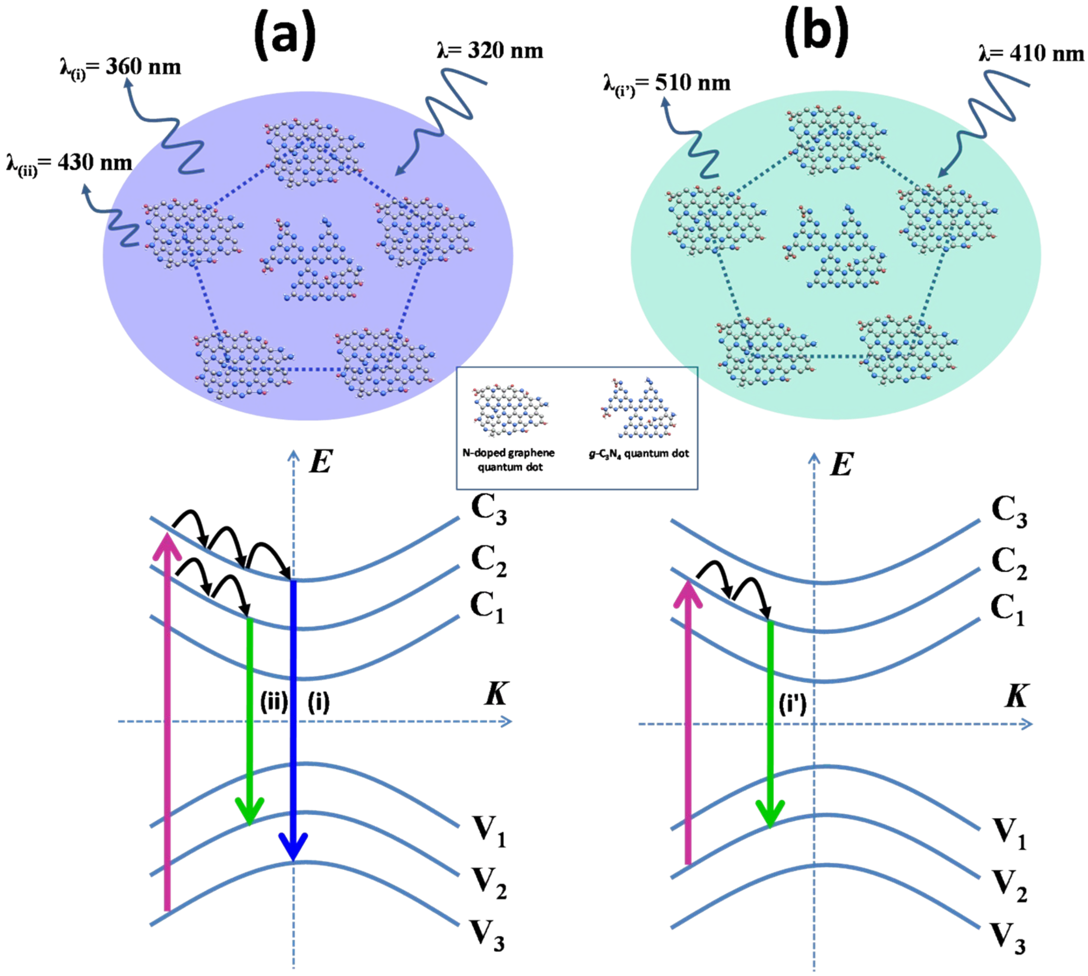

Figure S7. Optical band gap structures on NCD-3 sample under different illuminations: (a) 320 nm UV and (b) 450 nm blue light.

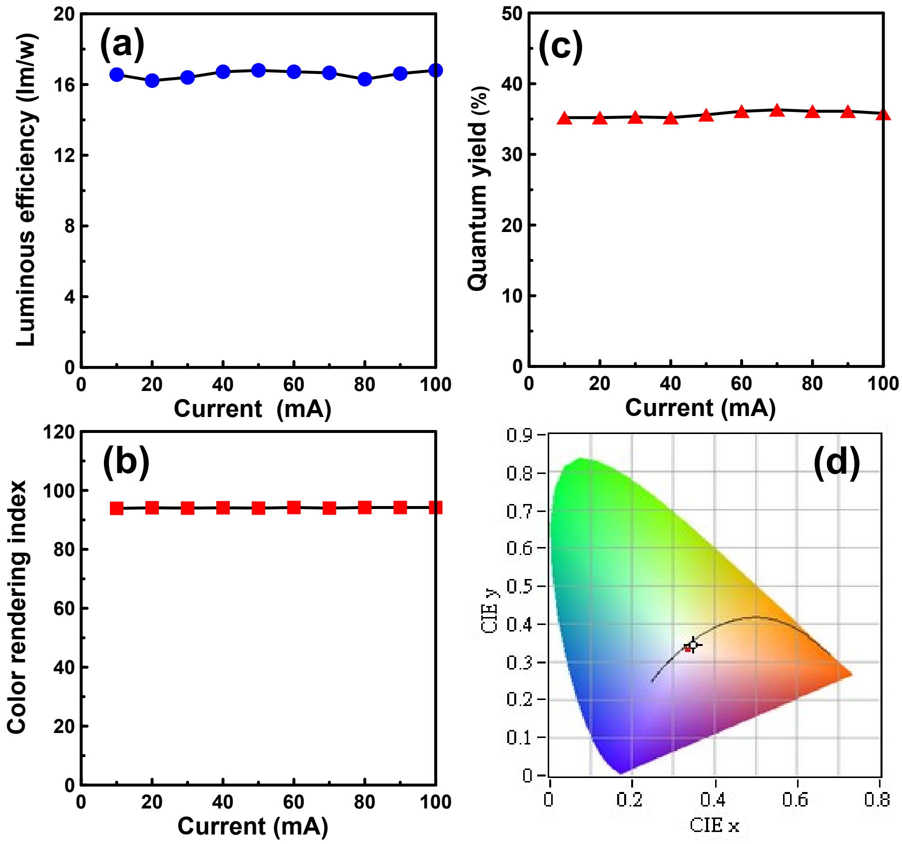

Figure S8. (a) Luminous efficiency, (b) color rendering index, and (c) quantum yield of LED using NCD-1 quantum dots at various working currents. (d) Color coordinates of the white LEDs lamp under 450 nm excitation.