Supplementary Information

Insight into the Multiple Quasi-Molecular States in Ethylenediamine Reduced Graphene Nanodots

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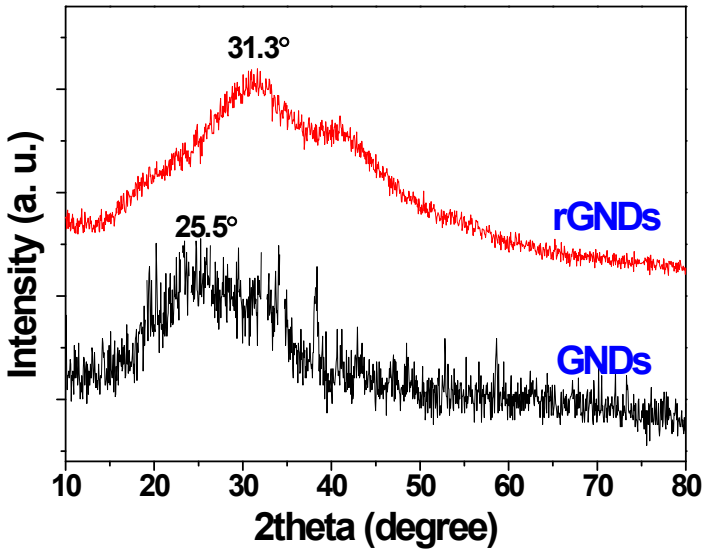

Figure S1 XRD pattern of GNDs and rGNDs.

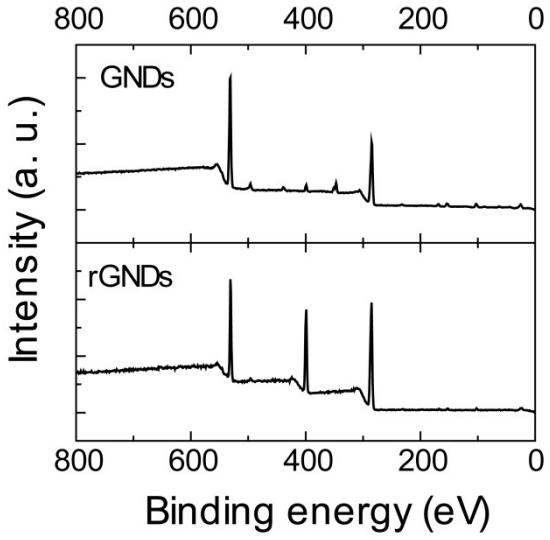

Figure S2 XPS full scan survey of GNDs and rGNDs.

Table S1 XPS C1s analysis results of the GNDs and rGNDs.

Sample	C1s fitting binding energy (eV) (relative atomic percentage (%))			
	C=C	C-C/C=N	C-O	C=O/C-N
GNDs	284.2 (43.2%)	285.5 (25.9%)	286.6 (12.5%)	287.7 (18.3%)
rGNDs	283.9 (28.5%)	285.0 (39.2%)	286.5 (21.8%)	287.5 (10.8%)

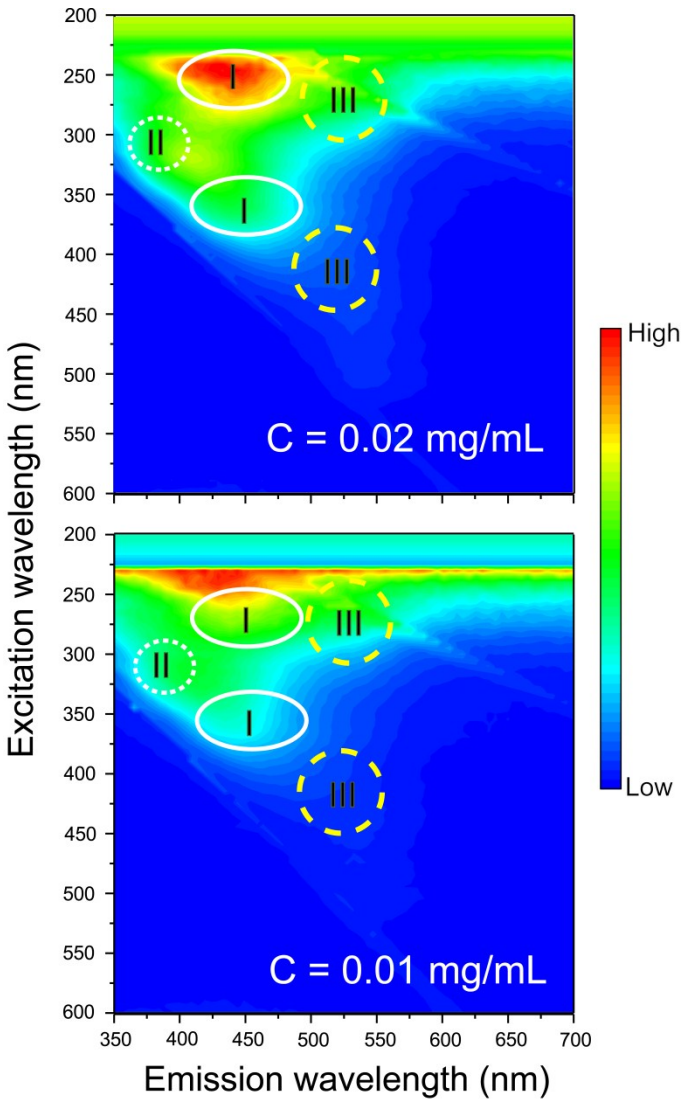

Figure S3 PLE contour maps of rGNDs in diluted solutions. (Upper) C = 0.02 mg/mL; (Lower) C= 0.01 mg/mL.

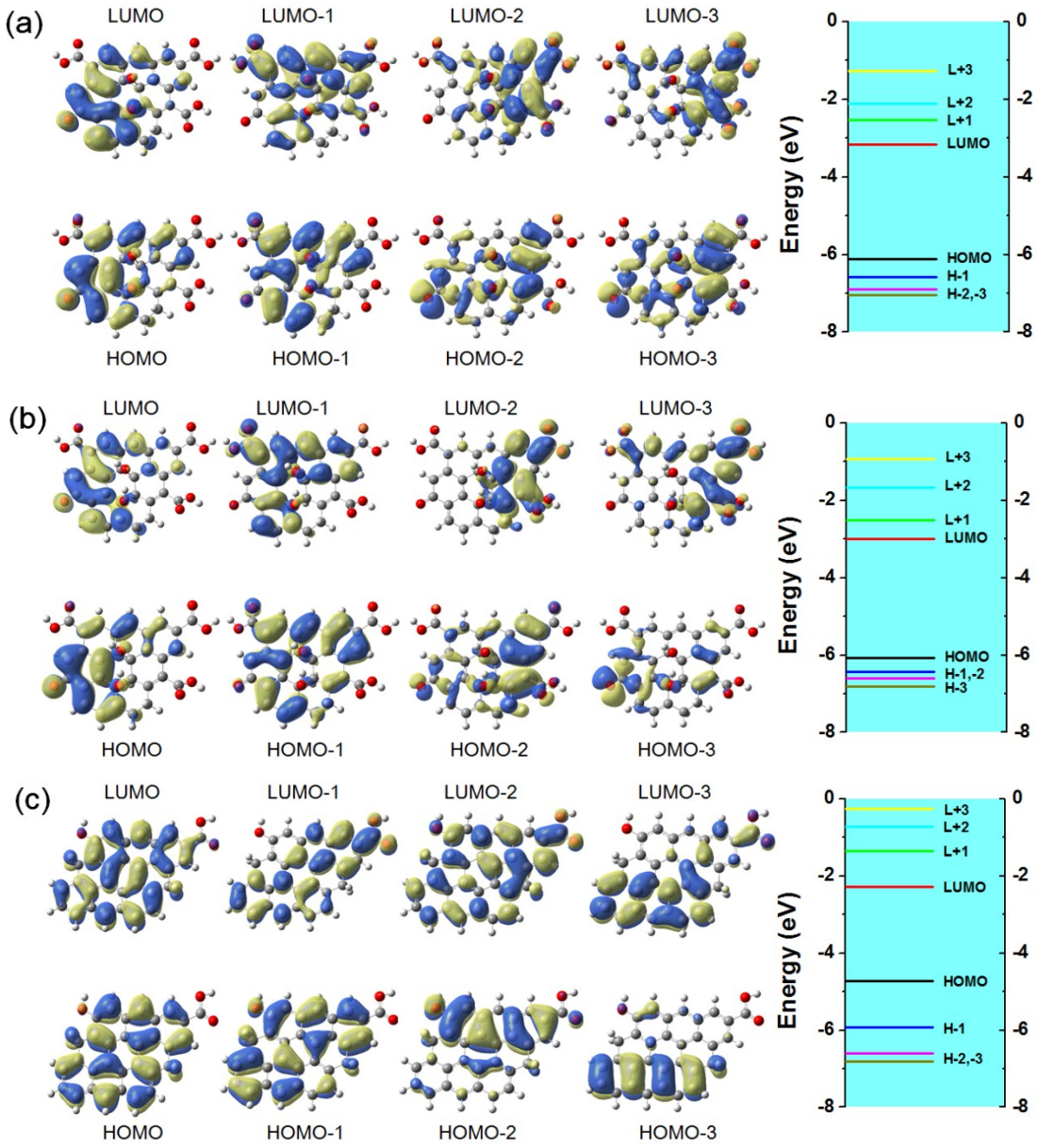

Figure S4 The wave functions of frontier orbitals and energy level diagrams of C=O-related (a), graphenol-related (b) and larger π-conjugated (c) quasi-molecular structures presented in Figure 7.

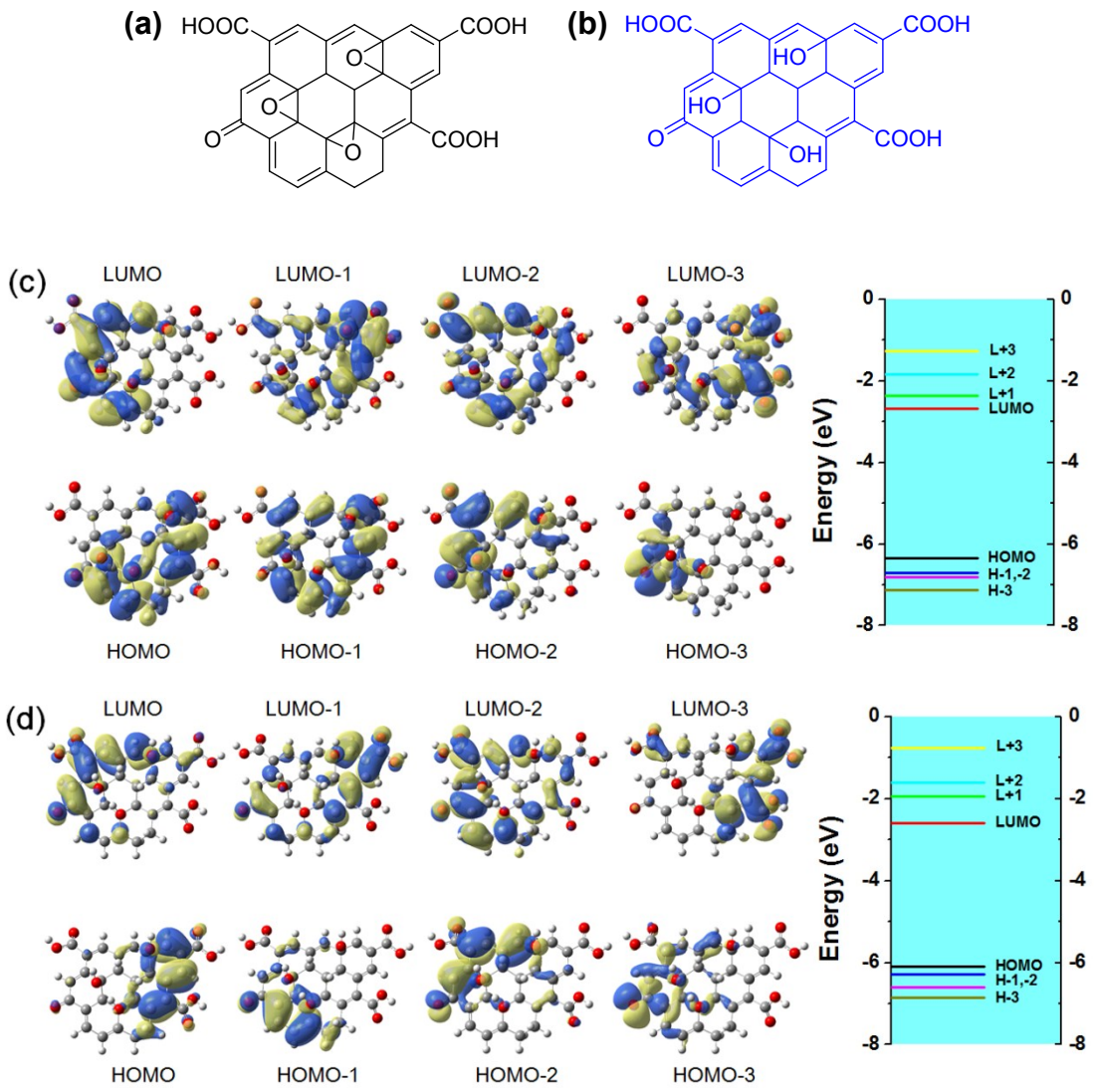

Figure S5 The proposed C=O-related (a) and graphenol (b) quasi-molecules bearing three epoxide and hydroxyl groups. The corresponding wave functions of frontier orbitals and energy level diagrams are shown in (c) and (d), respectively.

Quantum Yield Measurements.

The quantum yield was determined by the slope method.

$$\emptyset_x = \emptyset_x\left(K_x/K_s\right)\left(\eta_x/\eta_s\right)^2$$

Where Φ is the relative quantum yield, K is the slope determined by the curves between the measured integrated emission intensity and the optical density, η is the refractive index of the solvent. For the aqueous solutions, η_x/η_s=1. The subscript "*s*" refers to quinine sulfate dissolved in 0.5 M H_2SO_4 with absolute quantum yield (0.54), and "*x*" for the sample. To minimize re-absorption effects, absorption in the 1.0 cm fluorescence cuvette was kept below 0.10 at the excitation wavelength (360 nm).

Table S2 PLQY of rGNDs as a function of hydrothermal reaction temperature and duration time. C(EDA) = 1 M.

Sample	Temperature (°C)	Duration (h)	QY(%)	Peak position (nm)	FHWM (nm)
1	60	5	2.2	422	79
2	100	5	3.0	446	85
3	170	5	11.9	442	84
4	200	5	7.5	443	86
5	170	2	4.7	444	86
6	170	8	7.5	443	86

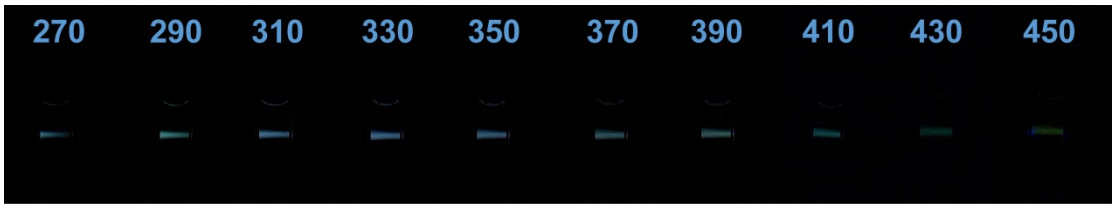

Figure S6 Photograph of oxidized GNDs solution (0.1 mg/mL) illuminated with Xe lamp. Filters are used to eliminate the scattering light.

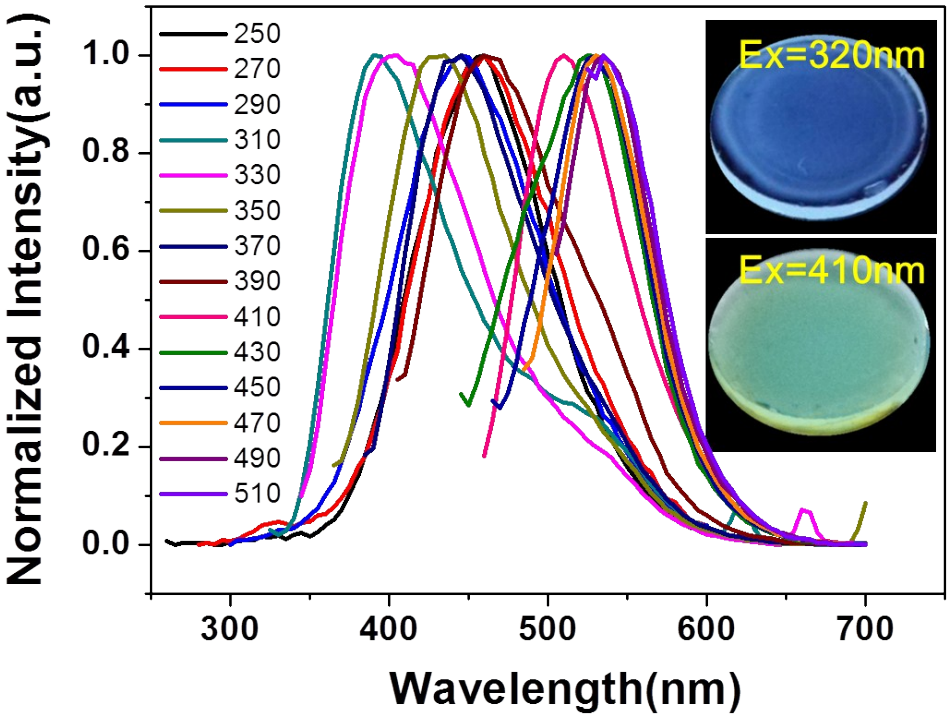

Figure S7 Normalzied PL spectra of rGNDs/PVA composite film as a function of excitation wavelength. Inset: Photograph of rGNDs/PVA composite film illuminated with 320 nm and 410 nm light.

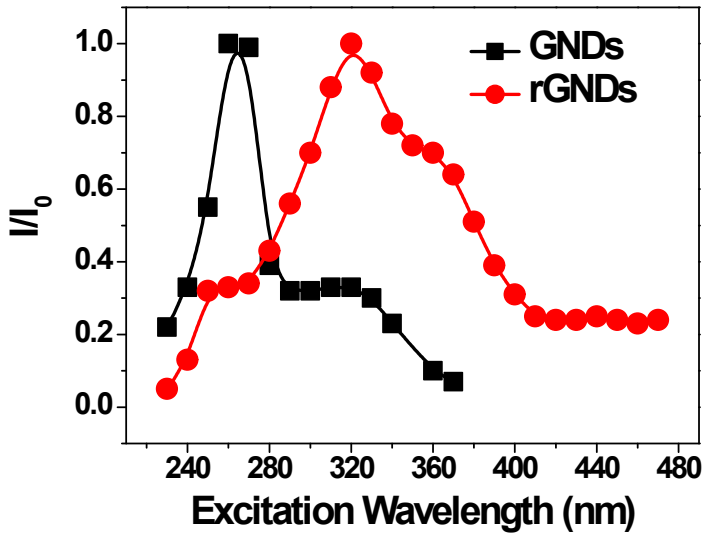

Figure S8 PL intensity ratio between the shifted peaks and their dominant emission (I/I_0) as a function of excitation wavelength.