Rhodamine B degradation by nanosized zeolitic imidazolate framework-8 (ZIF-8)

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Supporting Information

Functional Groups	IR absorption cm ⁻¹
C=N stretch	1574
-CH ₃ bend	1473, 1418
C-N symmetric stretching	1091
C-N in-plane stretching	1180, 1147
C-H bending in imidazole ring	1311, 954, 759, 693

Table S1. IR absorption frequencies of ZIF-8

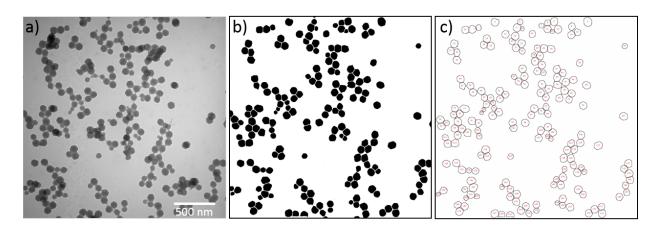


Figure S1. The ZIF-8 nanoparticle size distribution analysis was conducted based on the TEM image of over 180 nanoparticles (a), the image was then cropped (b) and analyzed (c) using ImageJ software.

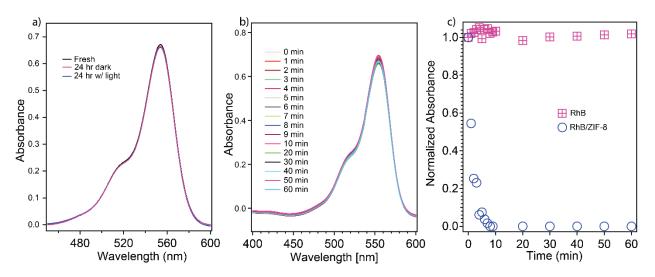


Figure S2. a) UV absorbance spectra of freshly prepared RhB in water (5 ppm) and spectra of the same concentration RhB solution under dark and ambient light after 24 hr and b) time-dependent absorbance of RhB under UV irradiation within 1 hr; and c) comparison of normalized absorbance of RhB in the presence and absence of ZIF-8 nanoparticles under UV condition with 1 hr.

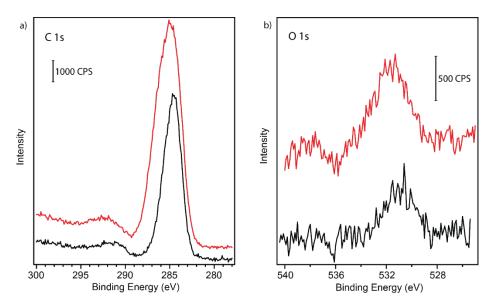


Figure S3. High resolution of C 1s and O 1s XPS spectra of ZIF-8 before (black) and after (red) RhB adsorption.

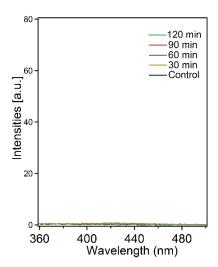


Figure S4. PL spectra of 2 mM of terephthalic acid in 0.5 mM NaOH solution under UV radiation for different period of time. The intensity scale is as same as the one shown in Figure 8a for comparison.

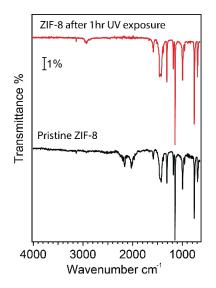


Figure S5. ATR-IR spectra of ZIF-8 before and after exposure to UV irradiation for 60 min. No chemical change was observed indicating the chemical stability of ZIF-8 under UV and its regeneration potential. The peaks in the range of 2200 to 1900 cm⁻¹ are corresponding to atmosphere CO_2 .

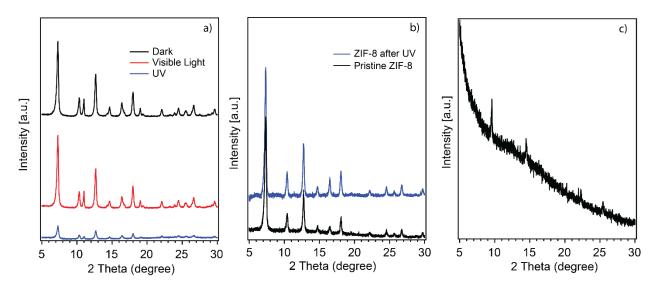


Figure S6. PXRD patterns of a) nanosized ZIF-8 after adsorbing rhodamine B in dark, visible light, and UV conditions, b) nanosized ZIF-8 before and after being immersed in water for 60 min under UV irradiation; and c) pure rhodamine B powder.

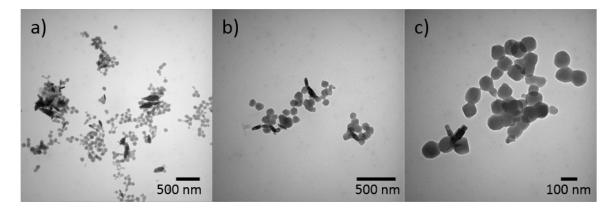


Figure S7. TEM images of ZIF-8 after adsorbing RhB (5 ppm) in water for 1 hour under visible light condition. a) – c) represent the magnifications of 30K, 50K, and 100K, respectively.

T-plot analysis

Based on our N₂ gas adsorption isotherm data, we applied the t-Plot method to assess the external surface areas of ZIF-8 nanocrystals before and after rhodamine B adsorption in visible light condition. We found that the calculated external surface area of ZIF-8 nanocrystals increased from 113. 25 m²/g to 151.09 m²/g after adsorbing rhodamine B, which again confirms rhodamine B adsorbed on the external surface of ZIF-8 nanocrystals.

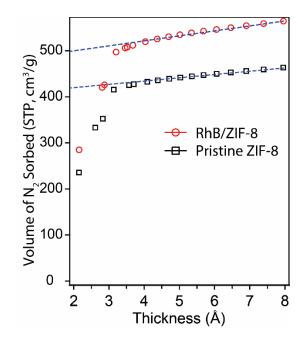


Figure S8. t-plots of ZIF-8 nanocrystals before and after rhodamine B adsorption under visible light for 1 hr.

The statistical thickness t (Å) was determined based on the Harkins-Jura Equation [Harkins et al., J. Chem. Phys. 1943, 11, 431]:

$$t = \sqrt{\frac{13.99}{0.034 - \log P/P_0}}$$

where P/P_0 is the relative pressure values obtained during the N₂ adsorption isotherm measurement. The external surface area (m²/g) was calculated using the built-in program in the Micromeritics software by applying this equation:

$$S_{ext} = \frac{\left(s \ cm^{3}/g \cdot \text{\AA STP}\right) * \left(10^{10} \ \text{\AA}/m\right) * (D \ cm^{3} \ liquid/cm^{3} \ STP)}{F * (10^{6} \ cm^{3}/m^{3})}$$

where s is the slope of the linear region of a V_{ads} -t plot; V_{ads} is the N₂ adsorbed amount at each relative pressure condition measured in the adsorption isotherm at 77K; D is the density conversion factor (0.001547 in the case of N₂ at 77K and 1 atm, calculated as shown below); F is the surface area conversion factor (0.975 as the instrument was calibrated using 1000 Å pore size silica).

$$D = \frac{\rho_{gas}}{\rho_{liquid}} = \frac{V_{liquid}}{V_{gas}} = \frac{0.03468 \, L/mol}{22.414 \, L/mol} = 0.001547$$

where ρ_{gas} and ρ_{liquid} are the density of N₂ at gas and liquid phases at 77K and 1 atm. The ratio of the density can be converted to the reciprocal of its volume at the same condition. The molar volume of N2 in gas phase is considered as the molar volume of an ideal gas; while the molar volume of N₂ in liquid phase is based on the isothermal properties for N₂ on NIST (<u>http://webbook.nist.gov/chemistry/fluid/</u>) by setting temperature to 77K and pressure at 1 atm.

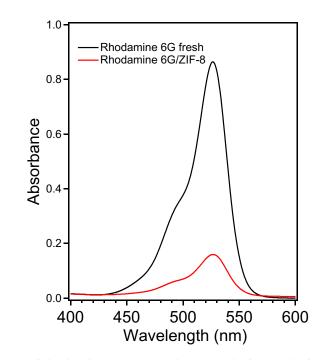


Figure S9. UV absorbance of rhodamine 6G (5 ppm in water) before and after mixing with nanosized ZIF-8 for 1 hr under ambient light.