

Supporting Information for:

Agar Aerogel Containing Small-Sized Zeolitic Imidazolate Framework Loaded Carbon Nitride: A Solar-Triggered Regenerable Decontaminant for Convenient and Enhanced Water Purification

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Number of pages: 25

Number of figures: 19

Number of Tables: 04

Supporting Figures:

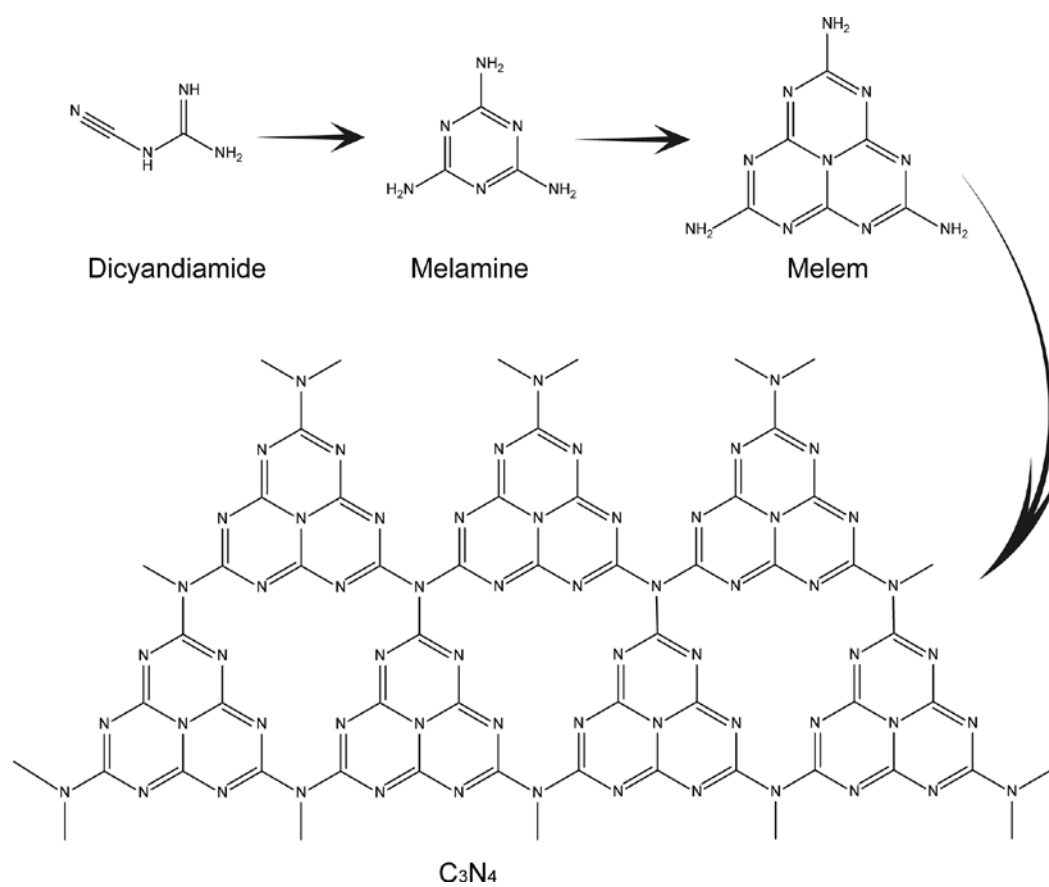


Figure S1. Reaction path for the formation of C₃N₄ from dicyandiamide.

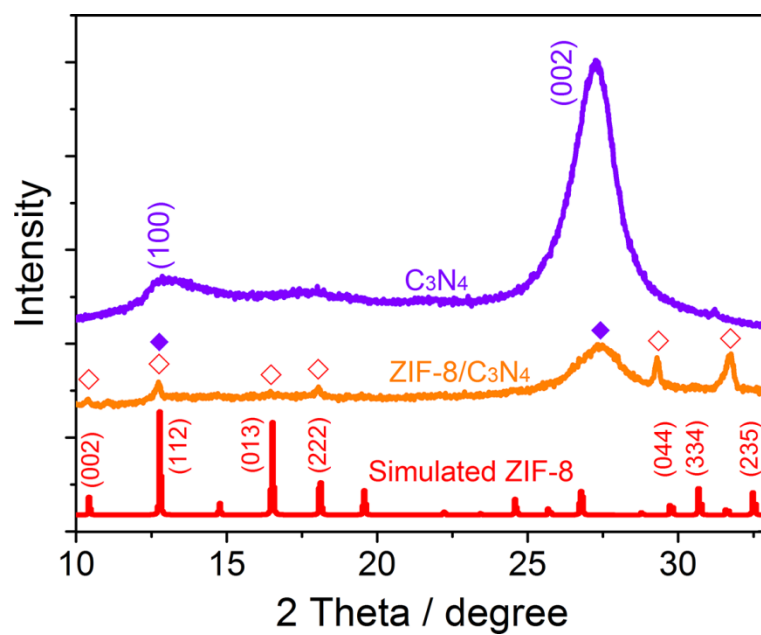


Figure S2. XRD patterns of C_3N_4 , simulated ZIF-8 and the as-obtained ZIF-8/ C_3N_4 .

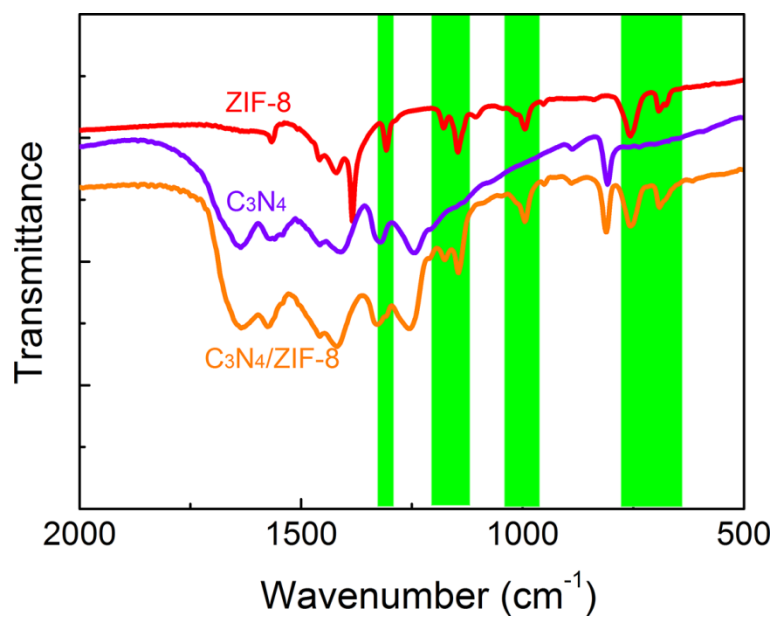


Figure S3. FT-IR spectra of C₃N₄, ZIF-8 and the as-obtained ZIF-8/C₃N₄.

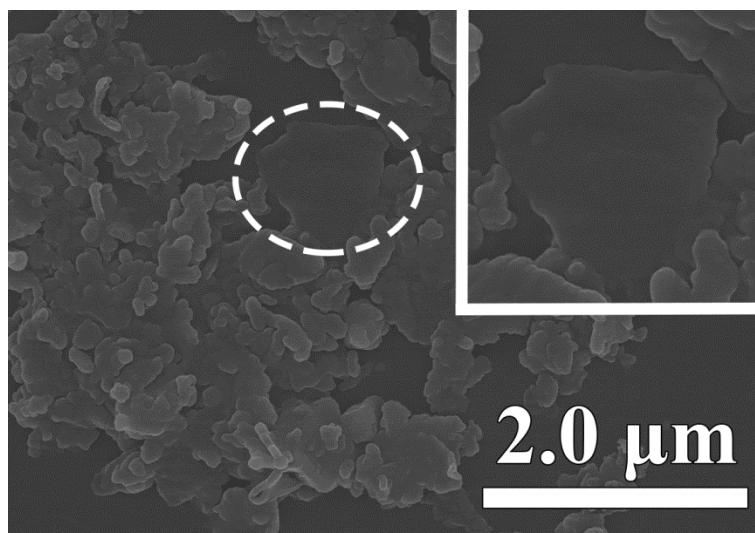


Figure S4. SEM image of C₃N₄ nanosheets.

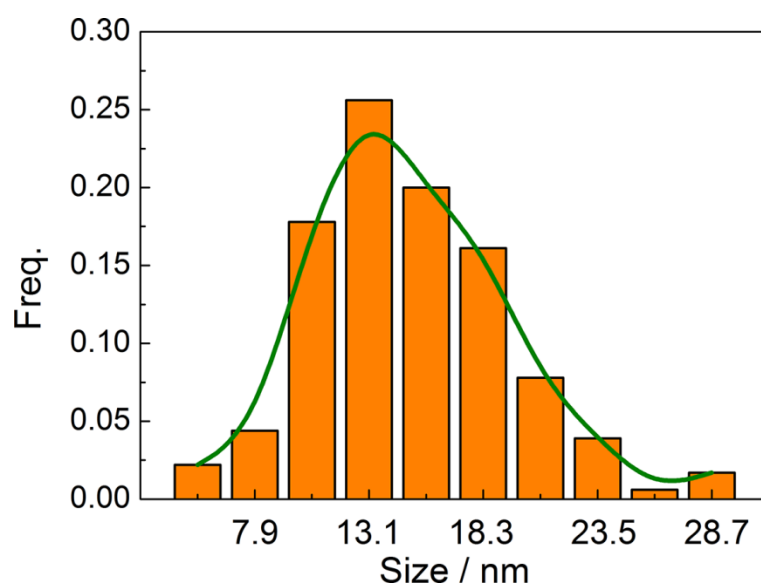


Figure S5. The size distribution of ZIF-8 nanoparticles on C₃N₄, over 150 particles were counted, indicating ZIF-8 nanoparticles possess average particle size, about 14.95 nm.

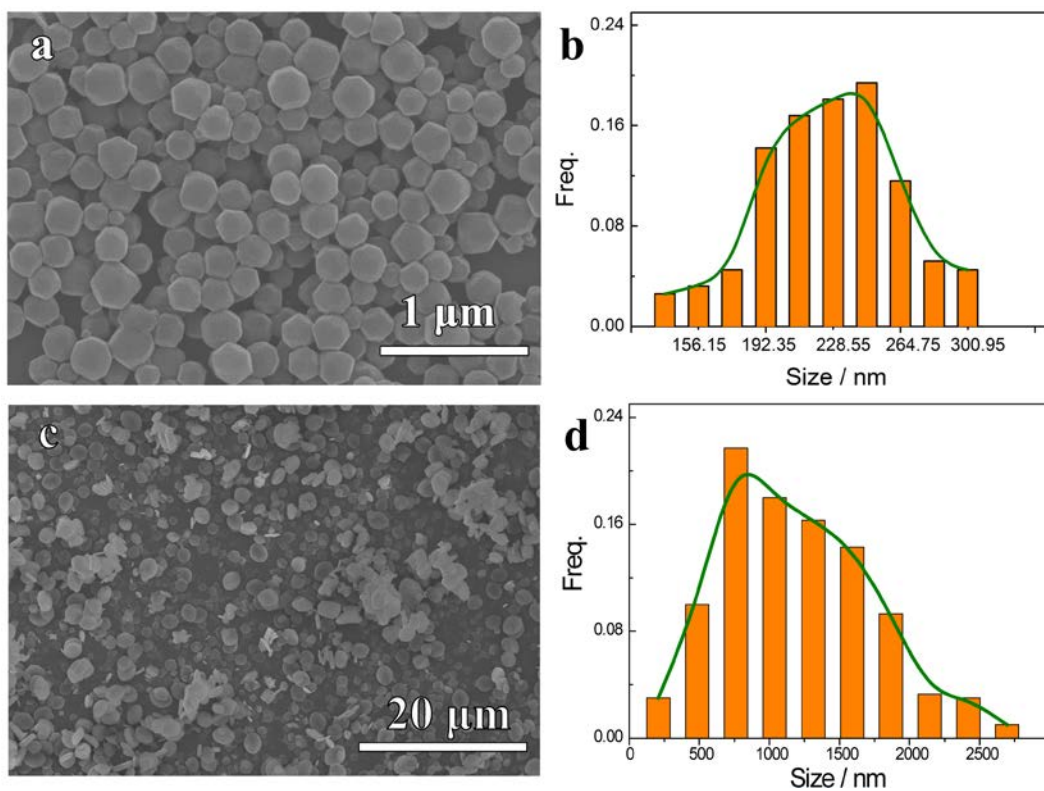


Figure S6. SEM image and size distribution of big-sized bulk ZIF-8, over 150 particles were counted. a, b) ZIF-8 nanoparticles, synthesized by a reported method,¹ possess average particle size of 227.61 nm. c,d) ZIF-8 nanoparticles with size of 1193.20 nm were synthesized by the same condition for ZIF-8/C₃N₄ but without the presence of C₃N₄.

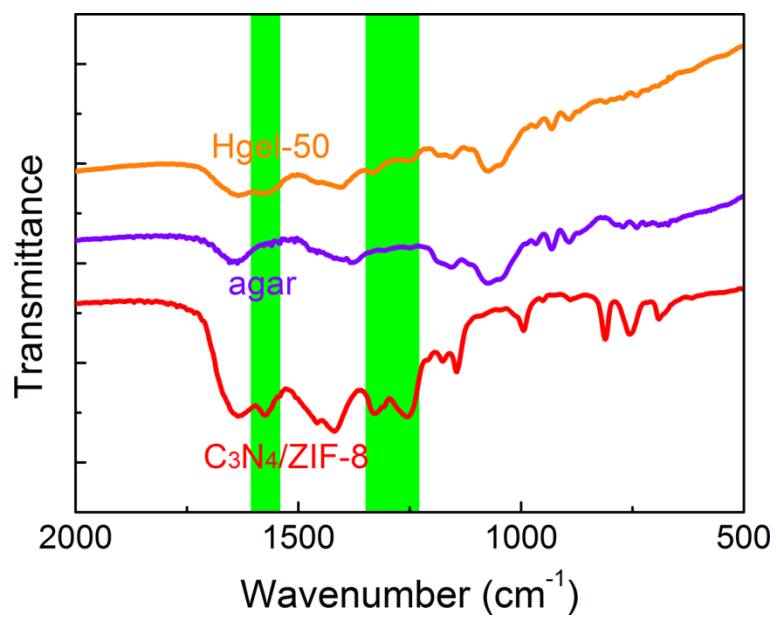


Figure S7. FT-IR spectra of agar, ZIF-8, C₃N₄ and Hgel-50.

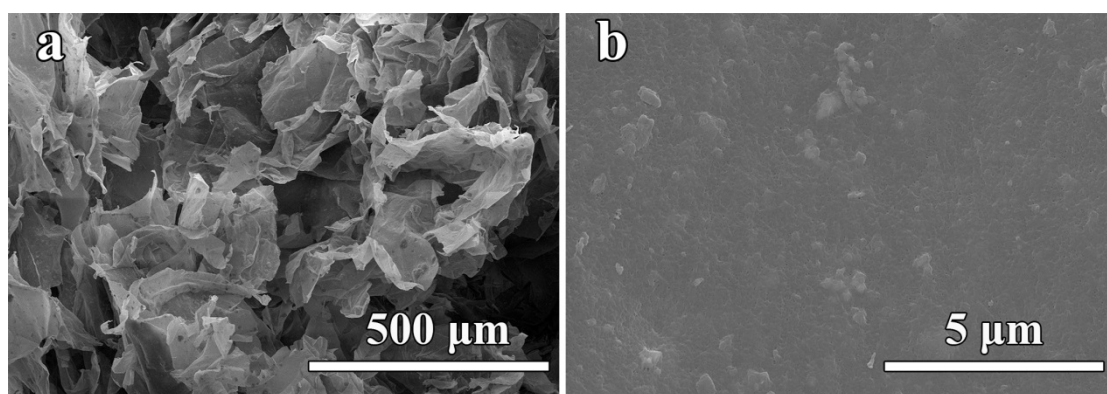


Figure S8. SEM of the hybrid aerogel containing 11.1% ZIF-8/C₃N₄.

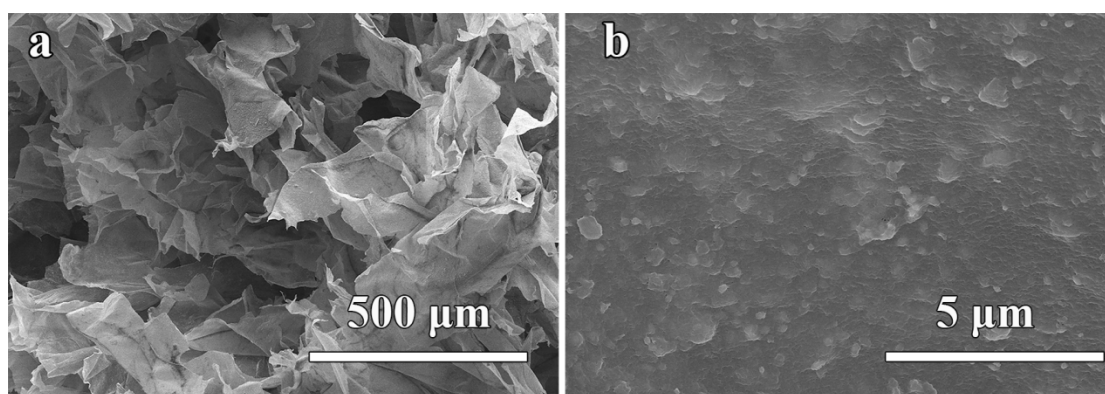


Figure S9. SEM of the hybrid aerogel containing 33.3% ZIF-8/C₃N₄.

Table S1. Adsorption capacities of various adsorbents for Congo red.

Kind of adsorbent	Adsorption capacity Q_t [mg g^{-1}]	
	Detected ^{a)}	Simulated ^{b)}
Pure aerogel	8.23	-
C_3N_4	14.87	-
Big-sized bulk ZIF-8	789.73	-
ZIF-8/ C_3N_4	504.42	352.71
11.1% ZIF-8/ C_3N_4 -aerogel	61.44	63.37
33.3% ZIF-8/ C_3N_4 -aerogel	178.63	173.46
50% ZIF-8/ C_3N_4 -aerogel	260.21	256.33

^{a)}The data was the equilibrium absorption value in Figure 2b, which was conducted by soaking 5 mg adsorbent into 20 mL CR solution at 200 ppm over 10 h in a shaker; ^{b)}The simulated capacity of ZIF-8/ C_3N_4 was calculated according to the proportions and data measured for big-sized bulk ZIF-8 and C_3N_4 ; the capacity of three hybrid aerogel was calculated based on the measured data for ZIF-8/ C_3N_4 and Pure aerogel.

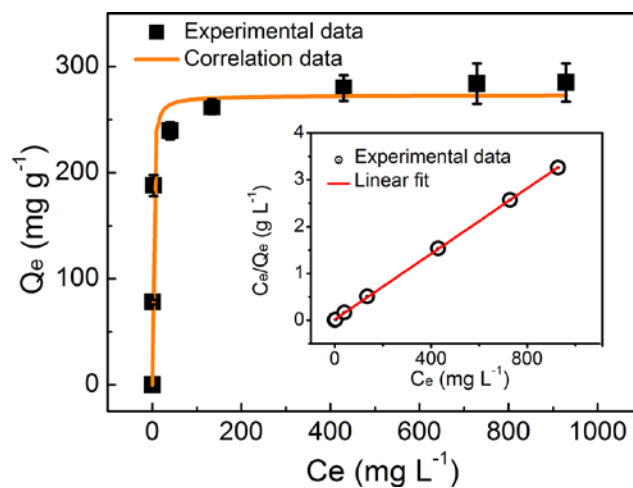


Figure S10. The adsorption isotherms of CR by Hgel-50 (correlation curve was drawn using the isotherm parameters calculated from the single-site adsorption isotherm model) and the linear fit of the model (inset).

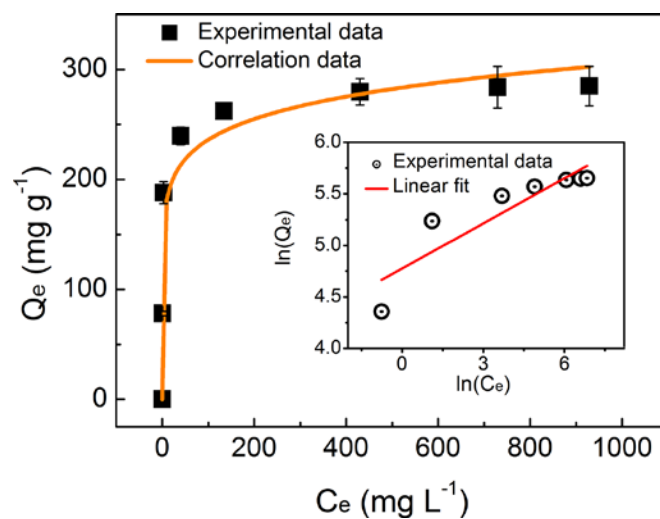


Figure S11. The adsorption isotherms of CR by Hgel-50 (correlation curve was drawn using the isotherm parameters calculated from the Freundlich isotherm model) and the linear fit of the model (inset).

Table S2. Thermodynamic parameters of Hgel-50 for CR adsorption.

	Single-site adsorption isotherm			Dual-site adsorption isotherm			Freundlich isotherm		
	Q_m	K_L	R^2	Q_m	K_d	R^2	K_F	$1/n$	R^2
	(mg g ⁻¹)	(L mg ⁻¹)		(mg g ⁻¹)	(L mg ⁻¹)		(mg g ⁻¹)		
Hgel-50	272.87	0.76	0.985	287.35	1.10	0.995	141.56	0.11	0.929
	±6.11	±0.14		±5.77	±0.07		±18.17	±0.02	
Hgel-Z	190.13	0.14	0.989	208.75	0.24	0.997	82.79	0.13	0.942
	±3.75	±0.02		±1.55	±0.02		±11.82	±0.03	

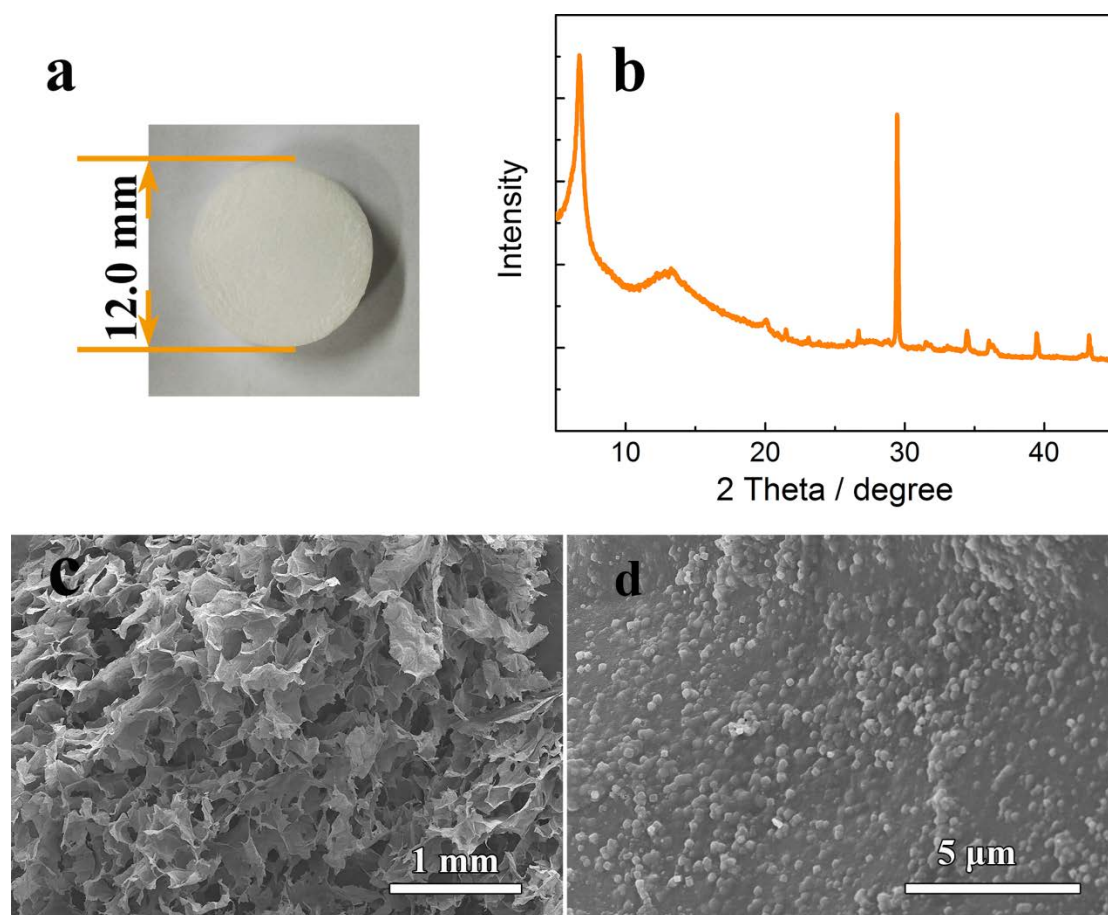


Figure S12. a) Photograph, b,c) SEM images and d) XRD pattern of aerogel containing 21.8% ZIF-8 (Hgel-Z).

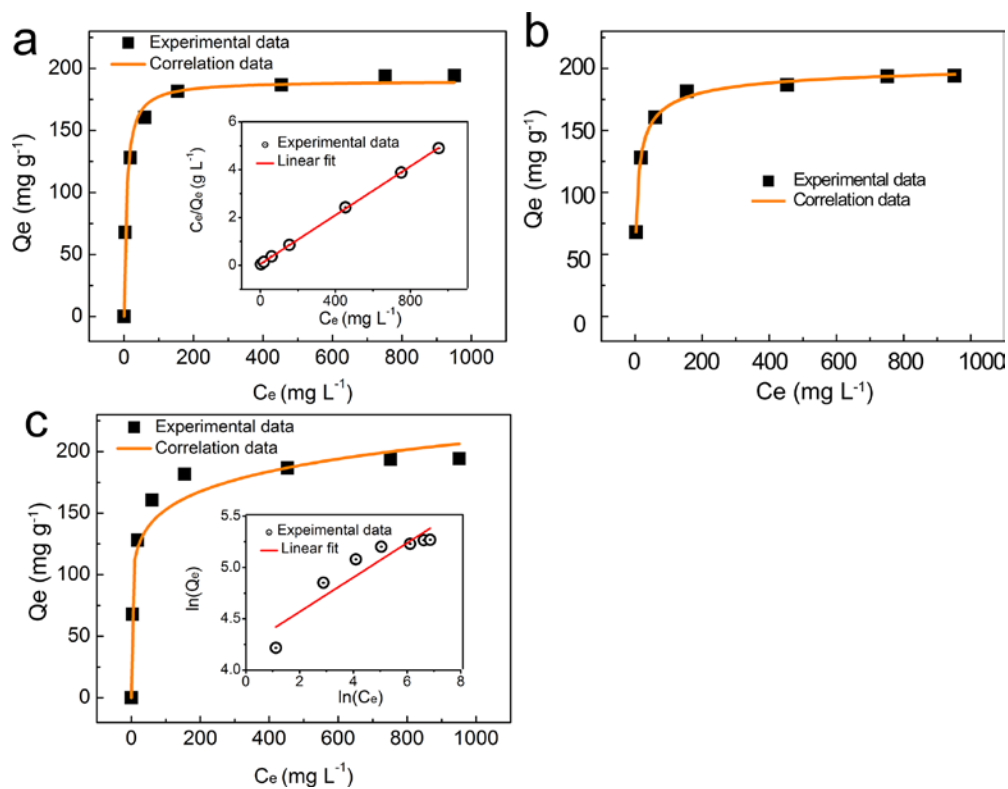


Figure S13. The single-site adsorption a), dual-site adsorption b) and Freundlich c) isotherm model for the adsorption isotherms of CR by Hgel-Z and the linear fit of the model (inset).

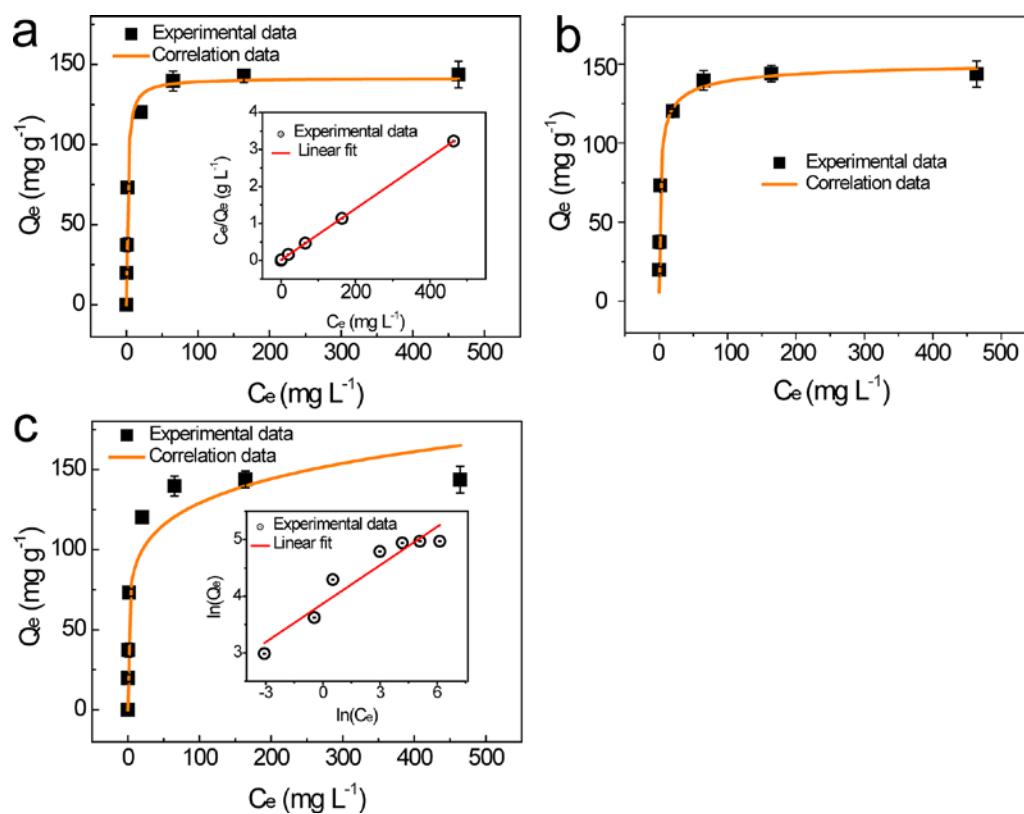


Figure S14. The single-site adsorption a), dual-site adsorption b) and Freundlich c) isotherm model for the adsorption isotherms of methylene blue by Hgel-50 and the linear fit of the model (inset).

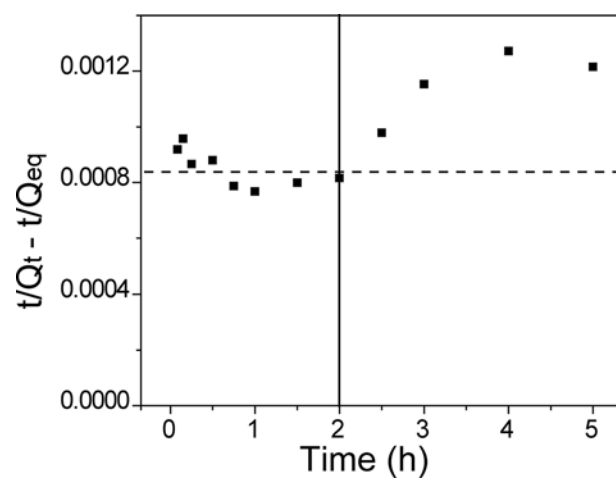


Figure S15. Invalidity of the pseudo-second-order conditions for the full time range of 5 hours.

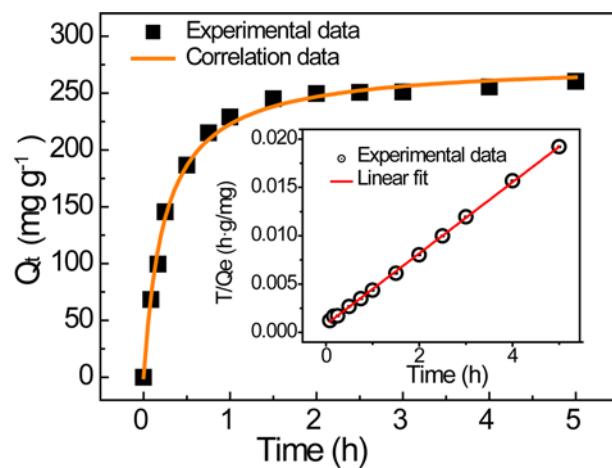


Figure S16. The adsorption kinetics of CR by Hgel-50 (correlation curve was drawn using the kinetic parameters calculated from the pseudo-second-order model of full time) and pseudo-second-order plots (inset).

Table S3. Adsorption kinetics parameters of Hgel-50 for CR adsorption.

$Q_{e,exp}$ (mg g ⁻¹)	Pseudo-first-order			Pseudo-second-order			Pseudo-second-order		
	$Q_{e,c}$ (mg g ⁻¹)	k_1 (h ⁻¹)	R^2	of full times			of lower times		
				$Q_{e,c}$ (mg g ⁻¹)	$k_2 \times 10^{-2}$ (g mg h ⁻¹)	R^2	$Q_{e,c}$ (mg g ⁻¹)	$k_2 \times 10^{-2}$ (g mg h ⁻¹)	R^2
260.21	249.90	3.05	0.991	276.69	1.49	0.995	288.59	1.28	0.996
	± 3.13	± 0.17		± 3.44	± 0.11		± 5.54	± 0.11	

Intraparticle diffusion model	Initial Phase			Secondary Phase		
	K_{p1} (mg g ⁻¹ h ^{-0.5})	C_I	R^2	K_{p2} (mg g ⁻¹ h ^{-0.5})	C_I	R^2
	256.24 \pm 25.84	1.03 \pm 15.29	0.961	20.84 \pm 4.28	215.31 \pm 7.04	0.792

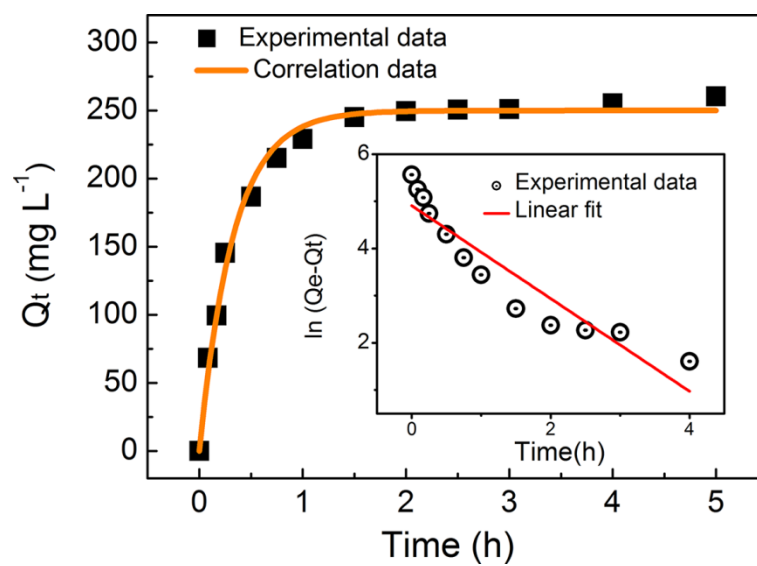


Figure S17. The adsorption kinetics of CR by Hgel-50 (correlation curve was drawn using the kinetic parameters calculated from the pseudo-first-order model of full time) and pseudo-first-order plots (inset).

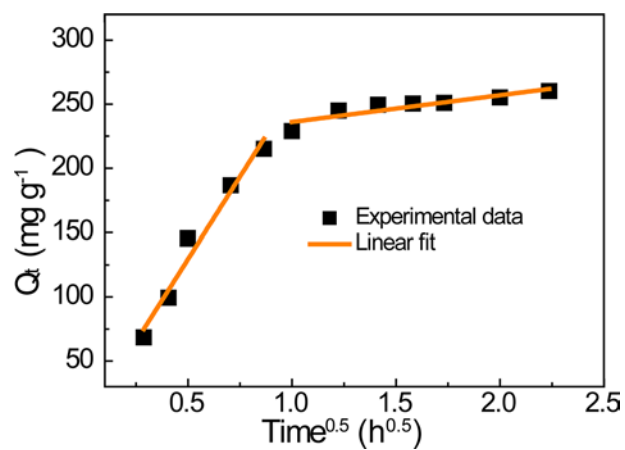


Figure S18. The intra-particle diffusion model for the adsorption of CR by Hgel-50.

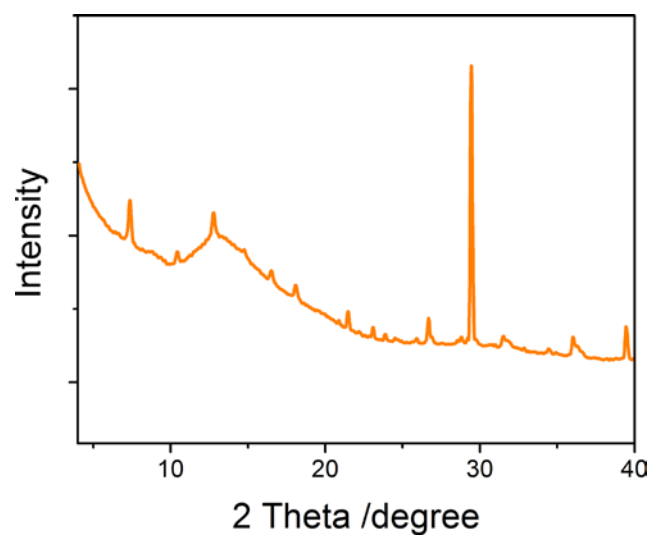


Figure S19. XRD pattern of the regenerated Hgel-50.

Table S4. Zn^{2+} concentration detected by atomic absorption spectrometer on pure water and water after treatment with Hgel-50.

	Pure water	CR solution after aerogel adsorption	CR solution after synergistic removal
Zn^{2+} concentration (ppm)	0.088 ± 0.016	0.092 ± 0.012	0.087 ± 0.019

Reference

1. Torad, N. L.; Hu, M.; Kamachi, Y.; Takai, K.; Imura, M.; Naito, M.; Yamauchi, Y. Facile synthesis of nanoporous carbons with controlled particle sizes by direct carbonization of monodispersed ZIF-8 crystals. *Chem. Commun.* **2013**, 49 (25), 2521-2523.