Supporting Information

Renewable 4-HIF/NaOH aerogel for efficient methylene blue removal via cation-π interaction induced electrostatic interaction

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General remarks

For zeta potential measurements, 0.01 g 4-HIF aerogel powder was suspended in the 5 mL of deionized water. The Zetasizer nano potential analyzer (Zeta PAL) was used to measure the zeta potential (ξ) at pH from 2 to 10. Each of the measurements was conducted at 25 °C and repeated 10 times. The 0.1 M solutions of sodium hydroxide (NaOH) and hydrochloric acid (HCl) solutions were used as a titration media to adjust the pH values.

0.45 μm polypropylene syringe filter was a miniature-scale water purification device in which one slice of filter paper was fixed in its plastic shell. Mixing the aerogel powder with pure water in the syringe, upon press the syringe, water drop down and the aerogel powder was stuck on the filter paper easily. Then the polypropylene syringe filter equipped with aerogel was obtained and can be used to remove dye quickly and conveniently as we demonstrated in Fig. 3(a).

Table S1. BET Analysis of alkaline 4-HIF aerogel

parameter	value
Surface area	130 m^2 g^{-1}
Pore volume	2.5 cm^3 g^{-1}
Pore radius	46 nm

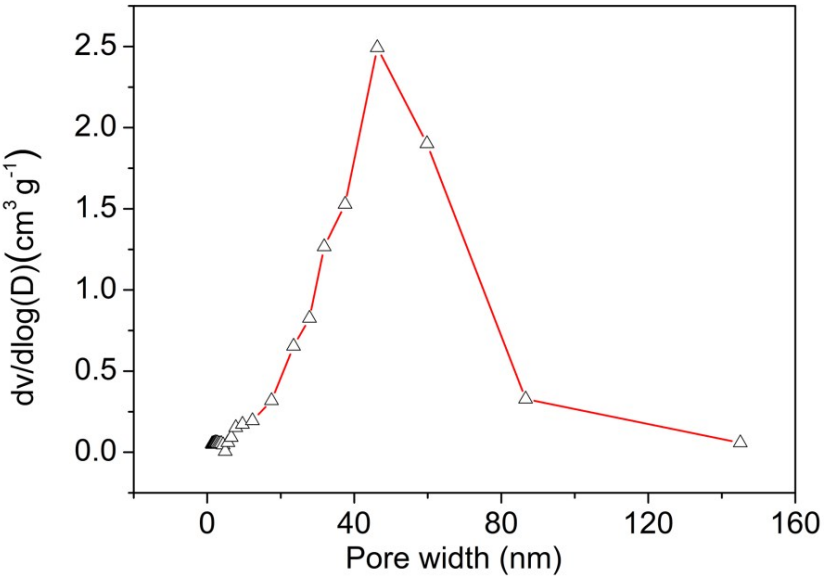

Figure S1. Pore size distribution curve of alkaline 4-HIF aerogel

Table S2. Weight ratio of elements of 4-HIF alkaline aerogel after adsorbing MB

Element	Weight %	Atomic %
C K	39.04	44.03
N K	40.26	38.94
O K	19.20	16.26
Na K	0.80	0.47
S K	0.70	0.29

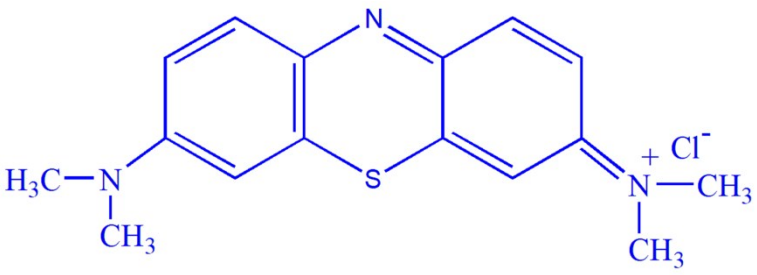

Figure S2. The molecular structures of methylene blue (MB)

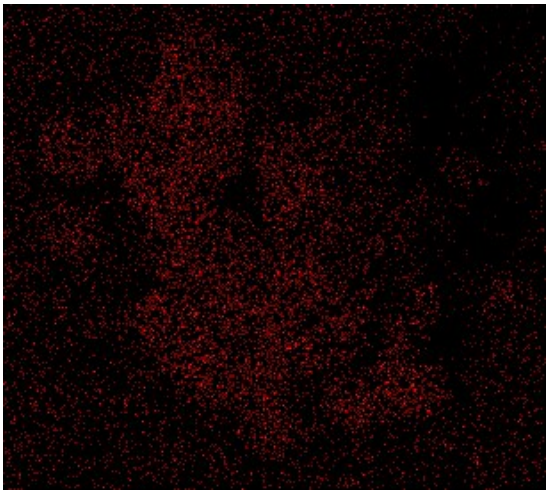

Figure S3. Elemental mapping of S in MB-4-HIF aerogel

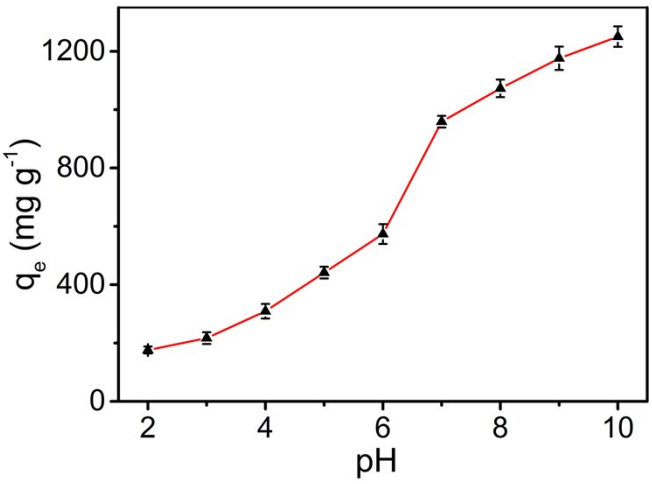

Figure S4. Effects of initial pH on the adsorption of MB onto the 4-HIF aerogel.

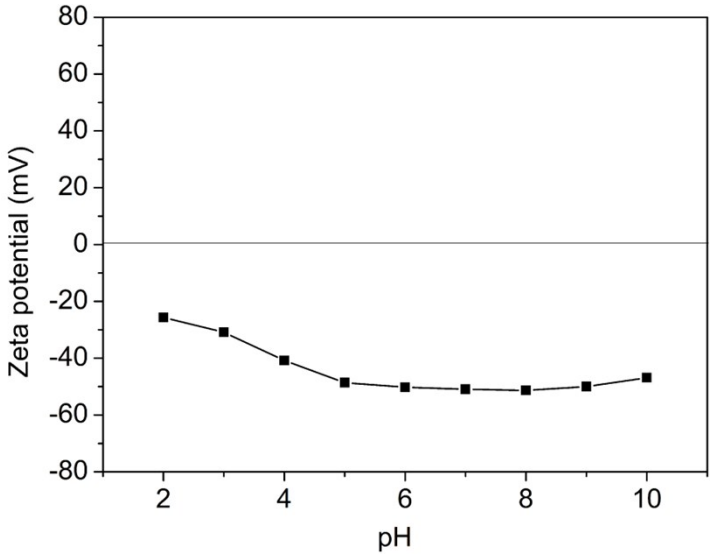

Figure S5. Zeta potentials of the alkaline 4-HIF aerogel at different pH solution.

Table S3. Kinetic parameters for the adsorption of MB

Temperature (K)		pseudo-first-order model		pseudo-second-order model		
	$q_{e,exp}$ (mg g^{-1})	K_1 (min^{-1})	R^2	q_e (mg g^{-1})	K_2 (g mg^{-1} min^{-1})	R^2
303	961.4	0.00675	0.966	909.1	6.71×10^{-5}	0.994

Table S4. Parameters of Langmuir and Freundlich models and coefficients of determination (R^2), for the adsorption of MB onto 4-HIF aerogel.

	Freundlich			Langmuir		
Experimental q_{max} (mg g^{-1})	K_f	1/n	R^2	q_m (mg g^{-1})	k_L (L mg^{-1})	R^2
1012.6	686.6	0.08757	0.833	1016.9	0.8939	0.999

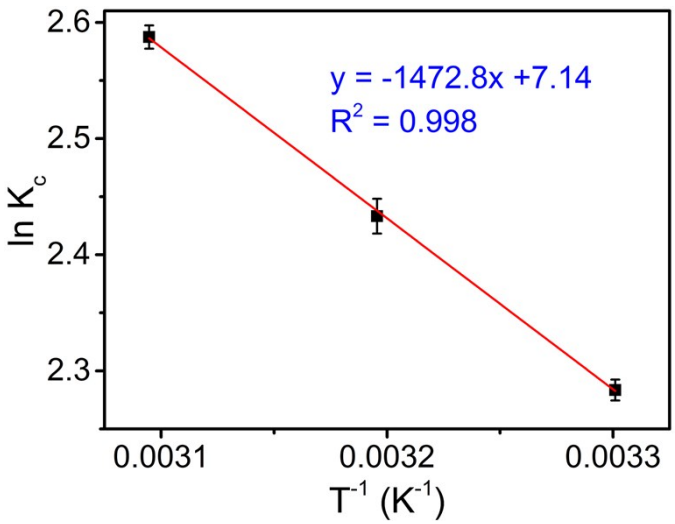

Figure S6. Van't Hoff graph for MB adsorption onto 4-HIF aerogel

Table S5. Thermodynamic parameters at different temperatures.

T (K^{-1})	q_e (mg g^{-1})	ΔG (kJ mol^{-1})	ΔH (kJ mol^{-1})	ΔS (J mol^{-1} K^{-1})
303	968.8	-5.757	12.311	59.609
313	1019.1	-6.345	-	-
323	1075.4	-6.951	-	-

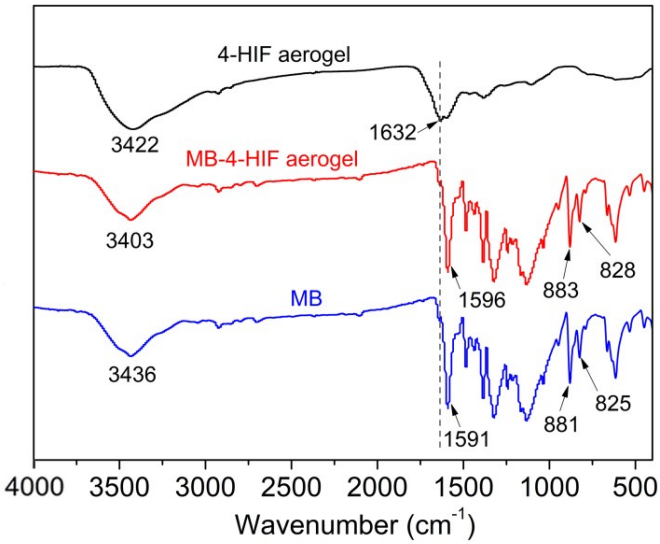

Figure S7. FT-IR spectra comparison of the 4-HIF aerogel, MB-4-HIF aerogel and MB.

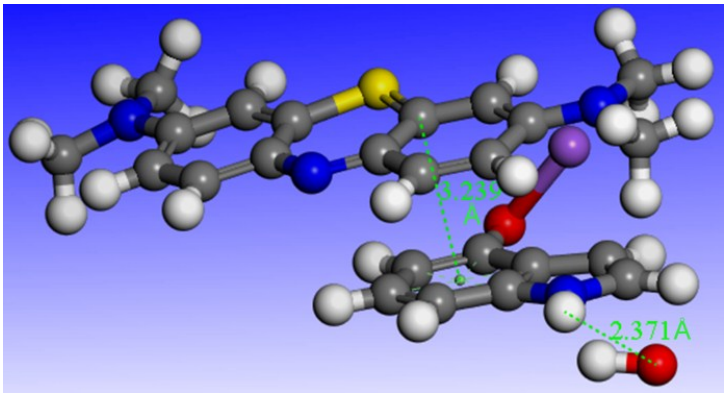

Figure S8. DFT simulation between MB and 4-HIF aerogel.

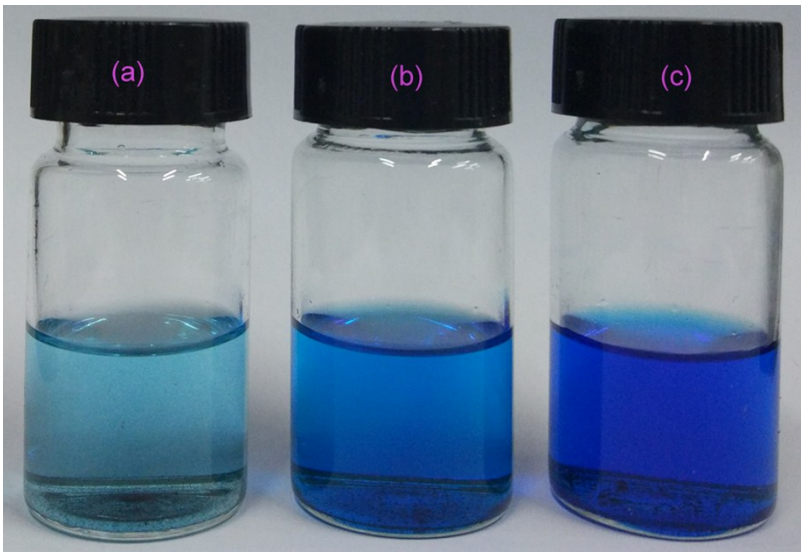

Figure S9. The photograph of desorbing MB-4-HIF aerogel by (a) ethanol, (b) 0.1 M HCl/ethanol at romm temperature and (c) 0.1 M HCl/ethanol after heating at 50 ^{o}C (each vial 5 mg saturated MB-4-HIF aerogel powder was added).