## **Supplementary Information**

### Nanofibrous membranes with surface migration of functional groups

## for ultrafast wastewater remediation

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Fig. S1 1H NMR spectra for MMA-SSNa copolymer.



**Fig. S2** N<sub>2</sub> adsorption–desorption isotherms for the nanofibrous membranes (A:MS-0, B:MS-2.5, C:MS-5, D:MS-10) and corresponding BJH (Barrett–Joyner– Halenda) pore-size distributions (insert).



**Fig. S3** The variation of UV-Vis spectra and digital photographs of the (A) MV and (B) RhB solutions after being adsorbed by UFAM with increasing adsorption time.

## **Adsorption Kinetics**



**Fig. S4** Applications of the pseudo-first-order (A), pseudo-second-order (B) and intraparticle diffusion (C) adsorption models for the MB adsorption onto UFAM.

Sample	Co	$q_e, exp -$ $(mg g^{-1})$	Pseudo-first-order			Pseudo-second-order		
	(μmol L <sup>-1</sup> )		K <sub>1</sub> (min <sup>-1</sup> )	q <sub>e</sub> (mg g <sup>-1</sup> )	$r_1^2$	$K_2$ (g mg <sup>-1</sup> min)	q <sub>e</sub> (mg g <sup>-1</sup> )	$r_2^2$
UFAM	100	214.27	1.7965	203.38	0.9401	10.38×10 <sup>-3</sup>	238.10	0.9914
	200	412.51	1.4944	441.69	0.9956	4.84×10-3	454.55	0.9964
	300	543.46	1.1625	566.91	0.9569	2.84×10-3	625	0.9995
	400	599.76	1.0681	612.10	0.9599	2.5×10-3	666.67	0.9999
	500	609.29	1.1373	547.25	0.9834	3.21×10-3	666.67	0.9995

**Table S1** Kinetic parameters of pseudo-first-order and pseudo-second-order

 adsorption models of UFAM for MB adsorption.

To better understand the adsorption ability of the UFAM toward MB, three types of kinetic models were applied to analyze the experimental data, including the pseudo-first-order equation, the pseudo-second-order equation and the intraparticle diffusion equation. The pseudo-first-order equation was based on the assumption that the adsorption rate is controlled by physical adsorption involving adsorption force through van der Waals force,  $\pi$ - $\pi$  force and hydrogen bonding between adsorbent and adsorbate, while the pseudo-second-order equation was based on the assumption that the adsorption rate is controlled by chemical adsorption through sharing or exchange of electrons between the adsorbate and adsorbent<sup>1</sup>, and they could be expressed as follows<sup>2, 3</sup>:

$$\ln(q_e - q_t) = \ln q_e - k_{1i}$$

$$\frac{t}{q_t} = \frac{1}{k_2 q_e^2} + \frac{1}{q_e}$$

Where  $k_1$  (min<sup>-1</sup>) and  $k_2$  (g mg<sup>-1</sup> min<sup>-1</sup>) were the rate constants of the pseudofirst-order and pseudo-second-order adsorption, respectively;  $q_e$  (mg g<sup>-1</sup>) and  $q_t$  (mg g<sup>-1</sup>) were the adsorption capacities at equilibrium and at time t (min), respectively. The linear plots of ln( $q_e$ - $q_t$ ) versus t and t/ $q_t$  versus t was shown in **Fig. S4A and S4B**, respectively, and the values of  $k_1$ ,  $k_2$  and  $q_e$  could be calculated from their slope and intercept. The calculated kinetics parameters and correlation coefficients for the adsorption of MB onto UFAM at different initial concentrations are listed in **Table S1**. It should be pointed out that the correlation coefficient values of the pseudosecond-order kinetic model ( $r^2 > 0.99$ ) were higher than that of pseudo-first-order kinetic model, indicating that the pseudo-second-order kinetic model was more appropriate to describe the adsorption process for UFAM for MB.

		Step I		Step II		
Sample	C (µmol L <sup>-1</sup> )	$K_{p I}$ (mg g <sup>-1</sup> min <sup>1/2</sup> )	r <sub>pI</sub> <sup>2</sup>	$K_{pII}$ (mg g <sup>-1</sup> min <sup>1/2</sup> )	r <sub>p II</sub> <sup>2</sup>	
	100	198.25	0.9853	4.67	0.8476	
	200	301.93	0.9942	35.36	0.8060	
UFAM	300	313.93	0.9999	82.91	0.9429	
	400	342.95	0.9932	112.40	0.9568	
	500	372.56	0.9668	77.23	0.9526	

**Table S2** Kinetic parameters of intra-particle diffusion adsorption model of UFAM

 for MB adsorption.

Since neither the pseudo-first-order nor the second-order model can identify the diffusion mechanism, the intra-particle diffusion model was used to further investigate the diffusion mechanism<sup>4</sup>. The intraparticle diffusion equation was described as follows:

$$q_t = k_p t^{1/2} + C$$

where  $k_p$  was the rate constant of intra-particle diffusion model;  $q_t (mg g^{-1})$  was the adsorption amount of dyes at time t (min); and C was a constant for the experiment (mg g<sup>-1</sup>). By plotting  $q_t$  versus  $t^{1/2}$ , two step curves were obtained as shown in **Fig. S4C**. It is generally believed that the two slopes indicated a two-steps adsorption process<sup>5</sup>: the external surface adsorption or diffusion in macro-pores occurred as the first step, and the second step corresponded to the intra-particle diffusion. Meanwhile, the values of the interception C were not equal to zero, which meant that the adsorption process was more than one diffusive resistance. The diffusion rate parameters ( $K_{pI}$ ,  $K_{p\Pi}$ ) and their correlation coefficients ( $r_{pI}^2$ ,  $r_{p\Pi}^2$ ) for the two sections of intra-particle plots were calculated and listed in **Table S2**. It is worthwhile mentioning that  $K_{pI}$  was much higher than  $K_{p\Pi}$ , indicated that the adsorption process was mainly caused by the diffusion and on the surface or in the macro pores at the first step. This result was **consistent with the comparison of c**orrelation coefficient values  $r_{pI}^2$  and  $r_{p\Pi}^2$ .

#### **Adsorption isotherms**

In order to further understand the adsorption process, two well-known models of Langmuir and Freundlich isotherms were applied to analyze the adsorption data.

Langmuir isotherm was based on the assumption that there is no interaction between the adsorbate molecules and the adsorption occurs uniformly on the active sites of the adsorbent<sup>6</sup>. On the other hand, Freundlich isotherm was an empirical equation to describe the multilayer adsorption on heterogeneous surface and reversible adsorption<sup>7</sup>, and their nonlinear forms can be expressed as follows:

$$\frac{C_e}{q_e} = \frac{1}{K_L q_{\max}} + \frac{C_e}{q_{\max}} \qquad (6)$$
$$\ln q_e = \ln K_F + \frac{1}{n \ln C_e} \qquad (7)$$

where  $C_e (mg L^{-1})$  is the equilibrium concentration of the solution;  $q_e (mg g^{-1})$  is the adsorption amount of MB per unit mass at equilibrium;  $q_{max} (mg g^{-1})$  is the maximum adsorption capacity;  $K_L (L mg^{-1})$  and  $K_F (mg g^{-1})$  were the rate parameters of the Langmuir and Freundlich adsorption isotherms, respectively. Two isotherm model parameters are summarized in **Fig. S5** and **Table S3**, and it was noted that the value of n at the Freundlich equilibrium (n=6.173) was remarkably greater than 1, indicating that the favorable adsorption towards MB. Nevertheless, the Langmuir model fitted the experimental data better than the Freundlich model based on the higher correlation coefficients, suggesting that monolayer Langmuir adsorption was more suitable to describe the adsorption process.



Fig. S5 Adsorption isothermal models for the MB adsorption onto UFAM

	Langmuir			Freundlich			
Sample	K <sub>L</sub> (min <sup>-1</sup> )	$q_m$ (mg g <sup>-1</sup> )	$r_L^2$	K <sub>F</sub> (g mg <sup>-1</sup> min)	n	$r_F^2$	
UFAM	0.26	625	0.999	309.20	6.173	0.931	

Table S3 Parameters of the adsorption isotherm of UFAM for MB adsorption.



Fig. S6 Effect of pH value on the MB adsorption for UFAM.



Fig. S7 The desorption capacities for MS-10 and UFAM with increasing time.



**Fig. S8** (A) FTIR spectra, (B) XPS wide spectra of UFAM samples before adsorption, after adsorption and after 10 desorption, respectively.

# Adsorption mechanism of the functionalized PES nanofibrous membranes

In order to understand the MB adsorption mechanism of this functionalized PES nanofibrous membrane, ATR-FTIR and XPS analysis were performed. As shown in Fig. S8, several new peaks at 1325, 1392 and 1486 cm-1 could be observed onto the surface of sample after adsorption, which were assigned to the stretching vibrations of C-N bonds of MB<sup>8</sup>. Meanwhile, new peak of N element was detected in the wide scan spectra for UFAM after adsorption, which indicated the successful adsorption of MB. On the contrary, these peaks were weakened significantly for the UFAM sample after 10 cycles of desorption, which implied the successful elution for MB dyes. It was worthwhile mentioning that the S 2s and S 2p peaks were obviously weakened in the XPS spectra after the adsorption of MB, which revealed that SO3- groups might be the reactive sites for MB adsorption of UFAM. Similarly, the S 2s and S 2p peaks were obviously enhanced for the sample after 10 cycles of desorption, suggesting the successful regeneration for functional SO<sup>3-</sup> groups. Such an electrostatic interaction between dye molecules and adsorbent species was also reported by Zhang et al<sup>9</sup>.



Fig. S9 SEM image of UFAM after 10 cycles of dynamic filtration.



Fig. S10 Chemical structures and abbreviations of dyes used in this study.



**Fig. S11** The schematic illustration of adsorption for the anionic and cationic dyes by the UFAM.



Fig. S12 SEM image of UFAM after 10 cycles of dynamic filtration separation.



Fig. S13 The SEM images and diameter distributions of UFAM.



Fig. S14 FTIR spectra of MS-10 and UFAM samples, respectively.



**Fig. S15** N<sub>2</sub> adsorption–desorption isotherms for the MS-10 and UFAM respectively, and corresponding BJH (Barrett–Joyner–Halenda) pore-size distributions (insert).

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