## Supplementary Materials

## A Sulfonate Ligand-Defected Zr-Based Metal-Organic Framework for The Enhanced Selective Removal of Anionic Dyes

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Commercial name	Chemical structure	Absorption (λ <sub>max</sub> _nm)	
Quinoline Yellow (QY)	$\bigcup_{O}^{O} \longrightarrow_{HN} \bigcup_{(SO_3Na)_2}^{O}$	440	
Sunset Yellow (SY)	NaO-S O O N=N O N=N O N=N O S=ONa O	482	
Rhodamine B (RhB)	N HOOC	555	
Malachite Green (MG)	$H_{3}C$ $H_{3}C$ $H_{3}C$ $H_{3}C$ $H_{3}C$ $H_{3}C$ CI	620	

## Table S1. Basic information on employed organic dyes



**Figure S1.** FT-IR spectra of pristine MOF-808, H<sub>3</sub>BTC linker, H<sub>2</sub>BTC-SO<sub>3</sub>Na linker, and MOF-808-S.



Figure S2. <sup>1</sup>H-NMR spectra of digested MOF-808.



Figure S3. TGA profiles of MOF-808 and MOF-808-S.



**Figure S4.** Pseudo-first-order and second-order models of the adsorption processes of quinoline yellow (a, b); and sunset yellow (c, d) on MOF-808-S.



**Figure S5.** Pseudo-first-order and second-order models of the adsorption processes of rhodamine B (a, b), and malachite green (c, d) on MOF-808-S.



**Figure S6.** Langmuir and Freundlich models of the adsorption processes of quinoline yellow (a, b); and sunset yellow (c, d) on MOF-808-S.



**Figure S7.** Langmuir and Freundlich models of the adsorption processes of rhodamine B (a, b), and malachite green (c, d) on MOF-808-S.

N.	Sample	Pseudo-first-order model			Pseudo-second-order model		
		Q <sub>e,cal</sub> (mg/g)	k*10 <sup>-2</sup> (min <sup>-1</sup> )	R <sup>2</sup> (%)	Q <sub>e,cal</sub> (mg/g)	k*10 <sup>-2</sup> (g/mg.min)	R <sup>2</sup> (%)
1	QY	187.5	-1.520	88.20	746.5	0.023	99.96
2	SY	55.3	-0.966	77.84	661.4	0.108	99.98
3	RhB	27.3	-0.970	56.63	183.2	0.210	99.97
4	MG	156.3	-1.530	80.88	298.1	0.010	99.18

**Table S2.** Coefficients of pseudo first-order and second-order model for the adsorptionprocess based on MOF-808-S.

**Table S3.** Coefficients of Langmuir and Freundlich models for adsorption processes basedon MOF-808-S.

N	Sample	Langmuir model			Freundlich model		
14.		K <sub>L</sub> (L/mg)	$Q_L(mg/g)$	R <sup>2</sup> (%)	Ν	$K_F(L/g)$	R <sup>2</sup> (%)
1	QY	0.297	770.1	96.18	11.2	458.0	65.22
2	SY	0.021	784.6	97.63	2.91	99.7	94.66
3	RhB	0.005	301.2	88.66	5.17	63.1	75.42
4	MG	0.004	383.1	93.01	2.84	27.8	83.05



Figure S8. FT-IR spectra of the fresh and recovered materials.



Figure S9. Pore size distribution of the fresh and reused MOF-808-S.



**Figure S10.** UV-Vis spectra of quinoline yellow-rhodamine B mixtures in the presence of 200 ppm for each dye at various time intervals employing MOF-808 and MOF-808-S as adsorbents