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Supporting Information

Rapid microwave-assisted synthesis of magnetic biochar@ZIF-67 as an efficient nanocomposite-based adsorbent for dye-contaminated water cleanup

Sepehr Haghdoust [a], Payam Arabkhani [b], Sajad Ghaderi [c], Mehrorang Ghaedi [*a], Arash Asfaram [*b]

[a] *Chemistry Department, Yasouj University, Yasouj 75918-74831, Iran.*

[b] *Medicinal Plants Research Center, Yasuj University of Medical Sciences, Yasuj, Iran.*

[c] *Cellular and Molecular Research Center, Yasuj University of Medical Sciences, Yasuj, Iran.*

[*] Corresponding author: E-mail address: arash.asfaram@yums.ac.ir (A. Asfaram)

Figure Captions:

Figure S1. Reusability experiments for the removal of TA and SY dyes by MWDS-B@ZIF-67.

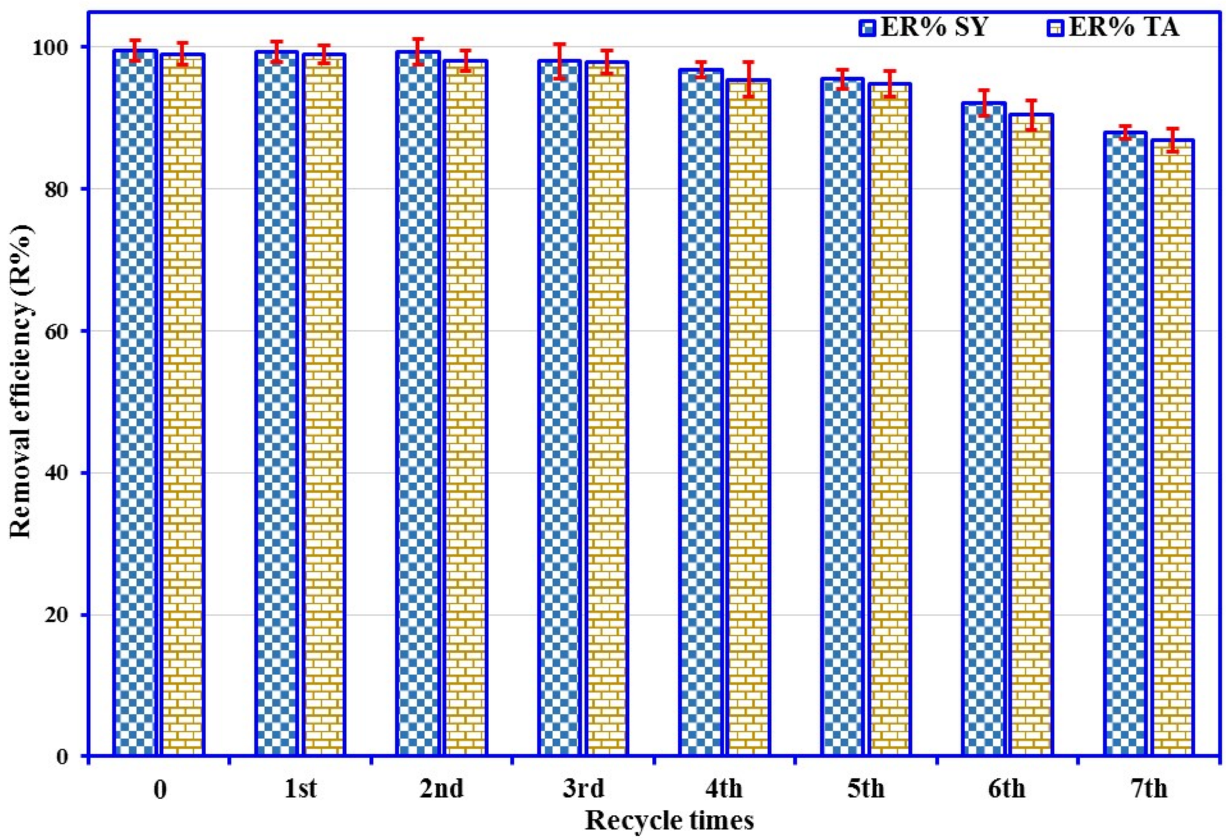

Figure S1. Reusability experiments for the removal of TA and SY dyes by MWDS-B@ZIF-67.

Table Captions:

Table S1. Calculated parameters of the adsorption isotherm models.

Table S2. Estimated parameters of the adsorption kinetic models.

Table S3. Thermodynamic parameters for the adsorption process.

Table S4. Comparison of the Langmuir maximum adsorption capacity (Q_{max}) and contact time of MWDS-B@ZIF-67 with other adsorbents.

Table S1. Calculated parameters of the adsorption isotherm models.

Isotherm	Plot	Parameters	TA	SY
Langmuir $\frac{C_e}{q_e} = \frac{1}{Q_m k_L} + \frac{C_e}{Q_m}$	C_e/q_e vs. C_e	Q_m (mg g^{-1})	95.91	64.87
		K_L (L mg^{-1})	8.515	3.352
		R^2	0.998	0.998
		$R_L=1/(1+(K_L \times C_0))$	0.003-0.029	0.007-0.069
Freundlich $ln q_e = ln K_F + \frac{1}{n} ln C_e$	$ln\ q_e$ vs. $ln\ C_e$	1/n	0.218	0.182
		K_F (L mg^{-1})	6.422	5.091
		R^2	0.969	0.973
Temkin $q_e = B_1 \ln K_T + B_1 \ln C_e$	q_e vs. $ln\ C_e$	B_1	8.49	5.77
		K_T(L mg^{-1})	1.000	1.000
		R^2	0.839	0.959
Dubinin-Radushkevich $ln\ q_e = lnQ_S - k\varepsilon^2$	$ln\ q_e$ vs. ε^2	Qs (mg g^{-1})	65.12	52.42
		$\beta \times 10^{-9}$	-3.70	-5.40
		E (kJ mol^{-1})	11.59	9.639
		R^2	0.808	0.887

Table S2. Estimated parameters of the adsorption kinetic models.

Model	Plot	Parameters	TA	SY
Pseudo-First order- kinetic $\ln(q_e - q_t) = \ln q_e - k_1 t$	*ln (q* $\ln(q_e - q_t)$ *vs. t*	k_1 (min^{-1})	0.273	0.316
		$q_{e\ (calc)}$ ($mg\ g^{-1}$)	48.22	47.93
		R^2	0.974	0.867
Pseudo-second order-kinetic $\frac{t}{q_t} = \frac{1}{k_2 q_e^2} + \frac{t}{q_e}$	t/q_t *vs. t*	k_2 (min^{-1})	0.008	0.014
		$q_{e\ (calc)}$ ($mg\ g^{-1}$)	44.82	32.41
		R^2	0.996	0.998
		h ($mg\ g^{-1} min^{-1}$)	16.83	14.59
Intraparticle diffusion $q_t = k_{diff} t^{1/2} + C$	q_t *vs.* $t^{1/2}$	K_{diff} ($mg\ g^{-1}\ min^{-1/2}$)	6.37	4.10
		C ($mg\ g^{-1}$)	12.57	11.74
		R^2	0.910	0.937
Elovich $q_t = \frac{1}{\beta}\ln(t) + \frac{1}{\beta}\ln(\alpha\beta)$	q_t *vs. ln t*	α ($mg\ g^{-1}\ min^{-1}$)	48.11	61.22
		β ($g\ mg^{-1}$)	0.1178	0.1839
		R^2	0.971	0.993
Experimental data		$q_{e\ (exp)}$ ($mg\ g^{-1}$)	39.76	29.53

Table S3. Thermodynamic parameters for the adsorption process.

	TA		SY	
T(k)	**k_d**	**ΔG°(kJ mol^{-1})**	**k_d**	**ΔG°(kJ mol^{-1})**
283.15	10.85	-5.61	16.14	-6.55
293.15	35.36	-8.69	28.27	-8.14
303.15	79.00	-11.01	51.17	-9.92
313.15	159.0	-13.20	79.00	-11.38
323.15	319.0	-15.49	119.0	-12.84
R^2	0.993		0.998	
ΔS° (J mol^{-1} k^{-1})	243.6		322.2	
ΔH° (kJ mol^{-1})	63.09		89.33	
$\Delta G° = -RT\ln K$				
$LnK^0 = \Delta H° - T\Delta S°_{/RT}$				

Table S4. Comparison of the Langmuir maximum adsorption capacity (Q_{max}) and contact time of MWDS-B@ZIF-67 with other adsorbents.

Adsorbent	**Q_{max} (mg g^{-1})**		**Time (min)**	**Ref.**
	TA	SY		
Low-cost agricultural by-product	4.71	-	70	1
Papaya seeds	51.0	-	-	2
Iron oxide nanoparticles	59.79	-	>180	3
Activated carbon biosorbents of Lantana Camara	90.90	-	-	4
Ni-Ag NPs-rGO	26.31	-	15	5
$Mn_{0.4}Zn_{0.6}Fe_2O_4$-NPs-D-YL-ISF7	90.83		-	6
Activated carbon derived from cassava sievate biomass	20.83	0.091	-	44
Positively charged triethylenetetramine biochar	85.47	74.07	30	45
Cross-linked chitosan	-	36.08	-	46
MWDS-B@ZIF-67	**95.91**	**64.87**		**This work**

References

1. S. Banerjee and M. Chattopadhyaya, *Arabian J. Chem.*, 2017, **10**, S1629-S1638.
2. C. T. Weber, G. C. Collazzo, M. A. Mazutti, E. L. Foletto and G. L. Dotto, *Water Sci. Technol.*, 2014, **70**, 102-107.
3. A. C. de Lima Barizao, M. F. Silva, M. Andrade, F. C. Brito, R. G. Gomes and R. Bergamasco, *J. Environ. Chem. Eng.*, 2020, **8**, 103618.
4. R. K. Gautam, P. K. Gautam, S. Banerjee, V. Rawat, S. Soni, S. K. Sharma and M. C. Chattopadhyaya, *J. Environ. Chem. Eng.*, 2015, **3**, 79-88.
5. R. Mirzajani and S. Karimi, *Ultras. Sonochem.*, 2019, **50**, 239-250.
6. A. Asfaram, M. Ghaedi, K. Dashtian and G. R. Ghezelbash, *ACS Sust. Chem. Eng.*, 2018, **6**, 4549-4563.