Preparation and characterization of monoliths HKUST-1 MOF via straightway conversion of $Cu(OH)_2$-based monoliths and its application for wastewater treatment: Artificial neural network and central composite design modeling

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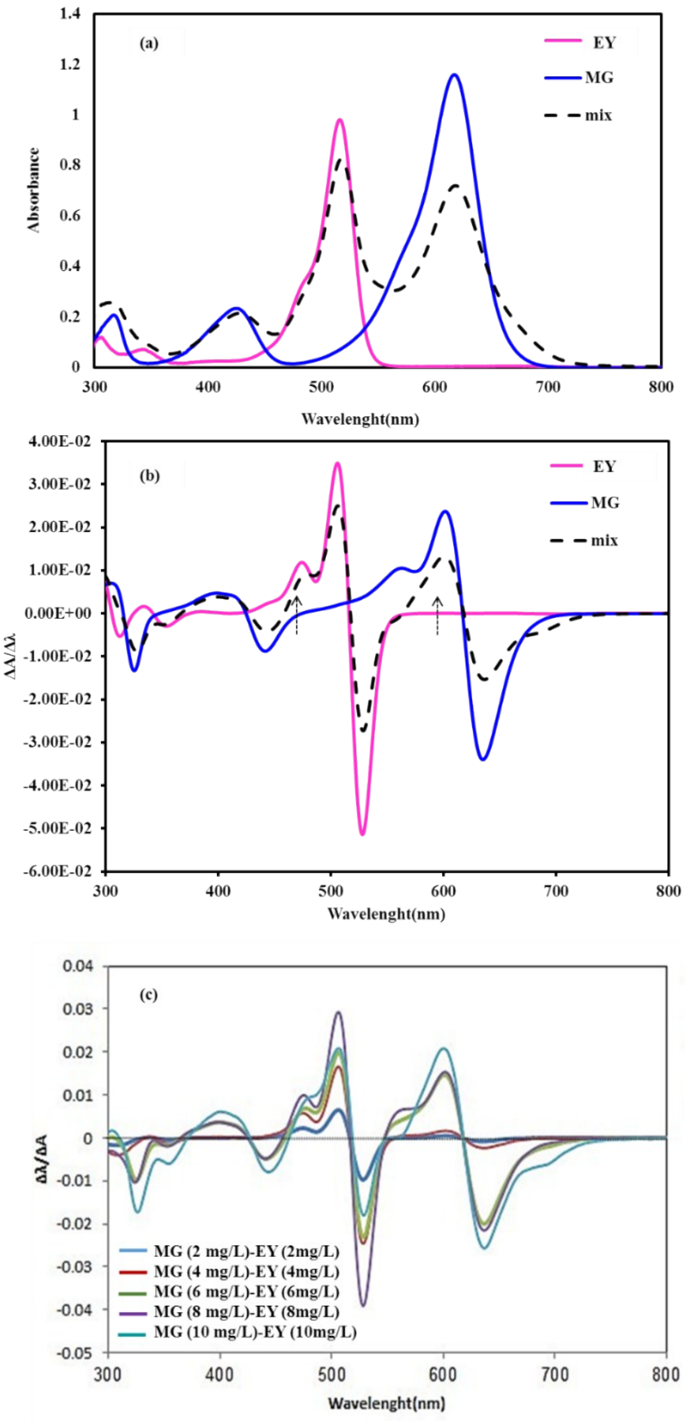

Fig. S1. The zero order derivatives for EY and MG dye at concentration of 8 mg/L for individual and mixed solutions (a), the first order derivative for individual and mixed solutions of EY and MG (b) (b) and the first derivative of two dye at different concentrations (c)

Table S1. The used intervals for the effective operational parameters

Factors	Levels			Star point α=2.0	
	Low (-1)	Central (0)	High (+1)	- α	+ α
(A) MG Concentration (mg L^{-1})	4	8	10	6	12
(B) EY Concentration (mg L^{-1})	4	8	10	6	12
(C) pH	4	6	8	2	10
(D) Monolith HKUST-1 mass (g)	0.005	0.015	0.025	0.01	0.02
(E) Sonication time (min)	2	3	4	1	5

Table S2. CCD matrix and obtained responses

Runs	A	B	C	D	E	$R\%_{MG}$	$R\%_{EY}$
1	6	10	4	0.02	2	97.17	99.87
2	10	6	8	0.01	4	91.32	94.63
3	6	10	8	0.02	2	100.45	99.62
4	8	8	6	0.015	3	94.82	83.72
5	8	8	6	0.015	3	95.32	83.76
6	8	8	6	0.005	3	89.67	86.54
7	8	8	10	0.015	3	98.65	97.81
8	12	8	6	0.015	3	95.01	87.9
9	10	10	8	0.01	2	98.25	89.12
10	10	10	8	0.02	4	99.98	96.7
11	8	8	6	0.015	3	94.78	82.94
12	10	10	4	0.02	2	97.89	101.49
13	8	8	6	0.015	3	94.57	83.12
14	8	8	6	0.015	3	94.49	83.47
15	6	6	8	0.02	4	94.98	101.23
16	10	6	8	0.02	4	95.27	99.62
17	10	10	4	0.01	4	92.42	85.68
18	8	4	6	0.015	3	89.21	97.22
19	10	10	8	0.01	4	97.01	81.65
20	6	10	8	0.02	4	99.67	101.1
21	6	10	8	0.01	2	97.63	92.56
22	6	6	8	0.01	2	91.82	96.4
23	6	6	4	0.01	2	87.45	98.57
24	6	10	4	0.01	2	92.38	95.41
25	10	6	4	0.01	2	88.36	99.78
26	8	8	6	0.015	5	92.86	94.2
27	6	6	4	0.02	4	91.03	98.4
28	10	10	4	0.01	2	93.94	94.2
29	10	10	4	0.02	4	96.14	98.42
30	6	6	4	0.01	4	85.65	97.11
31	6	10	8	0.01	4	96.45	90.25
32	10	6	8	0.02	2	96.9	97.43
33	10	10	8	0.02	2	100.8	99.034
34	8	8	6	0.015	3	94.87	83.48
35	8	8	6	0.01	3	94.92	82.98
36	10	6	8	0.01	2	92.94	95.07
37	6	6	8	0.01	4	90.57	99.2004
38	10	6	4	0.02	2	92.45	99.15
39	8	8	6	0.015	1	95.108	96.51
40	10	6	4	0.01	4	86.59	97.12
41	4	8	6	0.015	3	93.64	90.85
42	8	8	6	0.015	3	94.13	83.43
43	10	6	4	0.02	4	91.7	99.76
44	6	6	8	0.02	2	96.53	96.29
45	8	8	6	0.025	3	98.62	97.6
46	8	8	2	0.015	3	89.38	99.53
47	8	12	6	0.015	3	99.76	91.2
48	6	6	4	0.02	2	91.61	94.03
49	6	10	4	0.02	4	95.88	99.82
50	6	10	4	0.01	4	91.54	89.95

Table S3. analysis of variance (ANOVA) for removal of MG using nanoparticles of monolithic HKUST-1 MOF

Model Source	Sum of square	Degree of freedom	Mean square	F value	P value
Model	1906.42	20	95.32	391.32	< 0.0001
A	18.03	1	18.03	74.02	< 0.0001
B	92.89	1	92.89	381.35	< 0.0001
C	12.43	1	12.43	51.02	< 0.0001
D	288.28	1	288.28	1183.47	< 0.0001
E	12.10	1	12.10	49.69	< 0.0001
AB	17.43	1	17.43	71.55	< 0.0001
AC	20.86	1	20.86	85.64	< 0.0001
AD	17.18	1	17.18	70.51	< 0.0001
AE	21.13	1	21.13	86.75	< 0.0001
BC	3.62	1	3.62	14.84	0.0006
BD	149.66	1	149.66	614.41	< 0.0001
BE	45.33	1	45.33	186.07	< 0.0001
CD	11.31	1	11.31	46.43	< 0.0001
CE	7.12	1	7.12	29.24	< 0.0001
DE	35.40	1	35.40	145.31	< 0.0001
A^2	65.34	1	65.34	268.22	< 0.0001
B^2	222.63	1	222.63	913.96	< 0.0001
C^2	450.64	1	450.64	1849.98	< 0.0001
D^2	141.48	1	141.48	580.80	< 0.0001
E^2	273.57	1	273.57	1123.10	< 0.0001
Residual	7.06	29	0.24		
Lack of Fit	6.36	22	0.29	2.90	0.0762
Pure Error	0.70	7	0.100		< 0.0001
Cor Total	1913.49	49			< 0.0001

Table S4. Analysis of variance (ANOVA) for removal of EY using nanoparticles of monolithic HKUST-1 MOF

Model Source	Sum of square	Degree of freedom	Mean square	F value	P value
Model	652.21	20	32.61	316.02	< 0.0001
A	4.82	1	4.82	46.74	< 0.0001
B	267.96	1	267.96	2596.75	< 0.0001
C	188.83	1	188.83	1829.94	< 0.0001
D	168.22	1	168.22	1630.21	< 0.0001
E	15.46	1	15.46	149.80	< 0.0001
AB	0.012	1	0.012	0.12	0.7313
AC	0.18	1	0.18	1.76	0.1951
AD	0.39	1	0.39	3.77	0.0618
AE	0.10	1	0.10	1.01	0.3222
BC	0.21	1	0.21	2.06	0.1616
BD	1.72	1	1.72	16.63	0.0003
BE	0.073	1	0.073	0.71	0.4067
CD	1.51	1	1.51	14.63	0.0006
CE	1.653E-003	1	1.653E-003	0.016	0.9002
DE	0.13	1	0.13	1.30	0.2640
A^2	0.23	1	0.23	2.20	0.1492
B^2	0.062	1	0.062	0.60	0.4433
C^2	0.84	1	0.84	8.10	0.0080
D^2	0.53	1	0.53	5.17	0.0305
E^2	0.92	1	0.92	8.90	0.0057
Residual	2.99	29	0.10		
Lack of Fit	2.14	22	0.097	0.79	0.6863
Pure Error	0.86	7	0.12		
Cor Total	655.20	49			

Table S5. CCD model summary report.

	MG	**EY**
Std. Dev.	0.32	0.49
Mean	94.25	93.70
C.V. %	0.34	0.53
PRESS	8.99	23.66
R-Squared	0.9954	0.9963
Adj R-Squared	0.9923	0.9938
Pred R-Squared	0.9863	0.9876
Adeq Precision	74.748	61.488

Table S6. The effect of number of neurons in the hidden layer on the efficiency of the prosed ANN model for modeling of the MG dye removal

	Train data			**Test data**		
Number of neurons	MSE	AAD%	R^2	MSE	AAD%	R^2
1	0.000812	12.77	0.837	0.00213	7.32	0.960
2	0.000374	10.20	0.903	0.00215	5.01	0.980
3	0.000741	12.70	0.961	0.001568	6.05	0.947
4	7.51E-05	3.51	0.990	0.000189	1.69	0.995
5	3.54E-05	2.14	0.997	7.91E-05	1.08	0.998
6	0.00071	8.37	0.907	0.001302	6.69	0.966
7	0.000277	8.33	0.957	0.000735	3.85	0.985
8	0.000627	11.48	0.895	0.001705	7.93	0.966
9	0.000272	5.57	0.929	0.001266	4.31	0.990
10	0.000189	6.42	0.958	0.000661	3.49	0.991
11	2.07E-05	9.15	0.679	0.007998	0.49	0.999
12	0.000371	8.12	0.905	0.000994	4.66	0.981
13	**1.75E-05**	**1.07**	**0.997**	**7.43E-05**	**0.49**	**0.999**
14	0.000118	3.25	0.981	0.000381	2.41	0.995
15	6.58E-06	4.96	0.956	0.000664	0.30	1.000
16	6.74E-05	10.38	0.893	0.002039	1.48	0.996
17	2.58E-05	13.84	0.879	0.00494	0.73	0.998
18	0.000223	16.12	0.779	0.007068	3.53	0.987
19	2.33E-05	5.16	0.957	0.001123	0.51	0.999
20	1.25E-05	6.87	0.973	0.00105	0.38	0.999

Table S7. The effect of number of neurons in the hidden layer on the efficiency of the prosed ANN model for modeling of the EY dye removal

	Train data			Test data		
Number of neurons	MSE	AAD%	R^2	MSE	AAD%	R^2
1	0.007139	24.67	0.824	0.009515	24.13	0.889
2	0.012953	23.90	0.892	0.007743	20.06	0.637
3	0.006999	31.52	0.886	0.01035	16.85	0.796
4	0.005653	17.96	0.962	0.004053	25.86	0.949
5	0.008445	14.01	0.919	0.004416	28.96	0.892
6	0.009838	30.85	0.879	0.010379	22.36	0.786
7	0.005825	1.41	0.999	3.62E-05	19.53	0.924
8	0.002554	1.64	0.999	5.86E-05	3.38	0.970
9	**0.000233**	**0.73**	**1.000**	**1.59E-05**	**2.41**	**0.997**
10	0.008503	19.77	0.927	0.00492	27.41	0.886
11	0.00294	3.33	0.997	0.000231	6.96	0.938
12	0.013806	15.66	0.884	0.008759	15.87	0.801
13	0.003302	1.57	1.000	4.32E-05	4.93	0.955
14	0.005582	0.67	1.000	1.64E-05	8.68	0.934
15	0.000821	0.83	1.000	2.15E-05	5.07	0.991
16	0.001003	0.79	1.000	2.09E-05	3.04	0.986
17	0.006412	4.94	0.992	0.000724	10.66	0.888
18	0.002878	1.00	1.000	2.32E-05	4.76	0.968
19	0.001785	1.22	1.000	2.77E-05	3.39	0.970
20	0.008481	5.24	0.991	0.000689	12.19	0.840