Supporting Information

RSM-BBD Optimization of Room-Temperature Synthesized Meso-ZIF-8 for Synergistic Adsorption-Photocatalysis of RhB

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Experimental Section

2.4. BBD-RSM design and data analysis

2.4.1. Adsorption process

The adsorption and degradation process was optimized through statistical response surface methodology (RSM), which offers a powerful tool for evaluating multiple variables simultaneously. In this study, a Box–Behnken design (BBD) was applied to assess the linear, quadratic, and interaction effects of five independent factors (**Table S1**). The main objective was to maximize the response variable (adsorption efficiency) by systematically varying the amount of 2-HmIM, pollutant concentration, pH, catalyst loading, and contact time. The selection of these parameters was guided by prior literature on organic dye removal as well as preliminary experimental observations. Data analysis for the experimental design was carried out using

Nemrodw 2007 software[1]. The total number of experimental runs (N) was calculated according to **Eq. (S1)**. The obtained responses (RhB removal efficiency) were then fitted to a quadratic polynomial model, as expressed in **Eq. (S2)**:

$$\mathbf{N = 2^k + 2k + C_0} \qquad \textbf{(S1)}$$

$$Y = b_0 + \sum_{i=1}^{k} b_i x_i + \sum_{i=1}^{k} b_{i-i} x_i^2 + \sum_{i=1}^{k-1} \sum_{j=i+1}^{k} b_{i-j} x_i x_j + \varepsilon \qquad \textbf{(S2)}$$

In this context, k denotes the number of independent variables, while C_0 represents the number of center points. Y corresponds to the predicted response, and b_0, b_i, b_{ii} and b_{ij} are the regression coefficients associated with the intercept, linear, quadratic, and interaction terms, respectively. X_i and X_j indicate the coded values of the factors, with k=5 in the present study. To validate the model, an analysis of variance (ANOVA) was performed to evaluate the statistical significance of the regression. 2D and 3D surface plots were then produced to identify the optimal running conditions for achieving high RhB elimination.

In detail, each Erlenmeyer beaker was loaded with ZIF-8 (50mg–90mg) and 100 mL of an organic dye solution (RhB) at the concentration from 5 mg/ L to 15 mg/L for the time from 5 min to 65 min under the agitation (450 rpm). Forty-four experiments for each model were randomly performed to determine the removal efficiency R (%) **Eq. (S3)** as follows:

$$\%R = \frac{C0 - Ct}{C0} * 100 \qquad \textbf{(S3)}$$

Note that C_o, and C_t are defined as initial, and RhB concentrations (mg/L) in solution at time t, respectively.

Table S1: Coded levels of Experimental variables used in the adsorption process.

Factor \ Level	-1	0	1
Pollutant dose ppm	**5**	**10**	**15**
Linker amount	**30**	**50**	**70**
pH	**4**	**7**	**10**
Contact time min	**5**	**35**	**65**
Catalyst weight mg	**50**	**70**	**90**

2.4.2. Photocatalytic process

The photocatalytic degradation of Rhodamine B was carried out as follows: 70 mg of ZIF-8 was dispersed in 100 mL of RhB solution (10 ppm) to prepare a suspension at neutral pH (7). The mixture was stirred in the dark for 1 h to establish adsorption–desorption equilibrium between the dye molecules and the ZIF-8 surface. Subsequently, the suspension was exposed to UV light while being continuously agitated with a magnetic stirrer. At predetermined intervals, 3 mL aliquots were withdrawn and centrifuged at 13400 rpm for 15 min to remove residual ZIF-8 particles. The progress of RhB photodegradation was monitored using a Shimadzu UV-2600 spectrophotometer by recording the absorbance within the 200–800 nm range. To determine the reactive species participating in the photocatalytic process, a series of scavenger experiments was conducted. The chemical reagents L-ascorbic acid, isopropanol (IPA), and ethylene diamine disodium tetra-acetate (EDTA) were employed to capture the reactive species $O_2^{\cdot-}$, OH· And h^+ respectively.

Table S2. Planned Experimental conditions for evaluating RhB Removal efficiency.

N°Exp	Pollutant dose	HmIM amount	pH	Contact time	Catalyst weight	Adsorption of RhB
	Ppm			Min	Mg	%
1	5.0000	30.0000	7.0000	35.0000	70.0000	77.8661
2	15.0000	30.0000	7.0000	35.0000	70.0000	58.2187
3	5.0000	70.0000	7.0000	35.0000	70.0000	92.9625
4	15.0000	70.0000	7.0000	35.0000	70.0000	82.8094
5	5.0000	50.0000	4.0000	35.0000	70.0000	90.4654
6	15.0000	50.0000	4.0000	35.0000	70.0000	74.5907
7	5.0000	50.0000	10.0000	35.0000	70.0000	86.6061
8	15.0000	50.0000	10.0000	35.0000	70.0000	72.7570
9	5.0000	50.0000	7.0000	5.0000	70.0000	77.9796
10	15.0000	50.0000	7.0000	5.0000	70.0000	71.7747
11	5.0000	50.0000	7.0000	65.0000	70.0000	87.9682
12	15.0000	50.0000	7.0000	65.0000	70.0000	77.3739
13	5.0000	50.0000	7.0000	35.0000	50.0000	79.9092
14	15.0000	50.0000	7.0000	35.0000	50.0000	59.2665
15	5.0000	50.0000	7.0000	35.0000	90.0000	91.7140
16	15.0000	50.0000	7.0000	35.0000	90.0000	84.4466
17	10.0000	30.0000	4.0000	35.0000	70.0000	52.8978
18	10.0000	70.0000	4.0000	35.0000	70.0000	92.4853
19	10.0000	30.0000	10.0000	35.0000	70.0000	64.7839
20	10.0000	70.0000	10.0000	35.0000	70.0000	94.0570
21	10.0000	30.0000	7.0000	5.0000	70.0000	60.6090
22	10.0000	70.0000	7.0000	5.0000	70.0000	82.5147

23	10.0000	30.0000	7.0000	65.0000	70.0000	51.1788
24	10.0000	70.0000	7.0000	65.0000	70.0000	83.7917
25	10.0000	30.0000	7.0000	35.0000	50.0000	51.0806
26	10.0000	70.0000	7.0000	35.0000	50.0000	81.5324
27	10.0000	30.0000	7.0000	35.0000	90.0000	63.5069
28	10.0000	70.0000	7.0000	35.0000	90.0000	90.4224
29	10.0000	50.0000	4.0000	5.0000	70.0000	79.0766
30	10.0000	50.0000	10.0000	5.0000	70.0000	80.1572
31	10.0000	50.0000	4.0000	65.0000	70.0000	84.1356
32	10.0000	50.0000	10.0000	65.0000	70.0000	83.1532
33	10.0000	50.0000	4.0000	35.0000	50.0000	76.1788
34	10.0000	50.0000	10.0000	35.0000	50.0000	73.8703
35	10.0000	50.0000	4.0000	35.0000	90.0000	85.0688
36	10.0000	50.0000	10.0000	35.0000	90.0000	83.8900
37	10.0000	50.0000	7.0000	5.0000	50.0000	74.3615
38	10.0000	50.0000	7.0000	65.0000	50.0000	68.8114
39	10.0000	50.0000	7.0000	5.0000	90.0000	83.5462
40	10.0000	50.0000	7.0000	65.0000	90.0000	89.7348
41	10.0000	50.0000	7.0000	35.0000	70.0000	84.4794
42	10.0000	50.0000	7.0000	35.0000	70.0000	84.4953
43	10.0000	50.0000	7.0000	35.0000	70.0000	84.4454
44	10.0000	50.0000	7.0000	35.0000	70.0000	84.4491

Table S3. ANOVA of Rh-B Adsorption efficiency (%).

Terms	Coefficient	T-Value	P-Value %
Constant C	84.46729	7018	< 0.01 ***
A	-6.51458	-1082.49	< 0.01 ***
B	13.77711	2289	< 0.01 ***

C	0.27349	45.44	< 0.01 ***
D	1.00801	167.49	< 0.01 ***
E	6.70743	1115	< 0.01 ***
A^2	-1.20695	-136.25	< 0.01 ***
B^2	-8.37291	-945.19	< 0.01 ***
C^2	-0.58487	-66.02	< 0.01 ***
D^2	-3.75208	-423.56	< 0.01 ***
E^2	-3.65433	-412.52	< 0.01 ***
AB	2.37355	197.20	< 0.01 ***
AC	0.50640	42.07	< 0.01 ***
BC	-2.57859	-214.23	< 0.01 ***
AD	-1.09736	-91.17	< 0.01 ***
BD	2.67682	222.40	< 0.01 ***
CD	-0.51572	-42.85	< 0.01 ***
AE	3.34383	277.81	< 0.01 ***
BE	-0.88409	-73.45	< 0.01 ***
CE	0.28242	23.46	0.0170 ***
DE	2.93467	243.82	< 0.01 ***

Table S4. Comparison of Different materials for rhodamine B adsorption.

Materials	Adsorption capacity q_{max} (mg/g)	References
Co@C	48	[2]
Zn/Co@C	101.93	
PVP/ZIF-8	73.6	[3]
PVP/ZIF-67	87.9	
P-CZIF-67 -867	137.1	
ZIF-8@ZIF-67	143.26	[4]
ZIF-8	56.40	
ZIF-67	81.63	
HTNT	6.6	[5]
ZIF-67	34.2	
HTNT@ZIF-67	84.2	
ZIF-8 70	91.74	this study

Table S5.1 ZIF-8 materials Reusability Cycles: Mean ± Standard Deviation

Sample	Cycle	Mean	Standard Deviation
	1st run	95.182	0.116
	2nd run	94.730	0.374
ZIF-8 30	3rd run	93.610	0.396

	4th run	89.100	0.248
	5th run	83.283	0.054
ZIF-8 50	1st run	94.383	0.097
	2nd run	93.923	0.207
	3rd run	93.531	0.249
	4th run	83.874	0.044
	5th run	80.628	0.344
ZIF-8 70	1st run	91.624	0.403
	2nd run	90.912	0.114
	3rd run	90.210	0.401
	4th run	81.928	0.455
	5th run	78.812	0.214

Table S5.2. ZIF-8 Photodegradation with Scavengers: Mean ± Standard Deviation

Sample	Condition	Mean	Standard Deviation
ZIF-8 30	Adsphotodecolorization	95.182	0.305
	No scavangers	89.650	0.035
	Isopropanol / OH°	15.731	0.132
	EDTA / h+	24.686	0.154
	L-asc (O2°-)	19.852	0.225
	Adsphotodecolorization	94.383	0.083
	No scavangers	70.188	0.215

	Isopropanol / OH°	22.896	0.181
	EDTA / h+	26.109	0.211
	L-asc (O2°-)	24.401	0.233
ZIF-8 70	Adsphotodecolorization	91.624	0.259
	No scavangers	26.336	0.266
	Isopropanol / OH°	27.827	0.201
	EDTA / h+	29.649	0.348
	L-asc (O2°-)	26.637	0.227

Table S6. competitive photodegradation for pollutants compared to ZIF-8 material.

Catalyst	Pollutant	Excitation source	Photocatalytic efficiency (%)	Ref.
ZIF-8/gC_3N_4	Congo red	Sunlight simulation	100	[6]
AgBr/ZIF-8	Methylene blue	UV-V irradiation	99.5	[7]
CeO2@ZIF-8	Methyl orange	UV light	99.81	[8]
ZIF-8@gC3N4	Rhodamine B	Light irradiation	99.8	[9]

ZIF-8/Ag2CO3/CF	Rhodamine B	UV-V irradiation	91	[10]
ZIF-8/BiFeO3	Rhodamine B	UV irradiation	High	[11]
CuPC/ZIF-8	Rhodamine B	UV-Visible light	95.04	[12]
ZIF-8@ZnAl LDP	Methyl orange	UV-Visible light	58	[13]
ZIF-8 30	Rhodamine B	UV irradiation	89.64	This work

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