

Supporting Information

Synthesis and application of Fe/Ni modified ZIF-8 as an environmentally friendly photocatalyst for methylene blue dye degradation under visible light

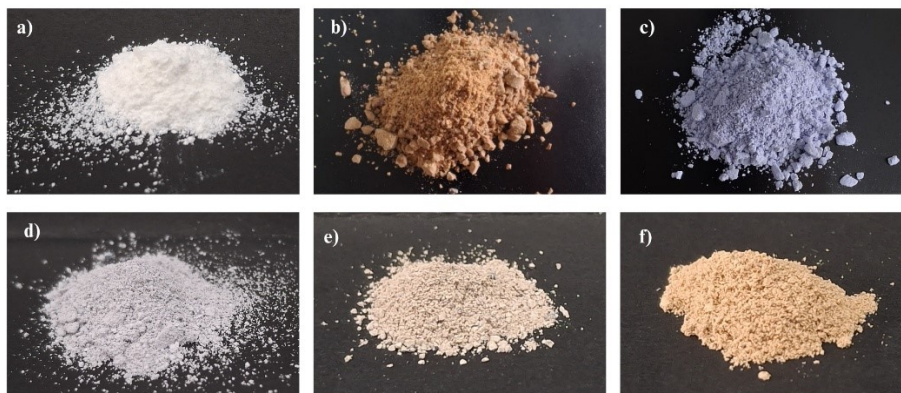


Fig. S1. Photographic images of (a) pristine ZIF-8 (white powder), (b) Fe@ZIF-8 (brownish-orange color), (c) Ni@ZIF-8 (dark bluish-gray hue), (d) Fe(5)/Ni(15)@ZIF-8 (light gray), (e) Fe(10)/Ni(10)@ZIF-8 (off-white), and (f) Fe(15)/Ni(5)@ZIF-8 (pale brown color).

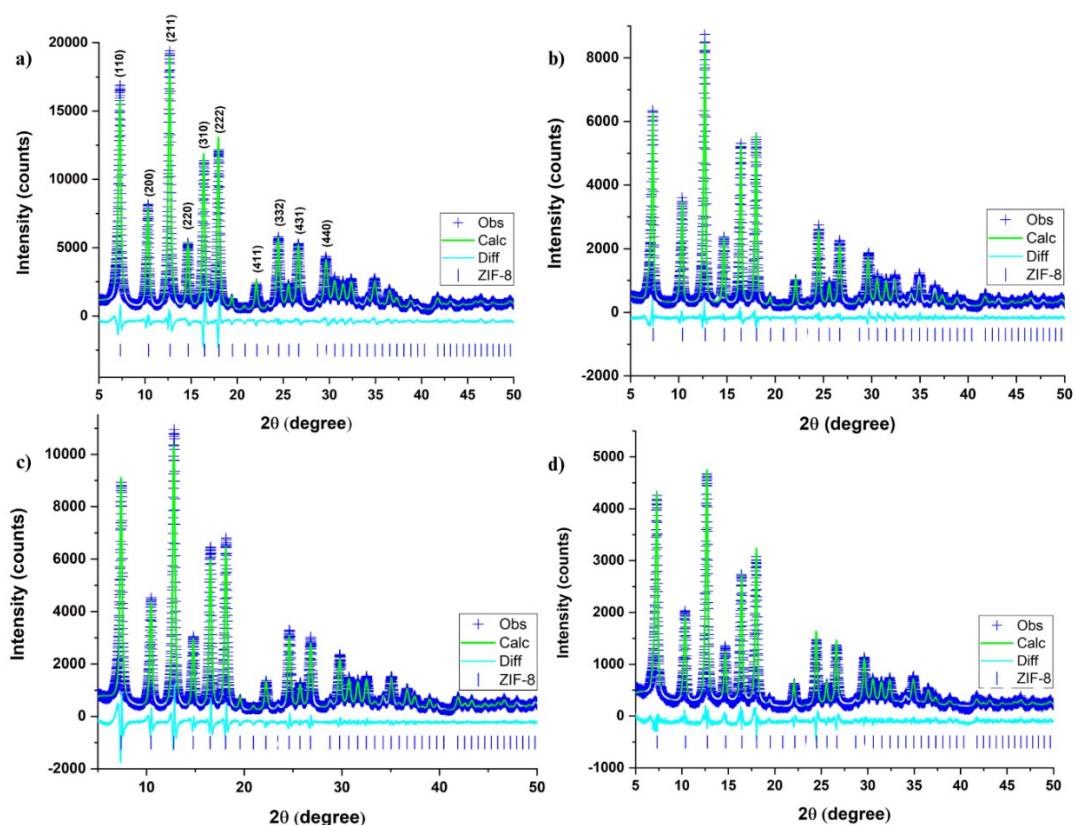


Fig. S2. XRD pattern from Le Bail refinement of (a) ZIF-8, (b) Fe(5)/Ni(15)@ZIF-8, (c) Fe(10)/Ni(10)@ZIF-8, and (d) Fe(15)/Ni(5)@ZIF-8

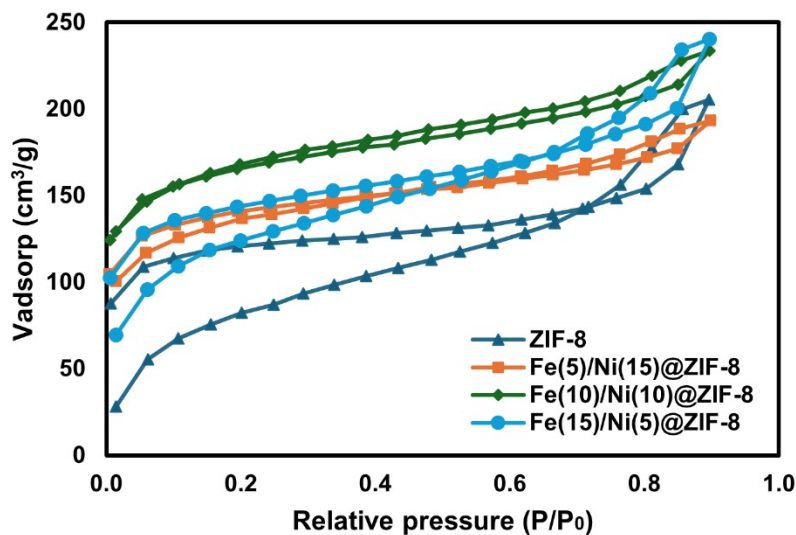


Fig. S3. N₂ adsorption-desorption isotherm of material photocatalysts

Table S1. Bond lengths and bond angles of the optimized structural model

a. Zn₄-MeIM₁₂

Parameter	Type	ZIF-8experimental	Zn ₄ calculate	Deviation
Bond lengths (Å)	Zn-N	1.98	2.00	1.12
	Fe-N			
	Ni-N			
	C1-N1	1.33	1.33	0.35
	C3-N1	1.37	1.36	0.37
	C1-C2	1.49	1.48	0.44
	C3=C4	1.34	1.36	1.17
Average deviation				0.69
Bond angles (°)	N-Zn-N	109.81	105.32	4.08
	N-Fe-N			
	N-Ni-N			
	C1-N1-C3	105.30	105.22	0.07
	N1-C3-C4	108.66	108.36	0.27
	N1-C3-H4	125.70	121.33	3.47
	N1-C1-C2	123.90	123.50	0.32
	C1-C2-H1	109.50	110.22	0.66
	H1-C2-H2	109.50	107.90	1.46
Average deviation				1.47

b. FeZn₃-MeIM₁₂

Parameter	Type	ZIF-8 _{experimental}	FeZn ₃ _{calculate}	Deviation
Bond lengths (Å)	Zn-N	1.98	1.99	0.32
	Fe-N		2.25	
	Ni-N			
	C1-N1	1.33	1.33	0.39
	C3-N1	1.37	1.36	0.29
	C1-C2	1.49	1.48	0.41
	C3=C4	1.34	1.36	1.15
Average deviation				0.51
Bond angles (°)	N-Zn-N	109.81	108.76	0.95
	N-Fe-N		109.36	
	N-Ni-N			
	C1-N1-C3	105.30	105.30	0.00
	N1-C3-C4	108.66	108.32	0.31
	N1-C3-H4	125.70	121.38	3.42
	N1-C1-C2	123.90	123.66	0.19
	C1-C2-H1	109.50	109.92	0.38
	H1-C2-H2	109.50	108.60	0.81
Average deviation				0.86

c. NiZn₃-MeIM₁₂

Parameter	Type	ZIF-8 _{experimental}	NiZn ₃ _{calculate}	Deviation
Bond lengths (Å)	Zn-N	1.98	2.01	1.35
	Fe-N			
	Ni-N		2.06	
	C1-N1	1.33	1.33	0.33
	C3-N1	1.37	1.36	0.36
	C1-C2	1.49	1.48	0.40
	C3=C4	1.34	1.36	1.16
Average deviation				0.72
Bond angles (°)	N-Zn-N	109.81	106.08	3.39
	N-Fe-N			
	N-Ni-N		130.53	
	C1-N1-C3	105.30	105.20	0.08
	N1-C3-C4	108.66	108.38	0.25
	N1-C3-H4	125.70	121.31	3.48
	N1-C1-C2	123.90	123.53	0.29
	C1-C2-H1	109.50	110.19	0.63
	H1-C2-H2	109.50	107.88	1.47
Average deviation				1.37

Table S2. AAS results showing the concentration of Fe, Ni, and Zn elements in MB solution before and after photodegradation using Fe/Ni@ZIF-8 photocatalyst.

Element	Sample	Abs	C (mg/L)	FP	C (mg/L)	Remarks
Fe	Before	0	-0.34494	5	-1.7247	ND
	After	0.002	-0.31177	1	-0.3118	ND
Ni	Before	0.002	-0.35179	5	-1.7589	ND
	After	0.164	2.541071	1	2.5411	Detected
Zn	Before	0.084	0.119726	5	0.5986	Detected
	After	1.244	1.849262	1	1.8493	Detected