

Electronic Supplementary Information

A machine learning-based nano-photocatalyst module for accelerating the design of Bi₂WO₆/MIL-53(Al) nanocomposites with enhanced photocatalytic activity

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Table S1 The dataset of BWO/MIL

No	Class	DR_{RhB}	R_{pH}	C_M	D_M	C_{HN}	S_{ur}	D_{sur}	V_{pH}	T_{stir}	T_{hyd}	T_{hy}	S_{ol}	T_{dry}	R_m
1	1	79	0	0	0	0.5	0	0.05	4	3	120	12	1	70	0.67
2	1	68	0	0	0	0.5	1	0.125	7	12	160	16	2	80	2
3	2	30	0	0	0	0.5	2	0.2	1	21	200	20	0	60	1.25
4*	2	31	0	0	1	0.5	0	0.05	7	12	200	20	0	60	1
5	2	2	0	0	1	0.5	1	0.125	1	21	120	12	1	70	0.5
6*	2	17	0	0	1	0.5	2	0.2	4	3	160	16	2	80	1.5
7	1	80	0	0	1	1.5	0	0.125	1	3	160	20	1	80	1.25
8	2	23	0	0	1	1.5	1	0.2	4	12	200	12	2	60	0.67
9	2	11	0	0	1	1.5	2	0.05	7	21	120	16	0	70	2
10	1	98	0	1	0	1.5	0	0.2	1	12	120	16	0	70	1.5
11	2	24	0	1	0	1.5	1	0.05	4	21	160	20	1	80	1
12	2	18	0	1	0	1.5	2	0.125	7	3	200	12	2	60	0.5
13	2	32	0	1	0	2.5	0	0.125	4	21	200	12	0	80	2
14	1	81	0	1	0	2.5	1	0.2	7	3	120	16	1	60	1.25
15	2	26	0	1	0	2.5	2	0.05	1	12	160	20	2	70	0.67
16	1	78	0	1	1	2.5	0	0.2	7	21	160	20	2	70	0.5
17	2	40	0	1	1	2.5	1	0.05	1	3	200	12	0	80	1.5
18	1	86	0	1	1	2.5	2	0.125	4	12	120	16	1	60	1
19	2	40	1	0	0	1.5	0	0.125	1	3	200	16	2	70	1
20	2	44	1	0	0	1.5	1	0.2	4	12	120	20	0	80	0.5
21	2	36	1	0	0	1.5	2	0.05	7	21	160	12	1	60	1.5
22*	2	43	1	0	0	2.5	0	0.2	7	21	200	16	1	80	0.67
23	2	28	1	0	0	2.5	1	0.05	1	3	120	20	2	60	2
24*	1	58	1	0	0	2.5	2	0.125	4	12	160	12	0	70	1.25
25	1	93	1	0	1	2.5	0	0.125	4	21	120	20	2	60	1.5
26	2	44	1	0	1	2.5	1	0.2	7	3	160	12	0	70	1

27	2	1	1	0	1	2.5	2	0.05	1	12	200	16	1	80	0.5
28	2	53	1	1	0	0.5	0	0.05	4	3	160	16	0	60	0.5
29*	2	26	1	1	0	0.5	1	0.125	7	12	200	20	1	70	1.5
30	2	53	1	1	0	0.5	2	0.2	1	21	120	12	2	80	1
31	1	69	1	1	1	0.5	0	0.05	7	12	120	12	2	80	1.25
32	2	9	1	1	1	0.5	1	0.125	1	21	160	16	0	60	0.67
33	2	16	1	1	1	0.5	2	0.2	4	3	200	20	1	70	2
34	1	95	1	1	1	1.5	0	0.2	1	12	160	12	1	60	2
35	2	29	1	1	1	1.5	1	0.05	4	21	200	16	2	70	1.25
36	2	41	1	1	1	1.5	2	0.125	7	3	120	20	0	80	0.67
37	1	87	0	1	1	2	0	0.1	4	6	120	12	1	60	1.5
38	1	73	0	1	1	3	0	0.2	4	12	120	12	1	60	0.67
39	1	81	0	1	1	4	0	0.3	4	24	120	12	1	60	1.25
40	1	74	0	1	1	3	0	0.1	4	6	140	12	1	60	0.67
41	1	76	0	1	1	4	0	0.2	4	12	140	12	1	60	1.25
42	1	82	0	1	1	2	0	0.3	4	24	140	12	1	60	1.5
43	1	57	0	1	1	2	0	0.1	4	12	160	12	1	60	1.25
44	1	63	0	1	1	3	0	0.2	4	24	160	12	1	60	1.5
45*	1	79	0	1	1	4	0	0.3	4	6	160	12	1	60	0.67
46*	1	89	0	1	1	4	0	0.1	4	24	120	12	1	60	0.67
47	1	88	0	1	1	2	0	0.2	4	6	120	12	1	60	1.25
48	1	77	0	1	1	3	0	0.3	4	12	120	12	1	60	1.5
49*	1	74	0	1	1	4	0	0.1	4	12	140	12	1	60	1.5
50	1	82	0	1	1	2	0	0.2	4	24	140	12	1	60	0.67
51	1	83	0	1	1	3	0	0.3	4	6	140	12	1	60	1.25
52	1	78	0	1	1	3	0	0.1	4	24	160	12	1	60	1.25
53	1	72	0	1	1	4	0	0.2	4	6	160	12	1	60	1.5
54	1	58	0	1	1	2	0	0.3	4	12	160	12	1	60	0.67
55	1	96	0	1	1	4	0	0.4	4	6	120	12	1	60	1.25

Table S2 Meanings of feature values in Table S1

Value	R_{pH}	C_M	D_M	S_{ur}	S_{ol}
0	NaOH	In oven	In vacuum	CTAB	H ₂ O
1	NH ₃ ·H ₂ O	Outdoor	In air	PVP	Glycol
2				SDS	Ethanol

Table S3 The new designed samples with higher DR_{RhB}

No	Class	DR_{RhB}	C_{HN}	S_{ur}	T_{hyd}	R_m	Fisher(1)
1	1	119.221	4	2	120	1.06	0.0323
2	1	119.216	4	2	120	1.05	0.0288
3	1	119.206	4	2	120	1.07	0.0357
4	1	119.191	4	2	120	1.04	0.0254
5	1	119.171	4	2	120	1.08	0.0391