Supporting Information for

Machine Learning-Driven Optimization of Plasma-Catalytic Dry Reforming of Methane

1. The training data set for the hybrid machine learning model

Table S1. Experimental dataset for plasma-catalytic DRM process

No.	Discharge power (W)	Total flow rate (mL/min)	CO_2/CH_4 molar ratio	Ni loading (wt%)
1	20	75	1	5
2	20	75	1	7.5
3	20	75	1	10
4	20	75	1	12.5
5	20	75	1	15
6	20	75	1.25	5
7	20	75	1.25	7.5
8	20	75	1.25	10
9	20	75	1.25	12.5
10	20	75	1.25	15
11	20	75	1.5	5
12	20	75	1.5	7.5
13	20	75	1.5	10
14	20	75	1.5	12.5
15	20	75	1.5	15
16	20	75	0.75	5
17	20	75	0.75	7.5
18	20	75	0.75	10
19	20	75	0.75	12.5
20	20	75	0.75	15
21	20	75	0.5	5
22	20	75	0.5	7.5
23	20	75	0.5	10
24	20	75	0.5	12.5
25	20	75	0.5	15
26	20	75	1	10
27	30	100	1.25	7.5
28	30	100	0.75	7.5
29	30	100	0.75	12.5
30	30	100	1.25	12.5
31	30	50	0.75	7.5
32	30	50	1.25	7.5
33	30	50	0.75	12.5
34	40	75	1.5	10
35	40	75	0.5	10
36	40	75	1	10
37	40	75	1	10
38	40	75	1	15
39	40	25	0.5	5

40	40	25	0.5	7.5
41	40	25	0.5	10
42	40	25	0.5	12.5
43	40	25	0.5	15
44	40	25	0.75	5
45	40	25	0.75	7.5
46	40	25	0.75	10
47	40	25	0.75	12.5
48	40	25	0.75	15
49	40	25	1.5	5
50	40	25	1.5	7.5
51	40	25	1.5	10
52	40	25	1.5	12.5
53	40	25	1.5	15
54	40	25	1.25	5
55	40	25	1.25	7.5
56	40	25	1.25	10
57	40	25	1.25	12.5
58	40	25	1.25	15
59	40	25	1	5
60	40	25	1	7.5
61	40	25	1	10
62	40	25	1	12.5
63	40	25	1	15
64	40	125	0.5	7.5
65	40	125	0.75	7.5
66	40	125	1	7.5
67	40	125	1.25	7.5
68	40	125	1.5	7.5
69	40	125	0.5	15
70	40	125	0.75	15
71	40	125	1	15
72	40	125	1.25	15
73	40	125	1.5	15
74	40	125	0.5	5
75	40	125	0.75	5
76	40	125	1	5
77	40	125	1.25	5
78	40	125	1.5	5
79	40	125	0.5	12.5
80	40	125	0.75	12.5
81	40	125	1	12.5
82	40	125	1.25	12.5
83	40	125	1.5	12.5

84	40	125	0.5	10
85	40	125	0.75	10
86	40	125	1	10
87	40	125	1.25	10
88	40	125	1.5	10
89	40	75	1	15
90	50	50	1.25	7.5
91	50	100	0.75	12.5
92	50	100	0.75	7.5
93	50	50	0.75	7.5
94	50	100	1.25	7.5
95	50	100	1.25	12.5
96	50	50	1.25	12.5
97	60	75	1	7.5
98	60	75	1.5	7.5
99	60	75	1	10
100	60	75	0.5	10

Table S2. Comparison of experimental results and model predictions under the same operating parameters

No.	Experimental data				Model predictions			
	CO_2 conversion (%)	CH_4 conversion (%)	CO yield (%)	H_2 yield (%)	CO_2 conversion (%)	CH_4 conversion (%)	CO yield (%)	H_2 yield (%)
1	13.3	20.1	8.4	6.5	16.1	20.4	8.5	7.4
2	14.8	21.4	9.5	7.2	18.6	23.6	12.3	8.6
3	15.2	21.0	9.9	7.4	13.9	21.8	11.6	8.1
4	14.5	19.0	9.3	7.0	15.4	19.6	10.0	8.0
5	12.8	15.4	7.9	6.1	12.8	15.8	7.3	6.0
6	11.7	25.0	9.8	7.9	11.7	24.9	8.1	7.8
7	13.3	25.7	11.0	8.6	13.1	26.1	10.4	8.1
8	13.7	24.9	11.3	8.7	14.7	25.7	10.8	8.1
9	13.1	22.4	10.7	8.3	13.5	23.2	9.1	8.0
10	11.3	18.4	9.3	7.4	10.6	18.6	7.8	7.7
11	9.7	29.5	11.0	9.1	9.5	29.1	12.6	9.0
12	11.3	29.8	12.1	9.7	11.7	29.2	12.6	9.4
13	11.8	28.5	12.3	9.9	12.2	27.5	11.8	10.0
14	11.2	25.6	11.7	9.4	10.8	25.2	11.6	9.3
15	9.4	21.0	10.3	8.5	9.9	19.8	11.3	8.4
16	14.4	15.0	6.5	4.9	15.1	14.5	5.8	4.9
17	15.9	16.6	7.7	5.6	16.3	16.5	7.0	5.7
18	16.3	16.7	8.1	5.8	15.9	16.3	6.5	6.4
19	15.6	15.2	7.6	5.5	16.1	15.4	9.0	5.1

20	13.8	12.0	6.2	4.6	13.9	10.7	6.1	5.1
21	15.1	9.4	4.3	3.1	14.7	8.8	4.9	3.9
22	16.6	11.6	5.6	3.9	15.3	11.2	5.6	3.8
23	16.9	12.1	6.0	4.1	16.9	12.4	5.4	4.0
24	16.2	11.0	5.5	3.8	16.9	11.0	6.4	3.9
25	14.3	8.4	4.1	3.0	14.4	7.7	4.2	3.1
26	15.5	21.0	9.8	7.3	14.9	21.2	11.4	7.5
27	11.4	22.5	9.8	7.4	10.8	22.6	9.2	8.1
28	14.0	14.2	6.7	4.7	13.0	14.7	7.6	4.6
29	13.7	14.2	6.6	4.6	13.2	14.2	5.3	4.3
30	11.2	20.6	9.5	7.2	11.7	21.5	8.2	6.5
31	23.5	26.2	10.9	9.3	23.3	26.3	10.1	9.5
32	19.7	37.1	14.7	12.5	20.1	36.2	13.7	11.7
33	23.0	24.3	10.7	9.0	23.3	24.0	11.2	8.5
34	15.8	37.8	15.4	12.8	16.3	37.5	14.0	12.5
35	23.3	19.4	8.4	6.9	22.9	20.1	9.7	7.1
36	20.5	29.3	12.6	10.2	20.4	28.8	13.3	11.1
37	20.5	29.3	12.6	10.2	20.2	29.4	12.0	10.1
38	17.8	24.8	10.6	8.9	13.5	19.4	8.3	7.2
39	33.7	29.8	12.8	12.0	33.1	30.4	12.9	12.2
40	34.9	31.6	13.9	12.6	33.6	30.3	13.6	12.9
41	35.1	31.7	14.2	12.7	33.6	32.1	14.2	12.1
42	34.1	30.3	13.6	12.2	33.3	31.3	12.6	12.5
43	32.0	27.2	12.1	11.3	33.0	27.1	13.0	11.4
44	31.8	37.2	15.4	14.1	31.0	38.1	14.3	14.5
45	33.1	38.5	16.5	14.7	35.1	39.3	16.4	15.5
46	33.2	38.2	16.8	14.7	31.3	37.5	15.0	15.3
47	32.3	36.3	16.2	14.3	32.7	35.8	15.9	14.5
48	30.2	32.8	14.7	13.2	31.5	33.0	15.5	13.6
49	23.5	57.3	21.3	19.3	22.7	56.3	23.4	19.5
50	24.8	57.2	22.3	19.8	25.7	57.9	21.0	20.1
51	25.1	55.5	22.5	19.8	25.5	54.5	23.1	20.2
52	24.2	52.2	21.8	19.2	22.7	51.6	22.2	19.9
53	22.3	47.3	20.2	18.1	23.7	46.1	20.3	18.0
54	26.7	50.9	19.7	17.7	25.1	50.9	21.0	17.6
55	28.0	51.3	20.8	18.3	27.2	51.0	20.3	18.7
56	28.2	50.1	20.9	18.3	28.0	50.3	22.7	18.8
57	27.3	47.3	20.3	17.7	28.1	47.8	20.9	18.2
58	25.4	42.8	18.7	16.6	24.9	41.9	18.4	17.3
59	29.5	44.2	17.8	16.0	28.2	44.5	16.0	15.6
60	30.8	45.1	18.8	16.6	29.8	43.9	17.4	16.1
61	31.0	44.3	19.0	16.6	31.7	44.1	18.8	16.2
62	30.0	41.9	18.4	16.1	31.0	41.4	18.9	16.0
63	28.0	38.0	16.9	15.0	28.1	38.3	18.1	15.5

64	11.6	7.9	2.6	1.5	12.1	8.2	3.8	1.9
65	10.9	12.1	4.6	3.1	10.8	12.1	6.0	2.7
66	9.9	15.9	6.2	4.4	9.5	15.5	5.5	4.7
67	8.4	19.4	7.5	5.6	7.6	18.4	7.9	5.6
68	6.4	22.6	8.5	6.5	5.6	22.6	9.8	6.5
69	9.5	9.0	1.3	0.8	9.2	8.5	1.3	1.0
70	9.0	11.8	3.2	2.2	9.2	11.4	4.8	2.6
71	8.0	14.3	4.8	3.5	8.3	14.3	3.9	4.3
72	6.6	16.5	6.0	4.5	7.3	14.9	5.5	3.9
73	4.7	18.3	6.8	5.4	4.3	19.3	7.7	5.6
74	10.1	4.3	1.3	0.7	10.1	3.3	0.9	0.5
75	9.4	8.9	3.3	2.3	9.8	7.1	2.3	3.1
76	8.3	13.2	5.0	3.6	8.3	13.1	7.4	3.5
77	6.8	17.2	6.3	4.8	6.0	17.3	6.8	5.1
78	4.8	20.9	7.3	5.8	4.9	21.4	8.4	5.7
79	11.3	10.2	2.6	1.6	11.4	9.7	2.7	2.2
80	10.7	13.5	4.5	3.1	10.6	13.0	3.7	3.1
81	9.7	16.5	6.1	4.3	10.6	16.9	4.9	5.0
82	8.3	19.1	7.3	5.4	8.1	18.5	6.8	6.0
83	6.4	21.3	8.2	6.3	6.1	21.0	8.7	6.6
84	12.0	9.8	3.0	1.8	11.8	8.2	2.9	2.0
85	11.4	13.6	5.0	3.3	10.9	13.9	6.0	3.4
86	10.4	17.0	6.6	4.6	10.2	18.0	6.6	4.1
87	8.9	20.0	7.9	5.7	8.5	20.8	7.8	6.0
88	7.0	22.8	8.8	6.7	7.6	23.7	10.9	6.7
89	18.1	25.4	11.0	9.0	17.4	24.2	10.8	9.6
90	26.5	48.4	20.5	17.4	26.8	47.4	21.5	17.8
91	18.6	23.0	8.6	6.8	17.4	23.3	8.2	7.1
92	19.0	21.9	8.8	7.0	18.3	22.2	10.5	7.1
93	31.6	36.4	16.5	14.0	33.0	35.8	17.3	14.1
94	15.2	31.1	12.2	9.8	14.7	30.7	12.9	10.5
95	14.9	30.4	11.9	9.5	14.6	30.2	10.9	8.7
96	25.9	45.8	20.1	16.9	26.5	45.1	18.9	17.0
97	26.7	40.3	17.5	14.4	27.6	41.6	18.7	14.2
98	20.8	50.7	20.7	17.2	21.7	51.7	21.4	17.7
99	27.0	41.0	17.8	14.4	27.9	40.0	18.9	14.5
100	31.0	30.1	13.2	11.0	32.0	29.6	11.8	10.6

2. Genetic algorithm optimization results

Genetic algorithm (GA) is a metaheuristic algorithm inspired by the principles of evolution and natural selection process in biology. In each epoch, combinations of hyperparameters with the best fitness undergo crossover to minimize the mean square error (MSE) and ultimately determine the optimal hyperparameters for the model. The details of this process are shown in Fig. S1.

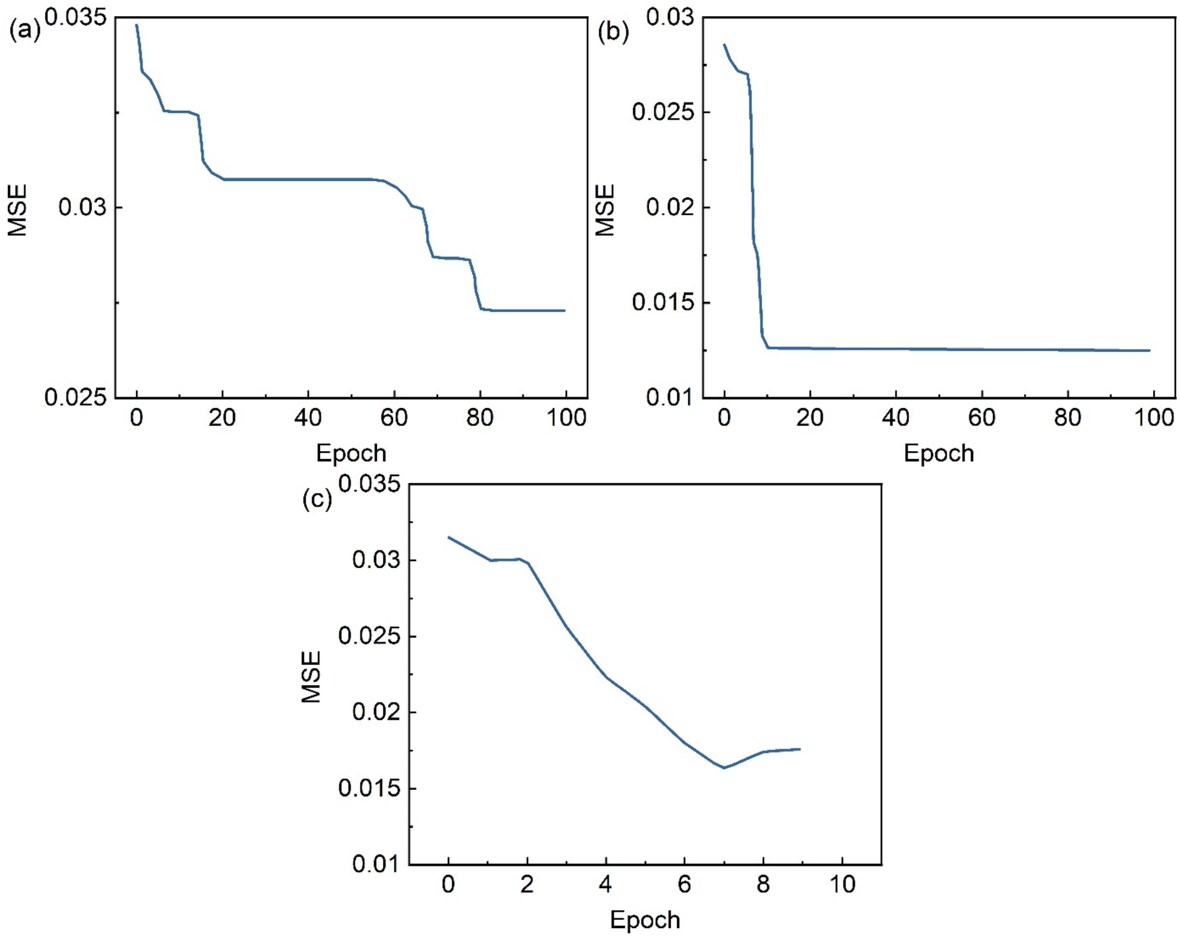

Fig. S1. MSE of the best fitness value in each epoch of the genetic algorithm optimization for: (a) ANN; (b) SVR; (c) RT.

3. Comparative analysis of the predicted and experimental results.

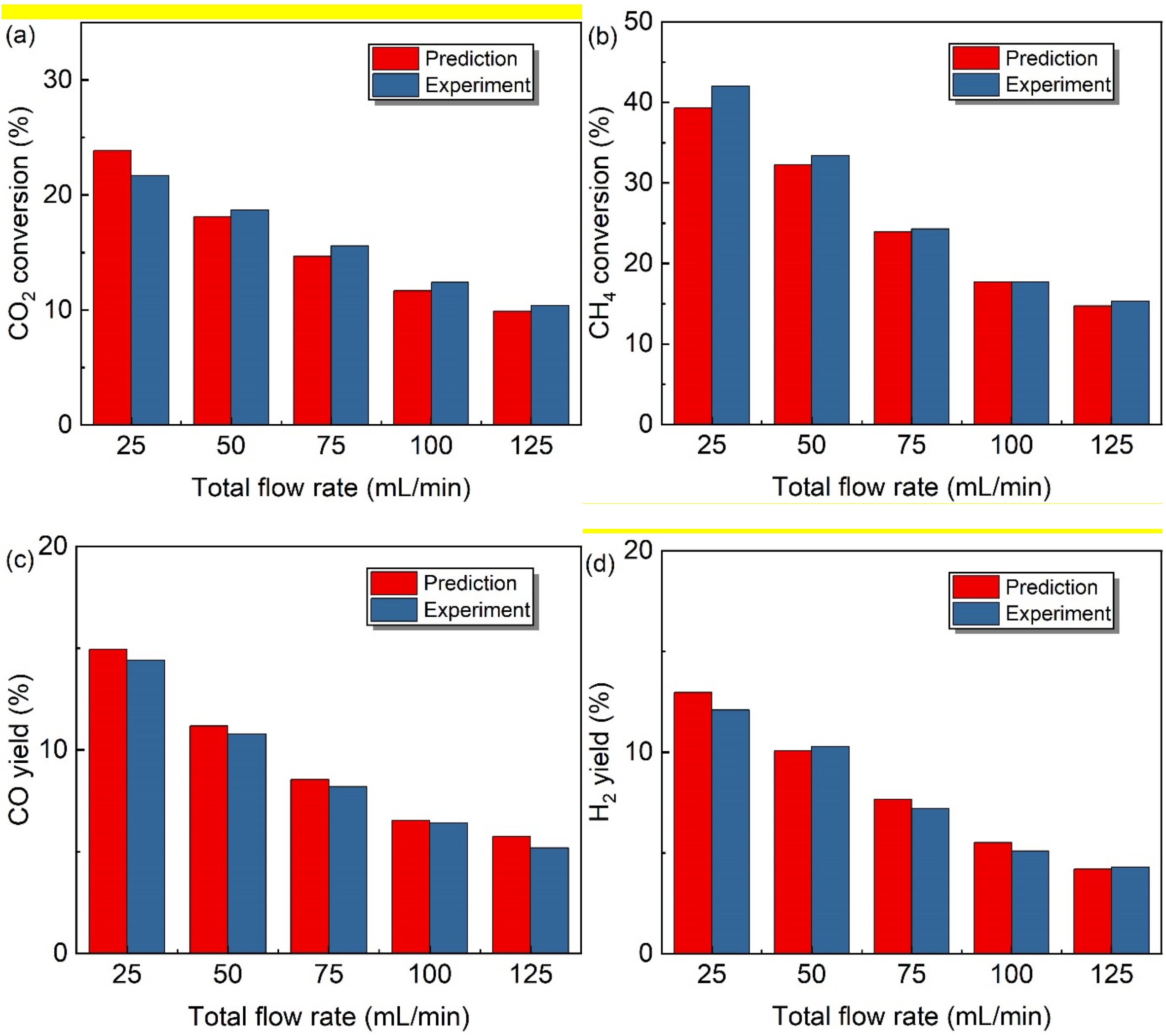

Fig. S2. Comparison of predicted values and unseen experimental data for model generalization evaluation: (a) CO_2 conversion; (b) CH_4 conversion; (c) CO yield; and (d) H_2 yield. (Ni loading = 7.5 wt%, CO_2/CH_4 = 1:1, discharge power = 30 W)

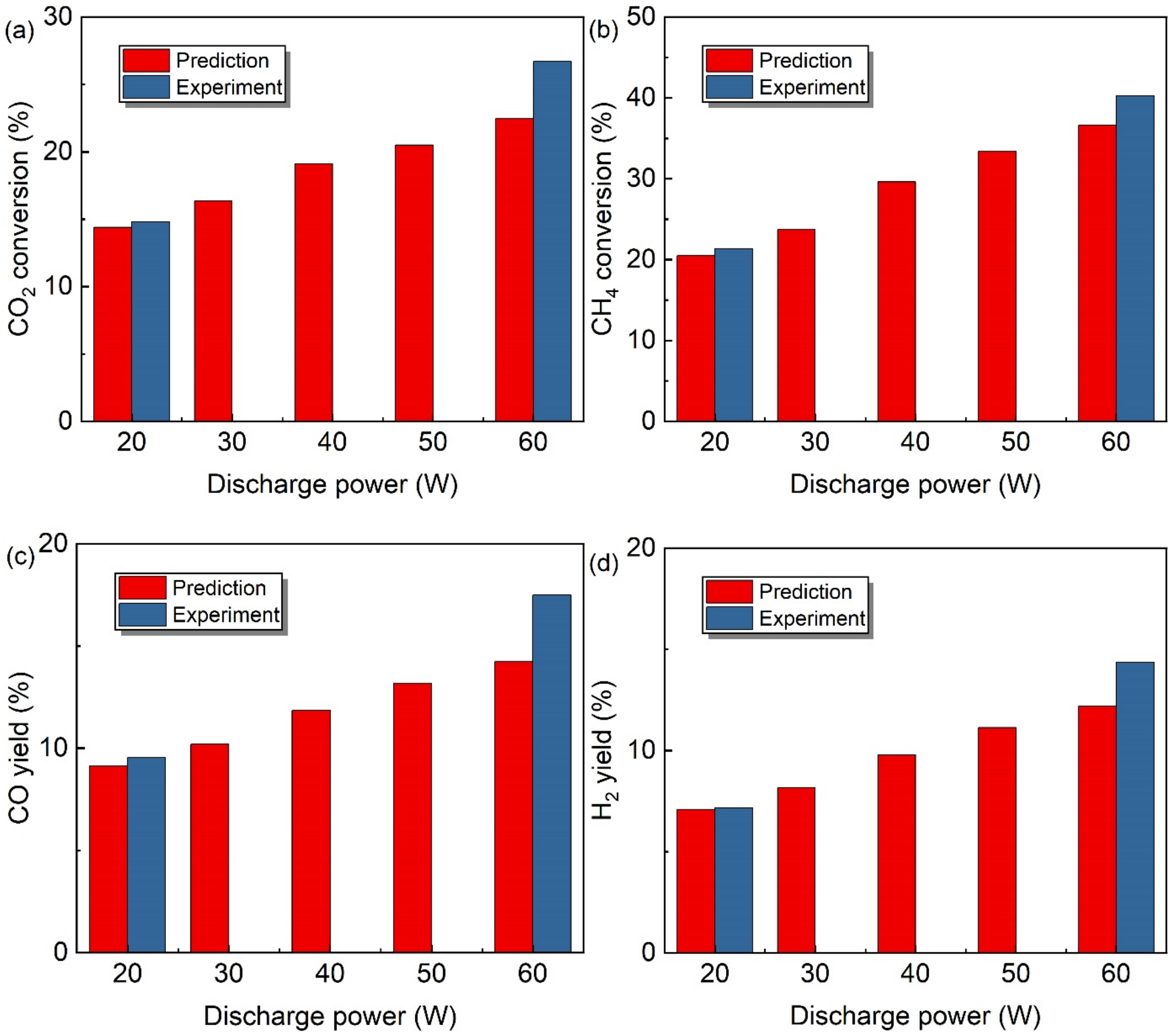

Fig. S3. Comparison of predicted values with available experimental data for key performance metrics: (a) CO_2 conversion; (b) CH_4 conversion; (c) CO yield; and (d) H_2 yield. (Ni loading = 7.5 wt%, CO_2/CH_4 = 1:1, total flow rate = 75 mL/min)

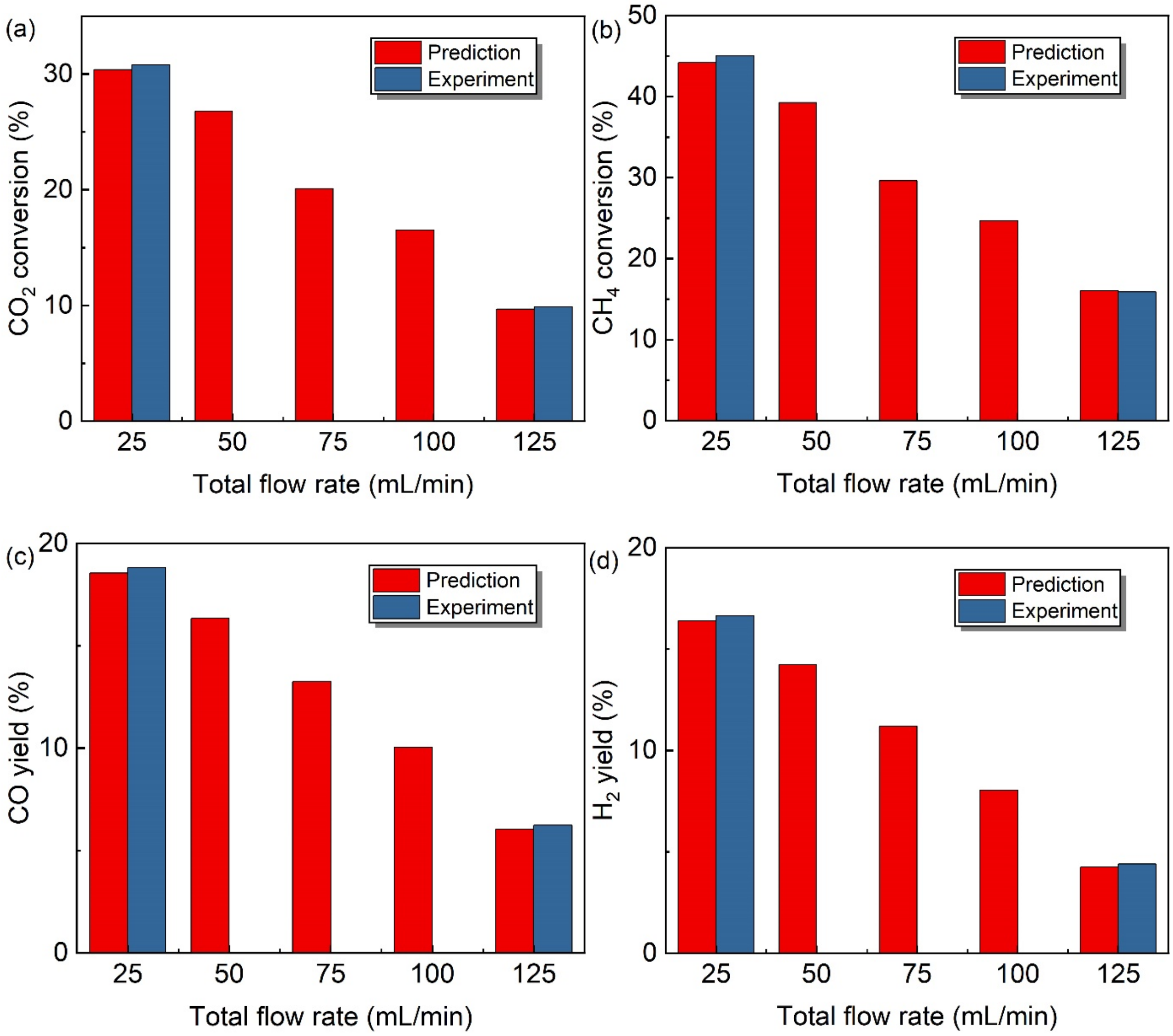

Fig. S4. Comparison of predicted values with available experimental data for key performance metrics: (a) CO_2 conversion; (b) CH_4 conversion; (c) CO yield; and (d) H_2 yield. (Ni loading = 7.5 wt%, CO_2/CH_4 = 1:1, discharge power = 40 W)

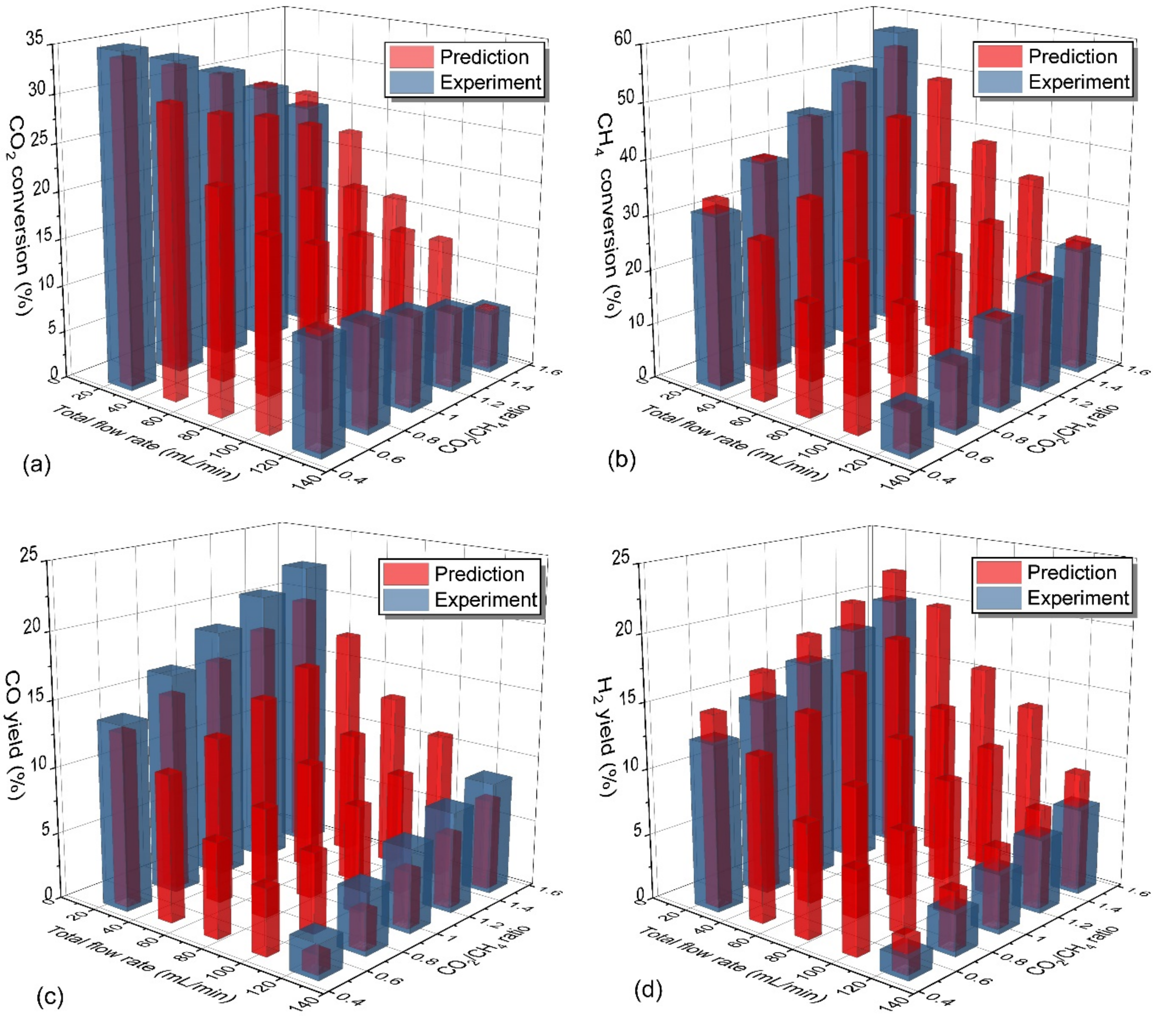

Fig. S5. Comparison of three-way predictions with available experimental results: (a) CO_2 conversion; (b) CH_4 conversion; (c) CO yield; and (d) H_2 yield. (Ni loading = 7.5 wt%, discharge power = 40 W)