

+Supporting Information (B): Detailed information of the original dataset

Machine learning-aided catalyst screening and multi-objective optimization for the indirect CO₂ hydrogenation to methanol and ethylene glycol process

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Table S1. Compiled experimental input-output data for the hydrogenation of ethylene carbonate to methanol and ethylene glycol through PCA and feature engineering improvements.

S. No	Data points	Inputs										Outputs										Reference
		Catalyst type	Cu load	Promoter	Content of promoter metal	Promoter	Content of promoter metal	Support type	Preparation method	Specific surface area	Calcination temperature	Preparation conditions	Reaction temperature	Reaction pressure	WHSV	THF	Solvent type	Conversion rate of EC	Yield of EG	Yield of MEG		
1		Cu-CuSO ₄ ·2H ₂ O	22	None	0	None	0	SiO ₂ -C	AE	201.3	450	350	180	3	0.63	100	THF	0.9998	0.986	0.8391	[1]	
2		Cu-CuSO ₄ ·2H ₂ O	22	None	0	None	0	SiO ₂ -C	AE	201.3	450	350	180	3	0.63	100	THF	0.9998	0.9896	0.8296	[1]	
3		Cu-CuSO ₄ ·2H ₂ O	22	None	0	None	0	SiO ₂ -C	AE	201.3	450	350	200	3	0.63	100	THF	1	0.8833	0.7782	[1]	
4		Cu-CuSO ₄ ·2H ₂ O	22	None	0	None	0	SiO ₂ -C	AE	201.3	450	350	180	3	0.105	100	THF	0.9998	0.7816	0.7633	[1]	
5		Cu-CuSO ₄ ·2H ₂ O	22	None	0	None	0	SiO ₂ -C	AE	201.3	450	350	180	3	0.105	100	THF	0.9998	0.8307	0.8009	[1]	
7		Cu-CuSO ₄ ·2H ₂ O	22	None	0	None	0	SiO ₂ -C	AE	201.3	450	350	180	3	0.315	100	THF	0.9985	0.8733	0.8609	[1]	
8		Cu-CuSO ₄ ·2H ₂ O	22	None	0	None	0	SiO ₂ -C	AE	201.3	450	350	180	3	0.42	100	THF	0.9983	0.895	0.7999	[1]	
9		Cu-CuSO ₄ ·2H ₂ O	22	None	0	None	0	SiO ₂ -C	AE	201.3	450	350	180	3	0.525	100	THF	0.9981	0.9006	0.8129	[1]	
10		Cu-CuSO ₄ ·2H ₂ O	22	None	0	None	0	SiO ₂ -C	AE	201.3	450	350	180	3	0.735	100	THF	0.9994	0.9003	0.7834	[1]	
11		Cu-CuSO ₄ ·2H ₂ O	22	None	0	None	0	SiO ₂ -C	AE	201.3	450	350	180	3	0.84	100	THF	0.9992	0.9006	0.8131	[1]	
12		Cu-CuSO ₄ ·2H ₂ O	22	None	0	None	0	SiO ₂ -C	AE	201.3	450	350	180	3	0.945	100	THF	0.9973	0.8963	0.7814	[1]	
13		Cu-CuSO ₄ ·2H ₂ O	22	None	0	None	0	SiO ₂ -C	AE	201.3	450	350	180	3	0.63	50	THF	1	0.9287	0.7944	[1]	
14		Cu-CuSO ₄ ·2H ₂ O	22	None	0	None	0	SiO ₂ -C	AE	201.3	450	350	180	3	0.63	150	THF	0.9963	0.9663	0.8256	[1]	
15		Cu-CuSO ₄ ·2H ₂ O	22	None	0	None	0	SiO ₂ -C	AE	201.3	450	350	180	3	0.63	200	THF	0.9996	0.9814	0.8488	[1]	
16		Cu-CuSO ₄ ·2H ₂ O	22	None	0	None	0	SiO ₂ -C	AE	201.3	450	350	180	3	0.175	100	THF	0.9988	0.888	0.7853	[1]	
17		Cu-CuSO ₄ ·2H ₂ O	22	None	0	None	0	SiO ₂ -C	AE	201.3	450	350	180	3	0.265	100	THF	0.9985	0.8856	0.8073	[1]	
18		Cu-CuSO ₄ ·2H ₂ O	22	None	0	None	0	SiO ₂ -C	AE	201.3	450	350	180	3	0.3475	100	THF	0.9996	0.8865	0.8055	[1]	
19		Cu-CuSO ₄ ·2H ₂ O	22	None	0	None	0	SiO ₂ -C	AE	201.3	450	350	180	3	0.4725	100	THF	0.9996	0.9055	0.8093	[1]	
20		Cu-CuSO ₄ ·2H ₂ O	22	None	0	None	0	SiO ₂ -C	AE	201.3	450	350	180	3	0.5775	100	THF	0.9998	0.9479	0.8274	[1]	
21		Cu-CuSO ₄ ·2H ₂ O	22	None	0	None	0	SiO ₂ -C	AE	201.3	450	350	180	3	0.6825	100	THF	0.9998	0.9453	0.8165	[1]	
22		Cu-CuSO ₄ ·2H ₂ O	22	None	0	None	0	SiO ₂ -C	AE	201.3	450	350	180	3	0.7875	100	THF	0.9993	0.9053	0.802	[1]	
23		Cu-CuSO ₄ ·2H ₂ O	22	None	0	None	0	SiO ₂ -C	AE	201.3	450	350	180	3	0.8925	100	THF	0.9998	0.9054	0.8029	[1]	
24		Cu-CuSO ₄ ·2H ₂ O	22	None	0	None	0	SiO ₂ -C	AE	201.3	450	350	180	3	0.63	62.6	THF	0.9997	0.9334	0.7953	[1]	
25		Cu-CuSO ₄ ·2H ₂ O	22	None	0	None	0	SiO ₂ -C	AE	201.3	450	350	180	3	0.63	74.5	THF	0.9997	0.929	0.7967	[1]	
26		Cu-CuSO ₄ ·2H ₂ O	22	None	0	None	0	SiO ₂ -C	AE	201.3	450	350	180	3	0.63	86.81	THF	0.9998	0.9454	0.7982	[1]	
27		Cu-CuSO ₄ ·2H ₂ O	22	None	0	None	0	SiO ₂ -C	AE	201.3	450	350	180	3	0.63	112.54	THF	0.9999	0.9623	0.8082	[1]	
28		Cu-CuSO ₄ ·2H ₂ O	22	None	0	None	0	SiO ₂ -C	AE	201.3	450	350	180	3	0.63	123.6	THF	0.9999	0.9759	0.8338	[1]	
29		Cu-CuSO ₄ ·2H ₂ O	22	None	0	None	0	SiO ₂ -C	AE	201.3	450	350	180	3	0.63	138.16	THF	0.9999	0.9868	0.8208	[1]	
30		Cu-CuSO ₄ ·2H ₂ O	22	None	0	None	0	SiO ₂ -C	AE	201.3	450	350	180	3	0.63	149.3	THF	0.9999	0.9866	0.8321	[1]	
31		Cu-CuSO ₄ ·2H ₂ O	22	None	0	None	0	SiO ₂ -C	AE	201.3	450	350	180	3	0.63	175.11	THF	0.9999	0.9884	0.8377	[1]	
32		Cu-CuSO ₄ ·2H ₂ O	22	None	0	None	0	SiO ₂ -C	AE	201.3	450	350	180	3	0.63	187.85	THF	0.9999	0.9836	0.8433	[1]	
33		Cu-CuSO ₄ ·2H ₂ O	22	None	0	None	0	SiO ₂ -C	AE	201.3	450	350	172	2.6	0.63	100	THF	0.9945	0.8064		[1]	
34		Cu-CuSO ₄ ·2H ₂ O	22	None	0	None	0	SiO ₂ -C	AE	201.3	450	350	174.71	3	0.63	100	THF	0.9993	0.9576	0.8157	[1]	
35		Cu-CuSO ₄ ·2H ₂ O	22	None	0	None	0	SiO ₂ -C	AE	201.3	450	350	177.26	3	0.63	100	THF	0.9971	0.9704	0.8258	[1]	
36		Cu-CuSO ₄ ·2H ₂ O	22	None	0	None	0	SiO ₂ -C	AE	201.3	450	350	182.11	3	0.63	100	THF	0.9991	0.9819	0.8319	[1]	
37		Cu-CuSO ₄ ·2H ₂ O	22	None	0	None	0	SiO ₂ -C	AE	201.3	450	350	184.86	3	0.63	100	THF	0.9998	0.9565	0.8319	[1]	
38		Cu-CuSO ₄ ·2H ₂ O	22	None	0	None	0	SiO ₂ -C	AE	201.3	450	350	187.35	3	0.63	100	THF	0.9998	0.9435	0.8291	[1]	
39		Cu-CuSO ₄ ·2H ₂ O	22	None	0	None	0	SiO ₂ -C	AE	201.3	450	350	192.42	3	0.63	100	THF	0.9997	0.9437	0.8353	[1]	
40		Cu-CuSO ₄ ·2H ₂ O	22	None	0	None	0	SiO ₂ -C	AE	201.3	450	350	195.02	3	0.63	100	THF	0.9994	0.9056	0.8014	[1]	
41		Cu-CuSO ₄ ·2H ₂ O	22	None	0	None	0	SiO ₂ -C	AE	201.3	450	350	197.4	3	0.63	100	THF	0.9997	0.915	0.7787	[1]	
42		CuSO ₂	31.2	None	0	None	0	SiO ₂	AE	489	450	300	180	3	1	180	1,4-dioxane	0.9735	0.9568	0.7206	[2]	
43		CuSO ₂	31.2	None	0	None	0	SiO ₂	AE	489	450	300	180	3	0.81	180	1,4-dioxane	0.9251	0.9262	0.6964	[2]	
44		CuSO ₂	31.2	None	0	None	0	SiO ₂	AE	489	450	300	180	3	1.5	180	1,4-dioxane	0.8602	0.846	0.6794	[2]	
45		uMe-CuSO ₂	30.6	Mo	0.1	None	0	SiO ₂	AE-IWI	465	500	300	180	3	0.75	180	1,4-dioxane	1	0.9888	0.7619	[2]	
46		uMe-CuSO ₂	30.6	Mo	0.1	None	0	SiO ₂	AE-IWI	465	500	300	180	3	1.25	180	1,4-dioxane	0.9902	0.9909	0.7559	[2]	
47		uMe-CuSO ₂	30.6	Mo	0.1	None	0	SiO ₂	AE-IWI	465	500	300	180	3	1.5	180	1,4-dioxane	0.9814	0.9821	0.7333	[2]	
48		uMe-CuSO ₂	30.6	Mo	0.1	None	0	SiO ₂	AE-IWI	465	500	300	180	3	1.5	180	1,4-dioxane	0.9547	0.9455	0.7041	[2]	
49		uMe-CuSO ₂	30.6	Mo	0.1	None	0	SiO ₂	AE-IWI	465	500	300	180	3	2	180	1,4-dioxane	0.8847	0.8759	0.6155	[2]	
50		uMe-CuSO ₂	30.2	Mo	0.49	None	0	SiO ₂	AE-IWI	448	500	300	180	3	0.75	180	1,4-dioxane	0.9997	0.998	0.7958	[2]	
51		uMe-CuSO ₂	30.2	Mo	0.49	None	0	SiO ₂	AE-IWI	448	500	300	180	3	1	180	1,4-dioxane	1	0			

186	xPu-CuSiO2	41.2	Pt	0.12	None	0	SiO2	AE-IWI	578	350	350	180	3	1	120	1.4-dioxane	0.9945	0.9704	0.9725	[6]
187	xPu-CuSiO2	41.2	Pt	0.12	None	0	SiO2	AE-IWI	578	350	350	180	3	1	130	1.4-dioxane	0.9945	0.9704	0.9725	[6]
188	xPu-CuSiO2	41.2	Pt	0.12	None	0	SiO2	AE-IWI	578	350	350	180	3	1	150	1.4-dioxane	0.9971	0.9737	0.9761	[6]
189	xPu-CuSiO2	41.2	Pt	0.12	None	0	SiO2	AE-IWI	578	350	350	180	3	1	160	1.4-dioxane	0.9971	0.9732	0.9785	[6]
190	xPu-CuSiO2	41.2	Pt	0.12	None	0	SiO2	AE-IWI	578	350	350	180	3	1	170	1.4-dioxane	0.9971	0.9732	0.9807	[6]
191	xPu-CuSiO2	40	Pt	0.21	None	0	SiO2	AE-IWI	569	350	350	180	3	1	70	1.4-dioxane	0.9874	0.9636	0.9201	[6]
192	xPu-CuSiO2	40	Pt	0.21	None	0	SiO2	AE-IWI	569	350	350	180	3	1	80	1.4-dioxane	0.9874	0.9647	0.8902	[6]
193	xPu-CuSiO2	40	Pt	0.21	None	0	SiO2	AE-IWI	569	350	350	180	3	1	90	1.4-dioxane	0.9874	0.9636	0.8614	[6]
194	xPu-CuSiO2	40	Pt	0.21	None	0	SiO2	AE-IWI	569	350	350	180	3	1	110	1.4-dioxane	0.9874	0.9676	0.8243	[6]
195	xPu-CuSiO2	40	Pt	0.21	None	0	SiO2	AE-IWI	569	350	350	180	3	1	120	1.4-dioxane	0.9874	0.9676	0.8128	[6]
196	xPu-CuSiO2	40	Pt	0.21	None	0	SiO2	AE-IWI	569	350	350	180	3	1	130	1.4-dioxane	0.9873	0.9679	0.8073	[6]
197	xPu-CuSiO2	40	Pt	0.21	None	0	SiO2	AE-IWI	569	350	350	180	3	1	150	1.4-dioxane	0.9902	0.9704	0.7906	[6]
198	xPu-CuSiO2	40	Pt	0.21	None	0	SiO2	AE-IWI	569	350	350	180	3	1	160	1.4-dioxane	0.9926	0.9723	0.7079	[6]
199	xPu-CuSiO2	40	Pt	0.21	None	0	SiO2	AE-IWI	569	350	350	180	3	1	170	1.4-dioxane	0.9952	0.9747	0.7068	[6]
200	xPu-CuSiO2	41.9	Pt	0.48	None	0	SiO2	AE-IWI	518	350	350	180	3	1	70	1.4-dioxane	0.9555	0.9295	0.8232	[6]
201	xPu-CuSiO2	41.9	Pt	0.48	None	0	SiO2	AE-IWI	518	350	350	180	3	1	80	1.4-dioxane	0.9555	0.9295	0.7978	[6]
202	xPu-CuSiO2	41.9	Pt	0.48	None	0	SiO2	AE-IWI	518	350	350	180	3	1	90	1.4-dioxane	0.9601	0.9332	0.7736	[6]
203	xPu-CuSiO2	41.9	Pt	0.48	None	0	SiO2	AE-IWI	518	350	350	180	3	1	110	1.4-dioxane	0.9641	0.9381	0.7343	[6]
204	xPu-CuSiO2	41.9	Pt	0.48	None	0	SiO2	AE-IWI	518	350	350	180	3	1	120	1.4-dioxane	0.9641	0.9381	0.7229	[6]
205	xPu-CuSiO2	41.9	Pt	0.48	None	0	SiO2	AE-IWI	518	350	350	180	3	1	130	1.4-dioxane	0.9641	0.9381	0.7112	[6]
206	xPu-CuSiO2	41.9	Pt	0.48	None	0	SiO2	AE-IWI	518	350	350	180	3	1	150	1.4-dioxane	0.9711	0.9482	0.6999	[6]
207	xPu-CuSiO2	41.9	Pt	0.48	None	0	SiO2	AE-IWI	518	350	350	180	3	1	160	1.4-dioxane	0.9711	0.9482	0.6827	[6]
208	xPu-CuSiO2	41.9	Pt	0.48	None	0	SiO2	AE-IWI	518	350	350	180	3	1	170	1.4-dioxane	0.9718	0.9481	0.6748	[6]
209	xPu-CuSiO2	41.9	Pt	0.48	None	0	SiO2	AE-IWI	518	350	350	180	3	1	180	1.4-dioxane	0.9718	0.9481	0.6666	[6]
210	CuSiO2	41.8	None	0	None	0	SiO2	AE	582	350	350	180	3	1	1	1.4-dioxane	0.9567	0.9311	0.8773	[6]
211	CuSiO2	41.8	None	0	None	0	SiO2	AE	582	350	350	180	3	1	55	1.4-dioxane	0.9682	0.942	0.8259	[6]
212	xPu-CuSiO2	41.2	Pt	0.12	None	0	SiO2	AE-IWI	578	350	350	180	3	1	45	1.4-dioxane	0.9157	0.892	0.8124	[6]
213	xPu-CuSiO2	41.2	Pt	0.12	None	0	SiO2	AE-IWI	578	350	350	180	3	1	50	1.4-dioxane	0.9406	0.9161	0.8408	[6]
214	xPu-CuSiO2	41.2	Pt	0.12	None	0	SiO2	AE-IWI	578	350	350	180	3	1	55	1.4-dioxane	0.9659	0.9405	0.8702	[6]
215	xPu-CuSiO2	40	Pt	0.21	None	0	SiO2	AE-IWI	569	350	350	180	3	1	45	1.4-dioxane	0.9477	0.9204	0.8469	[6]
216	xPu-CuSiO2	40	Pt	0.21	None	0	SiO2	AE-IWI	569	350	350	180	3	1	50	1.4-dioxane	0.961	0.939	0.8796	[6]
217	xPu-CuSiO2	40	Pt	0.21	None	0	SiO2	AE-IWI	569	350	350	180	3	1	55	1.4-dioxane	0.9748	0.9522	0.9146	[6]
218	xPu-CuSiO2	41.9	Pt	0.48	None	0	SiO2	AE-IWI	518	350	350	180	3	1	45	1.4-dioxane	0.8899	0.8756	0.7793	[6]
219	xPu-CuSiO2	41.9	Pt	0.48	None	0	SiO2	AE-IWI	518	350	350	180	3	1	50	1.4-dioxane	0.9164	0.8923	0.8014	[6]
220	xPu-CuSiO2	41.9	Pt	0.48	None	0	SiO2	AE-IWI	518	350	350	180	3	1	55	1.4-dioxane	0.9343	0.9045	0.824	[6]
221	CuSiO2-S	24.8	None	0	None	0	SiO2-S	AE	55	450	300	180	3	0.3	120	1.4-dioxane	0.8812	0.8731	0.5596	[7]
222	CuSiO2-S	24.8	None	0	None	0	SiO2-S	AE	55	450	300	180	3	0.3	140	1.4-dioxane	0.9793	0.9689	0.6291	[7]
223	CuSiO2-S	24.8	None	0	None	0	SiO2-S	AE	55	450	300	180	3	0.3	160	1.4-dioxane	0.9999	0.9688	0.6688	[7]
224	CuSiO2-S	24.8	None	0	None	0	SiO2-S	AE	55	450	300	180	3	0.3	180	1.4-dioxane	0.9999	0.9697	0.6507	[7]
225	CuSiO2-S	24.8	None	0	None	0	SiO2-S	AE	55	450	300	180	3	0.3	200	1.4-dioxane	0.9999	0.9699	0.6442	[7]
226	CuSiO2-F-3	17.8	None	0	None	0	SiO2-F-3	OSHP	112	450	300	180	3	0.3	10	1.4-dioxane	0.8444	0.8444	0.4704	[7]
227	CuSiO2-F-3	17.8	None	0	None	0	SiO2-F-3	OSHP	112	450	300	180	3	0.3	100	1.4-dioxane	0.9694	0.9616	0.6458	[7]
228	CuSiO2-F-3	17.8	None	0	None	0	SiO2-F-3	OSHP	112	450	300	180	3	0.3	120	1.4-dioxane	0.9851	0.9774	0.6614	[7]
229	CuSiO2-F-3	17.8	None	0	None	0	SiO2-F-3	OSHP	112	450	300	180	3	0.3	140	1.4-dioxane	0.9989	0.9923	0.6585	[7]
230	CuSiO2-F-3	17.8	None	0	None	0	SiO2-F-3	OSHP	112	450	300	180	3	0.3	160	1.4-dioxane	0.9995	0.9914	0.6335	[7]
231	CuSiO2-F-3	17.8	None	0	None	0	SiO2-F-3	OSHP	112	450	300	180	3	0.3	180	1.4-dioxane	0.9995	0.9908	0.6299	[7]
232	CuSiO2-F-3	17.8	None	0	None	0	SiO2-F-3	OSHP	112	450	300	180	3	0.3	200	1.4-dioxane	0.9999	0.9983	0.6144	[7]
233	CuSiO2-F-3.3	19.1	None	0	None	0	SiO2-F-3.3	OSHP	105	450	300	180	3	0.3	60	1.4-dioxane	0.7948	0.7748	0.4861	[7]
234	CuSiO2-F-3.3	19.1	None	0	None	0	SiO2-F-3.3	OSHP	105	450	300	180	3	0.3	80	1.4-dioxane	0.9555	0.9317	0.8039	[7]
235	CuSiO2-F-3.3	19.1	None	0	None	0	SiO2-F-3.3	OSHP	105	450	300	180	3	0.3	100	1.4-dioxane	0.9996	0.9909	0.6997	[7]
236	CuSiO2-F-3.3	19.1	None	0	None	0	SiO2-F-3.3	OSHP	105	450	300	180	3	0.3	120	1.4-dioxane	0.9996	0.9906	0.677	[7]
237	CuSiO2-F-3.3	19.1	None	0	None	0	SiO2-F-3.3	OSHP	105	450	300	180	3	0.3	140	1.4-dioxane	0.9912	0.9012	0.6898	[7]
238	CuSiO2-F-3.3	19.1	None	0	None	0	SiO2-F-3.3	OSHP	105	450	300	180	3	0.3	160	1.4-dioxane	0.9995	0.9906	0.6874	[7]
239	CuSiO2-F-3.3	19.1	None	0	None	0	SiO2-F-3.3	OSHP	105	450	300	180	3	0.3	180	1.4-dioxane	0.9998	0.9899	0.6717	[7]
240	CuSiO2-F-3.3	19.1	None	0	None	0	SiO2-F-3.3	OSHP	105	450	300	180	3	0.3	200	1.4-dioxane	0.9999	0.9919	0.6573	[7]
241	CuSiO2-F-3.35	23.3	None	0	None	0	SiO2-F-3.35	OSHP	97	450	300	180	3	0.3	60	1.4-dioxane	0.9791	0.97	0.7291	[7]
242	CuSiO2-F-3.35	23.3	None	0	None	0	SiO2-F-3.35	OSHP	97	450	300	180	3	0.3	80	1.4-dioxane	0.9984	0.9804	0.742	[7]
243	CuSiO2-F-3.35	23.3	None	0	None	0	SiO2-F-3.35	OSHP	97	450	300	180	3	0.3	100	1.4-dioxane	0.9996	0.9904	0.7199	[7]
244	CuSiO2-F-3.35	23.3	None	0	None	0	SiO2-F-3.35	OSHP	97	450	300	180	3	0.3	120	1.4-dioxane	0.9999	0.9902	0.7261	[7]
245	CuSiO2-F-3.35	23.3	None	0	None	0	SiO2-F-3.35	OSHP	97	450	300	180	3	0.3	140	1.4-dioxane	0.9999	0.9908	0.7149	[7]
246	CuSiO2-F-3.35	23.3	None	0	None	0	SiO2-F-3.35	OSHP	97	450	300	180	3	0.3	160	1.4-dioxane	0.9999	0.9915	0.7081	[7]
247	CuSiO2-F-3.35	23.3	None	0	None	0	SiO2-F-3.35	OSHP	97	450	300	180	3	0.3	180	1.4-dioxane	0.9995	0.9912	0.71	[7]
248	CuSiO2-F-3.35	23.3	None	0	None	0	SiO2-F-3.35	OSHP	97	450	300	180	3	0.3	200	1.4-dioxane	0.9914	0.9014	0.72	[7]
249	CuSiO2-S	24.8	None	0	None	0	SiO2-S	AE	55	450	300	180	3	0.3	130	1.4-dioxane	0.9336	0.9249	0.5993	[7]
250	CuSiO2-S	24.8	None	0	None	0	SiO2-S	AE	55	450	300	180	3	0.3	150	1.4-dioxane	0.9903	0.9808	0.6529	[7]
251	CuSiO2-S	24.8	None	0	None	0	SiO2-S	AE	55	450	300	180	3	0.3	170	1.4-dioxane	0.9993	0.9903	0.6405	[7]
252	CuSiO2-S	24.8	None	0	None	0	SiO2-S	AE	55	450	300	180	3	0.3	190	1.4-dioxane	0.9996	0.9896	0.6474	[7]
253	CuSiO2-F-3	17.8	None	0	None	0	SiO2-F-3	OSHP	112	450	300	180	3	0.3	90	1.4-dioxane	0.9116	0.9046	0.5623	[7]
254	CuSiO2-F-3	17.8	None	0	None	0	SiO2-F-3	OSHP	112	450	300	180	3	0.3	110	1.4-dioxane	0.9778	0.9706	0.6454	[7]
255	CuSiO2-F-3	17.8	None	0	None	0	SiO2-F-3													

376	Ni-CuSiO2-AE	29.8	Ni	1.61	None	0	SiO2	AE	551	400	350	170	3	0.6	60	1,4-dioxane	0.7266	0.7103	0.3774	[9]
377	Ni-CuSiO2-AE	29.8	Ni	1.61	None	0	SiO2	AE	551	400	350	170	3	0.6	80	1,4-dioxane	0.8353	0.8163	0.466	[9]
378	Ni-CuSiO2-AE	29.8	Ni	1.61	None	0	SiO2	AE	551	400	350	170	3	0.6	100	1,4-dioxane	0.9623	0.9432	0.5353	[9]
379	Ni-CuSiO2-AE	29.8	Ni	1.61	None	0	SiO2	AE	551	400	350	170	3	0.6	120	1,4-dioxane	0.9875	0.9668	0.5429	[9]
380	Ni-CuSiO2-AE	29.8	Ni	1.61	None	0	SiO2	AE	551	400	350	170	3	0.6	140	1,4-dioxane	0.9915	0.9669	0.6136	[9]
381	CuSiO2	32.2	None	0	None	0	SiO2	AE	534	400	350	170	3	0.6	50	1,4-dioxane	0.858	0.8411	0.6373	[9]
382	CuSiO2	32.2	None	0	None	0	SiO2	AE	534	400	350	170	3	0.6	70	1,4-dioxane	0.9118	0.8941	0.6723	[9]
383	CuSiO2	32.2	None	0	None	0	SiO2	AE	534	400	350	170	3	0.6	90	1,4-dioxane	0.9661	0.9439	0.7395	[9]
384	CuSiO2	32.2	None	0	None	0	SiO2	AE	534	400	350	170	3	0.6	110	1,4-dioxane	0.9919	0.9711	0.7532	[9]
385	CuSiO2	32.2	None	0	None	0	SiO2	AE	534	400	350	170	3	0.6	130	1,4-dioxane	0.9955	0.9754	0.7172	[9]
386	Ni-CuSiO2-AE	30.3	Ni	0.23	None	0	SiO2	AE	538	400	350	170	3	0.6	50	1,4-dioxane	0.8701	0.8487	0.7387	[9]
387	Ni-CuSiO2-AE	30.3	Ni	0.23	None	0	SiO2	AE	538	400	350	170	3	0.6	70	1,4-dioxane	0.9037	0.8807	0.8799	[9]
388	Ni-CuSiO2-AE	30.3	Ni	0.23	None	0	SiO2	AE	538	400	350	170	3	0.6	90	1,4-dioxane	0.9968	0.9729	0.8009	[9]
389	Ni-CuSiO2-AE	30.3	Ni	0.23	None	0	SiO2	AE	538	400	350	170	3	0.6	110	1,4-dioxane	0.998	0.9742	0.7426	[9]
390	Ni-CuSiO2-AE	30.3	Ni	0.23	None	0	SiO2	AE	538	400	350	170	3	0.6	130	1,4-dioxane	0.9966	0.973	0.7079	[9]
391	Ni-CuSiO2-IE	30.9	Ni	0.23	None	0	SiO2	IE	529	400	350	170	3	0.6	50	1,4-dioxane	0.9336	0.9178	0.5794	[9]
392	Ni-CuSiO2-IE	30.9	Ni	0.23	None	0	SiO2	IE	529	400	350	170	3	0.6	70	1,4-dioxane	0.966	0.9475	0.6221	[9]
393	Ni-CuSiO2-IE	30.9	Ni	0.23	None	0	SiO2	IE	529	400	350	170	3	0.6	90	1,4-dioxane	0.9832	0.9649	0.6268	[9]
394	Ni-CuSiO2-IE	30.9	Ni	0.23	None	0	SiO2	IE	529	400	350	170	3	0.6	110	1,4-dioxane	0.9919	0.9714	0.647	[9]
395	Ni-CuSiO2-IE	30.9	Ni	0.23	None	0	SiO2	IE	529	400	350	170	3	0.6	130	1,4-dioxane	0.9922	0.9678	0.6524	[9]
396	Ni-CuSiO2-IM	29.7	Ni	0.21	None	0	SiO2	IM	494	400	350	170	3	0.6	50	1,4-dioxane	0.9588	0.939	0.6952	[9]
397	Ni-CuSiO2-IM	29.7	Ni	0.21	None	0	SiO2	IM	494	400	350	170	3	0.6	70	1,4-dioxane	0.9948	0.9706	0.675	[9]
398	Ni-CuSiO2-IM	29.7	Ni	0.21	None	0	SiO2	IM	494	400	350	170	3	0.6	90	1,4-dioxane	0.9968	0.9731	0.643	[9]
399	Ni-CuSiO2-IM	29.7	Ni	0.21	None	0	SiO2	IM	494	400	350	170	3	0.6	110	1,4-dioxane	0.9982	0.9768	0.6152	[9]
400	Ni-CuSiO2-IM	29.7	Ni	0.21	None	0	SiO2	IM	494	400	350	170	3	0.6	130	1,4-dioxane	0.9972	0.9732	0.6041	[9]
401	Ni-CuSiO2-AE	29.5	Ni	0.09	None	0	SiO2	AE	614	400	350	170	3	0.6	50	1,4-dioxane	0.9501	0.9273	0.7285	[9]
402	Ni-CuSiO2-AE	29.5	Ni	0.09	None	0	SiO2	AE	614	400	350	170	3	0.6	70	1,4-dioxane	0.9967	0.9694	0.9336	[9]
403	Ni-CuSiO2-AE	29.5	Ni	0.09	None	0	SiO2	AE	614	400	350	170	3	0.6	90	1,4-dioxane	0.9975	0.9694	0.8559	[9]
404	Ni-CuSiO2-AE	29.5	Ni	0.09	None	0	SiO2	AE	614	400	350	170	3	0.6	110	1,4-dioxane	0.9977	0.9698	0.7723	[9]
405	Ni-CuSiO2-AE	29.5	Ni	0.09	None	0	SiO2	AE	614	400	350	170	3	0.6	130	1,4-dioxane	0.9968	0.9699	0.7614	[9]
406	Ni-CuSiO2-AE	30.8	Ni	0.42	None	0	SiO2	AE	551	400	350	170	3	0.6	50	1,4-dioxane	0.9468	0.9263	0.7005	[9]
407	Ni-CuSiO2-AE	30.8	Ni	0.42	None	0	SiO2	AE	551	400	350	170	3	0.6	70	1,4-dioxane	0.9898	0.9676	0.7563	[9]
408	Ni-CuSiO2-AE	30.8	Ni	0.42	None	0	SiO2	AE	551	400	350	170	3	0.6	90	1,4-dioxane	0.9953	0.9733	0.7333	[9]
409	Ni-CuSiO2-AE	30.8	Ni	0.42	None	0	SiO2	AE	551	400	350	170	3	0.6	110	1,4-dioxane	0.9971	0.973	0.7151	[9]
410	Ni-CuSiO2-AE	30.8	Ni	0.42	None	0	SiO2	AE	551	400	350	170	3	0.6	130	1,4-dioxane	0.9949	0.9647	0.677	[9]
411	Ni-CuSiO2-AE	29.8	Ni	1.61	None	0	SiO2	AE	551	400	350	170	3	0.6	50	1,4-dioxane	0.6465	0.6302	0.3112	[9]
412	Ni-CuSiO2-AE	29.8	Ni	1.61	None	0	SiO2	AE	551	400	350	170	3	0.6	70	1,4-dioxane	0.7831	0.766	0.4222	[9]
413	Ni-CuSiO2-AE	29.8	Ni	1.61	None	0	SiO2	AE	551	400	350	170	3	0.6	90	1,4-dioxane	0.9803	0.982	0.5011	[9]
414	Ni-CuSiO2-AE	29.8	Ni	1.61	None	0	SiO2	AE	551	400	350	170	3	0.6	110	1,4-dioxane	0.9733	0.9544	0.5374	[9]
415	Ni-CuSiO2-AE	29.8	Ni	1.61	None	0	SiO2	AE	551	400	350	170	3	0.6	130	1,4-dioxane	0.9886	0.9668	0.5778	[9]
416	CuSiO2	60	None	0	None	0	SiO2	DP	72	450	350	180	2	0.13	100	1,4-dioxane	0.9853	0.967	0.2953	[10]
417	Cu-MgSiO2	56.9	Mg	3.1	None	0	SiO2	DP	56	450	350	180	2	0.13	100	1,4-dioxane	0.9951	0.9892	0.3294	[10]
418	Cu-MgSiO2	56.7	Mg	3.3	None	0	SiO2	DP	56	450	350	180	3	0.13	100	1,4-dioxane	0.9889	0.9779	0.3472	[10]
419	Cu-MgSiO2	56.9	Mg	3.1	None	0	SiO2	DP	56	450	350	180	3	0.13	100	1,4-dioxane	0.993	0.984	0.4226	[10]
420	Cu-MgSiO2	57.3	Mg	2.7	None	0	SiO2	DP	56	450	350	180	3	0.13	100	1,4-dioxane	0.993	0.986	0.4805	[10]
421	Cu-MgSiO2	57.6	Mg	2.4	None	0	SiO2	DP	56	450	350	180	3	0.13	100	1,4-dioxane	0.995	0.9859	0.3333	[10]
422	48-Mg1/2ZrSiO	53.3	Mg	2.5	Zr	4.2	SiO2	DP	82	450	350	180	3	0.13	100	1,4-dioxane	0.992	0.986	0.499	[10]
423	48-Mg1/2ZrSiO	53	Mg	2.5	Zr	4.5	SiO2	DP	82	450	350	180	3	0.13	100	1,4-dioxane	0.9901	0.9803	0.6476	[10]
424	48-Mg1/2ZrSiO	52.9	Mg	2.5	Zr	4.6	SiO2	DP	82	450	350	180	3	0.13	100	1,4-dioxane	0.992	0.986	0.5128	[10]
425	48-Mg1/2ZrSiO	52.8	Mg	2.5	Zr	4.7	SiO2	DP	82	450	350	180	3	0.13	100	1,4-dioxane	0.992	0.986	0.4773	[10]
426	CuSiO2	60	None	0	None	0	SiO2	DP	72	450	350	180	3	0.13	100	1,4-dioxane	0.9928	0.982	0.4483	[10]
427	48-Mg1/2ZrSiO	53	Mg	2.5	Zr	4.5	SiO2	DP	82	450	350	180	3	0.13	100	1,4-dioxane	0.9921	0.9824	0.2988	[10]
428	48-Mg1/2ZrSiO	53	Mg	2.5	Zr	4.5	SiO2	DP	82	400	350	180	3	0.13	100	1,4-dioxane	0.9902	0.9785	0.336	[10]
429	48-Mg1/2ZrSiO	53	Mg	2.5	Zr	4.5	SiO2	DP	82	500	350	180	3	0.13	100	1,4-dioxane	0.9882	0.9785	0.3949	[10]
430	48-Mg1/2ZrSiO	53	Mg	2.5	Zr	4.5	SiO2	DP	82	550	350	180	3	0.13	100	1,4-dioxane	0.9902	0.9785	0.3762	[10]
431	48-Mg1/2ZrSiO	53	Mg	2.5	Zr	4.5	SiO2	DP	82	450	300	180	3	0.13	100	1,4-dioxane	0.9897	0.9806	0.2479	[10]
432	48-Mg1/2ZrSiO	53	Mg	2.5	Zr	4.5	SiO2	DP	82	450	400	180	3	0.13	100	1,4-dioxane	0.9975	0.9795	0.2002	[10]
433	48-Mg1/2ZrSiO	53	Mg	2.5	Zr	4.5	SiO2	DP	82	450	450	180	3	0.13	100	1,4-dioxane	0.9918	0.9817	0.1792	[10]
434	48-Mg1/2ZrSiO	53	Mg	2.5	Zr	4.5	SiO2	DP	82	450	350	160	3	0.13	100	1,4-dioxane	0.9921	0.9734	0.2473	[10]
435	48-Mg1/2ZrSiO	53	Mg	2.5	Zr	4.5	SiO2	DP	82	450	350	190	3	0.13	100	1,4-dioxane	0.9901	0.9794	0.436	[10]
436	48-Mg1/2ZrSiO	53	Mg	2.5	Zr	4.5	SiO2	DP	82	450	350	200	3	0.13	100	1,4-dioxane	0.9901	0.98028	0.4272	[10]
437	48-Mg1/2ZrSiO	53	Mg	2.5	Zr	4.5	SiO2	DP	82	450	350	180	2	0.13	100	1,4-dioxane	0.992	0.9821	0.4781	[10]
438	48-Mg1/2ZrSiO	53	Mg	2.5	Zr	4.5	SiO2	DP	82	450	350	180	4	0.13	100	1,4-dioxane	0.99	0.9801	0.79	[10]
439	48-Mg1/2ZrSiO	53	Mg	2.5	Zr	4.5	SiO2	DP	82	450	350	180	4	0.13	100	1,4-dioxane	0.7538	0.7463	0.3765	[10]
440	48-Mg1/2ZrSiO	53	Mg	2.5	Zr	4.5	SiO2	DP	82	450	350	180	4	0.13	135	1,4-dioxane	0.8999	0.8999	0.4964	[10]
441	48-Mg1/2ZrSiO	53	Mg	2.5	Zr	4.5	SiO2	DP	82	450	350	180	4	0.065	100	1,4-dioxane	0.888	0.8781	0.3095	[10]
442	48-Mg1/2ZrSiO	53	Mg	2.5	Zr	4.5	SiO2	DP	82	450	350	180	4	0.195	100	1,4-dioxane	0.992	0.9821	0.5379	[10]
443	48-Mg1/2ZrSiO	53	Mg	2.5	Zr	4.5	SiO2	DP	82	450	350	180	4	0.26	100	1,4-dioxane	0.992	0.9821	0.4881	[10]
444	3u-MgO/SBA-15	18.3	MgO	0	None	0	SBA-15	AE	474	400	300	180	3	0.5	200	1,4-dioxane	0.994	0.9585	0.6	

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