

Supporting Information

C-H and C-C bonds activation of propane to propylene and ethylene selectivity assisted by CO₂ over titania catalysts

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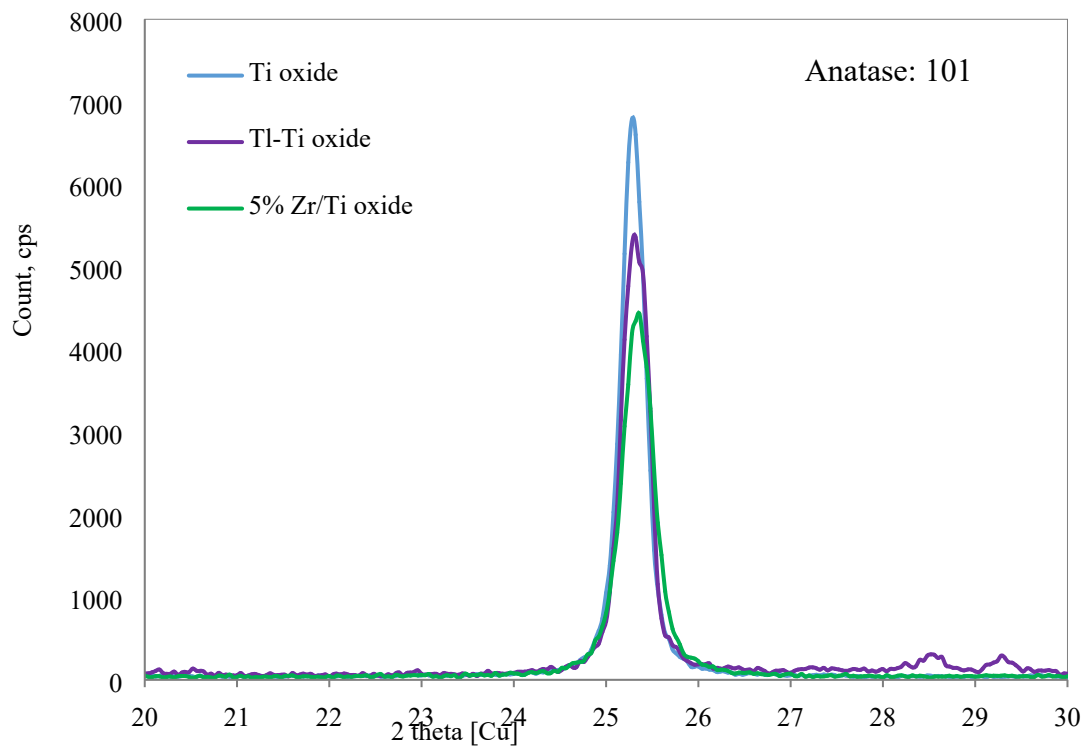


Figure S1. XRD pattern and defect of anatase crystalline phase (1 0 1) of TiO_2 , 5% Zr/Ti oxide and 10.5% Tl/Ti oxide catalysts

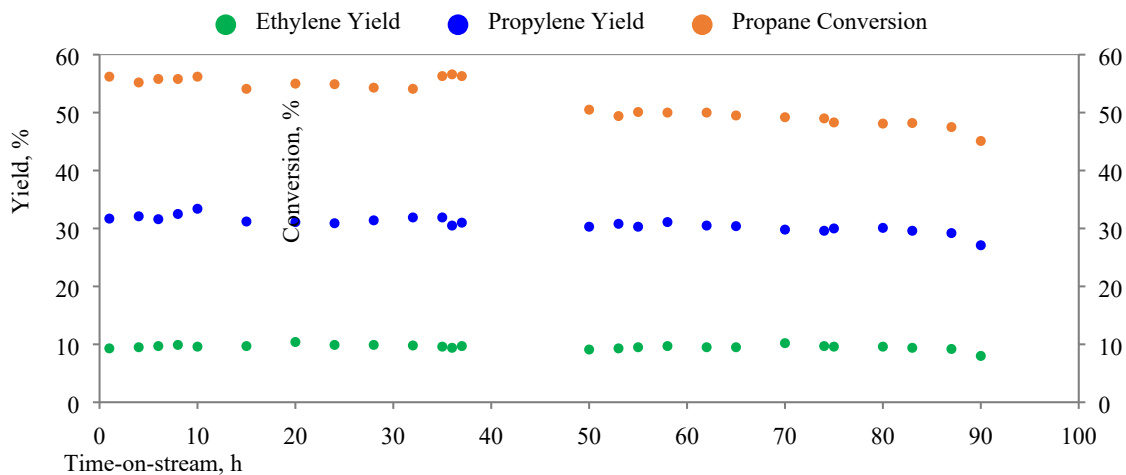


Figure S2. Time-of-stream cycle of propane conversion: 5% Zr/Ti oxide. Reaction condition:

600 °C, 1 atm, WHSV = 40 h⁻¹, CO₂/propane ratio = 20.4 molar ratio

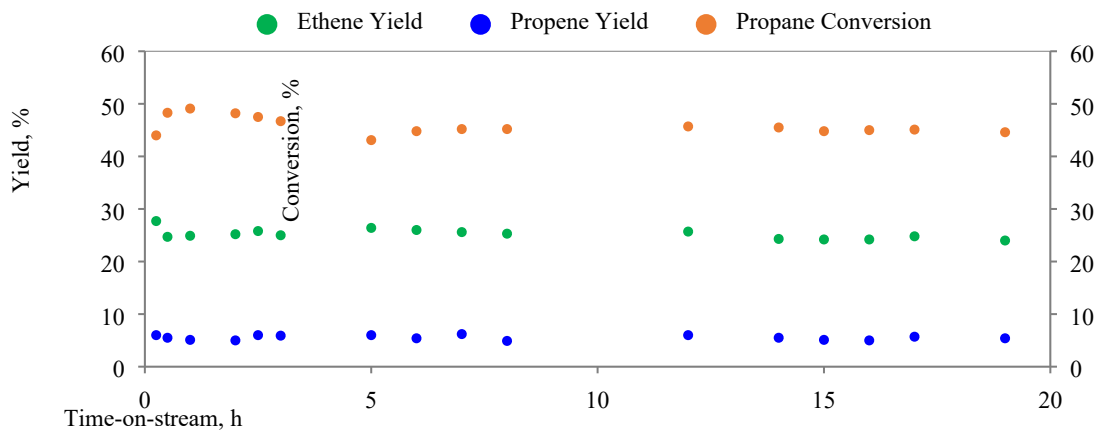


Figure S3. Time-of-stream cycle of propane conversion: 10.5% Ti/Ti oxide. Reaction condition:

600 °C, 1 atm, WHSV = 40 h⁻¹, CO₂/propane ratio = 20.4 molar ratio

Table S1. Gas analysis of propane dehydrogenation assisted by CO₂ over 5% Zr/Ti oxide catalyst, CO₂/propane molar ratio of 20.4 at 600 °C

Time hours	H ₂ mol%	CO mol%	methane mol%	CO ₂ mol%	Ethylene mol%	Ethane mol%	Propylene mol%	Propane mol%
0	0.05	0.60	0.25	90.66	0.37	0.349	1.25	1.73
4	0.05	0.69	0.26	90.29	0.38	0.267	1.27	1.77
6	0.06	0.62	0.27	89.79	0.38	0.295	1.25	1.74
8	0.06	0.72	0.24	89.75	0.39	0.269	1.29	1.75
10	0.06	0.75	0.23	90.69	0.38	0.277	1.32	1.73
15	0.06	0.65	0.25	90.59	0.38	0.272	1.23	1.81
20	0.05	0.65	0.27	90.83	0.41	0.259	1.23	1.78
24	0.05	0.61	0.26	90.95	0.39	0.297	1.22	1.78
28	0.05	0.68	0.28	90.74	0.39	0.227	1.24	1.81
32	0.05	0.72	0.25	90.75	0.39	0.236	1.26	1.81
35	0.05	0.63	0.24	90.67	0.38	0.336	1.26	1.73
36	0.05	0.48	0.27	88.06	0.37	0.399	1.2	1.71
37	0.05	0.55	0.26	88.97	0.38	0.362	1.22	1.73

Table S2. The propane conversion, selectivity and yield over 5% Zr/Ti oxide catalyst at 600 °C

Reaction Time (h)	Propene Selectivity (%)	Ethene Selectivity (%)	Propane Conversion (%)	Propylene Yield (%)	Ethylene Yield (%)	olefins Yield (%)	CO ₂ Conversion (%)
0	56.4	16.5	56.2	31.7	9.3	41	5.2
4	58.2	17.2	55.2	32.1	9.5	41.6	5.6
6	56.7	17.3	55.8	31.6	9.7	41.3	6.1
8	58.3	17.7	55.8	32.5	9.9	42.4	6.1
10	59.4	17.0	56.2	33.4	9.6	43	5.1
15	57.8	17.9	54.1	31.2	9.7	40.9	5.2
20	56.6	18.9	55	31.1	10.4	41.6	5.0
24	56.4	18.1	54.9	30.9	9.9	40.8	4.9
28	57.8	18.2	54.3	31.4	9.9	41.2	5.1
32	59.0	18.1	54.1	31.9	9.8	41.7	5.1
35	56.7	17.0	56.3	31.9	9.6	41.5	5.2
36	53.8	16.5	56.6	30.5	9.4	39.8	7.9
37	55.1	17.3	56.3	31.0	9.7	40.7	6.9

Table S3. Gas analysis of propane dehydrogenation assisted by CO₂ over 10.5% Tl/Ti oxide catalyst, CO₂/propane molar ratio of 20.4 at 600 °C

Time hours	H ₂ mol%	CO mol%	methane mol%	CO ₂ mol%	Ethylene mol%	Ethane mol%	Propylene mol%	Propane mol%
0	0.04	1.03	1.33	90.1	1.16	0.19	0.25	2.35
0.5	0.05	1.02	1.19	91.0	1.04	0.16	0.23	2.17
1	0.05	1.03	1.2	90.1	1.05	0.16	0.21	2.14
2	0.04	1.05	1.28	88.4	1.06	0.16	0.21	2.18
2.5	0.04	1.05	1.32	88.4	1.08	0.17	0.25	2.2
3	0.04	1.03	1.23	90.1	1.05	0.17	0.25	2.24
5	0.04	1.06	1.29	88.0	1.11	0.17	0.25	2.39
6	0.04	1.06	1.25	87.5	1.09	0.17	0.23	2.32
7	0.04	1.06	1.21	87.6	1.07	0.15	0.26	2.3
8	0.05	1.06	1.2	87.5	1.06	0.15	0.21	2.3

Table S4. The propane conversion, selectivity and yield over 10.5% Tl/Ti oxide catalyst at 600 °C

Reaction Time (h)	Propylene Selectivity (%)	Ethylene Selectivity (%)	Propane Conversion (%)	Propylene Yield (%)	Ethylene Yield (%)	Olefins Yield (%)	CO ₂ Conversion (%)
0	16.9	80.3	34.8	5.9	28	33.9	3.2
0.5	13.5	62.5	39.8	5.4	24.9	30.3	3.9
1	12.3	61.7	40.7	5	25.1	30.1	4.3
2	12.4	63.9	39.7	4.9	25.4	30.3	4.4
2.5	15.2	66.7	38.9	5.9	26	31.9	4.2
3	15.4	66.4	38.0	5.8	25.2	31.0	-
5	17.5	78.9	33.8	5.9	26.6	32.5	1.2
6	14.9	73.4	35.7	5.3	26.2	31.5	1.1
7	16.9	71.3	36.2	6.1	25.8	31.9	1.0
8	13.4	70.4	36.3	4.9	25.5	30.4	1.0