Electronic Supplementary Material (ESI) for Catalysis Science & Technology.

Catalytic Performance and Stability of Fe-Doped CeO2 in Propane Oxidative Dehydrogenation Using Carbon Dioxide as Oxidant

Hedun Wang and George Tsilomelekis*

Supporting Information

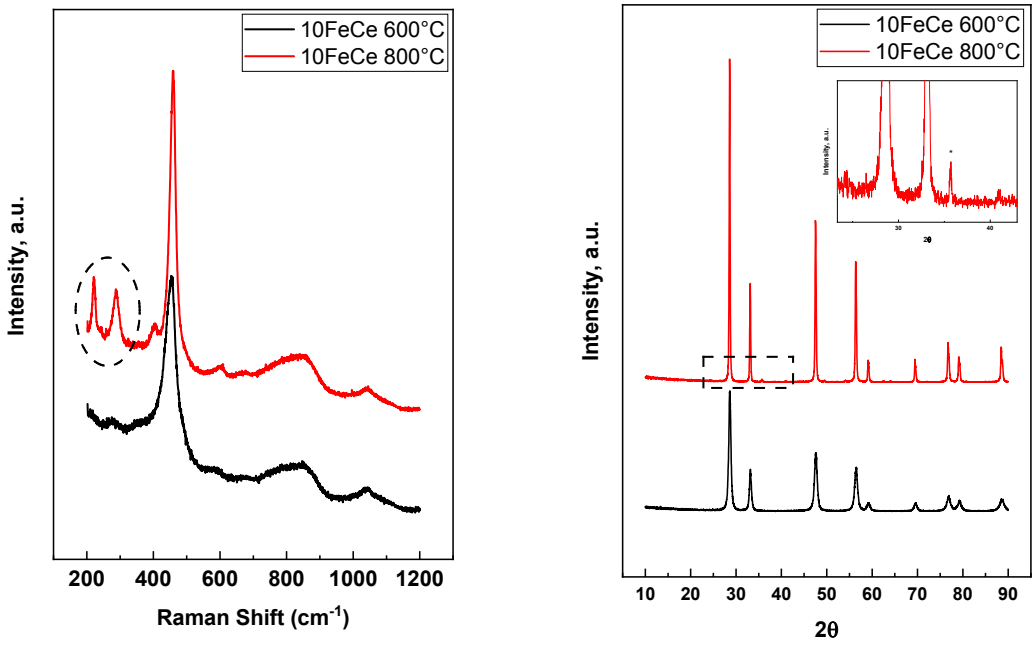

Figure S1: Raman and XRD of 600°C and 800°C calcined 10FeCe

Table S1: Specific surface are and crystallite size of synthesized catalysts with various Fe/Ce molar ratio

Sample	BET specific surface area m^2/gr	Crystallite size nm
1FeCe	59.9	12
2.5FeCe	53.9	9.8
5FeCe	65.5	10.7
10FeCe600	62.2	8.7
10FeCe800	9.6	>100
15FeCe	65.2	8.6

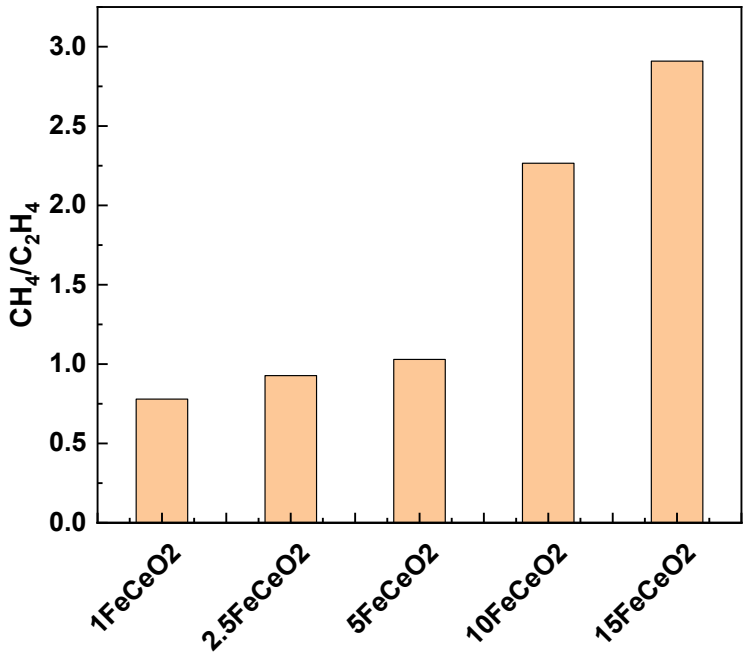

Figure S2: molar ratio of methane-to-ethylene of all Fe doped CeO2 catalysts. Data pertain to initial reaction conditions, 20ml/min total flow (w/F=0.6 g.s/cc) and constant temperature at 550°C.

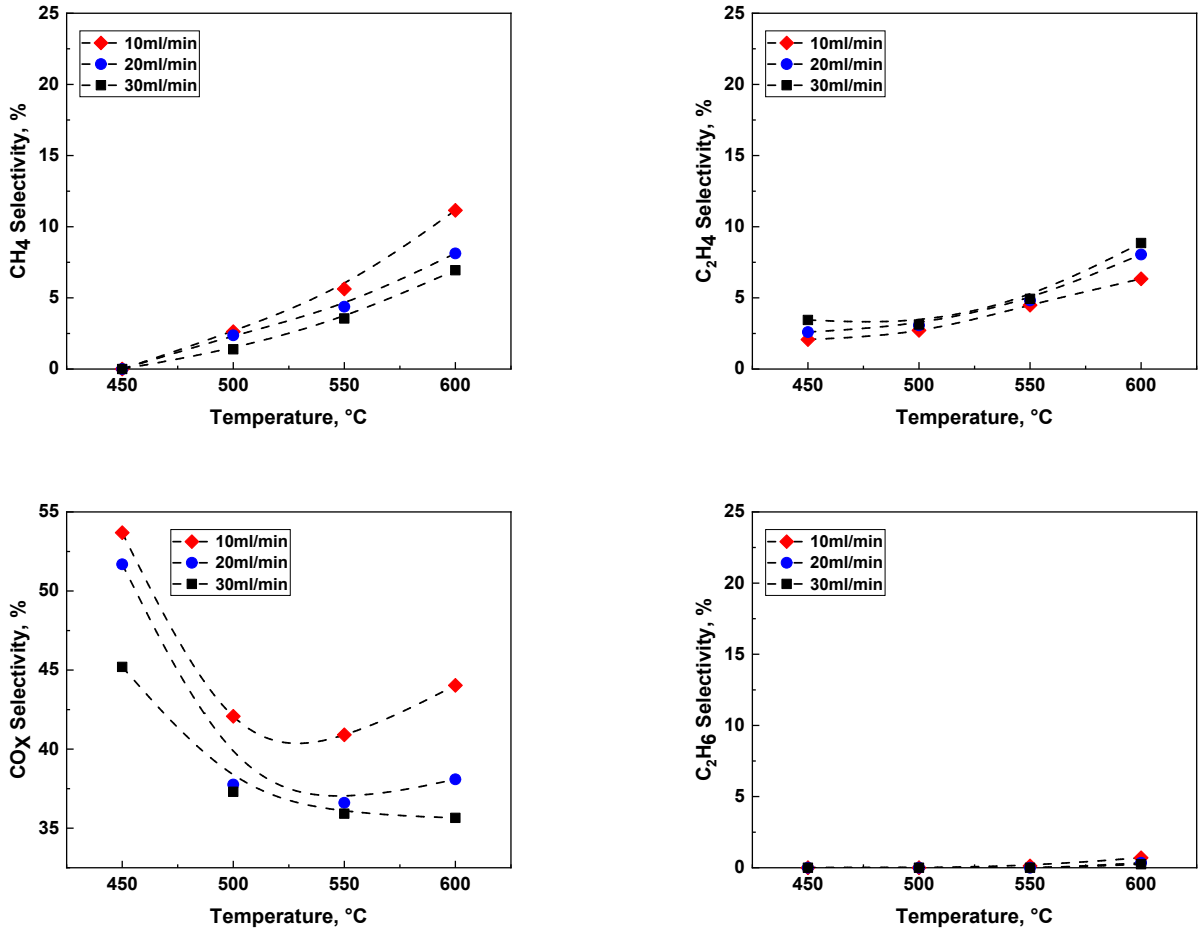

Figure S3: Effect of temperature as well as residence time on methane, ethane, ethylene and COx selectivity of the most selective, 10FeCeO2, catalyst. Data pertain to initial reaction conditions

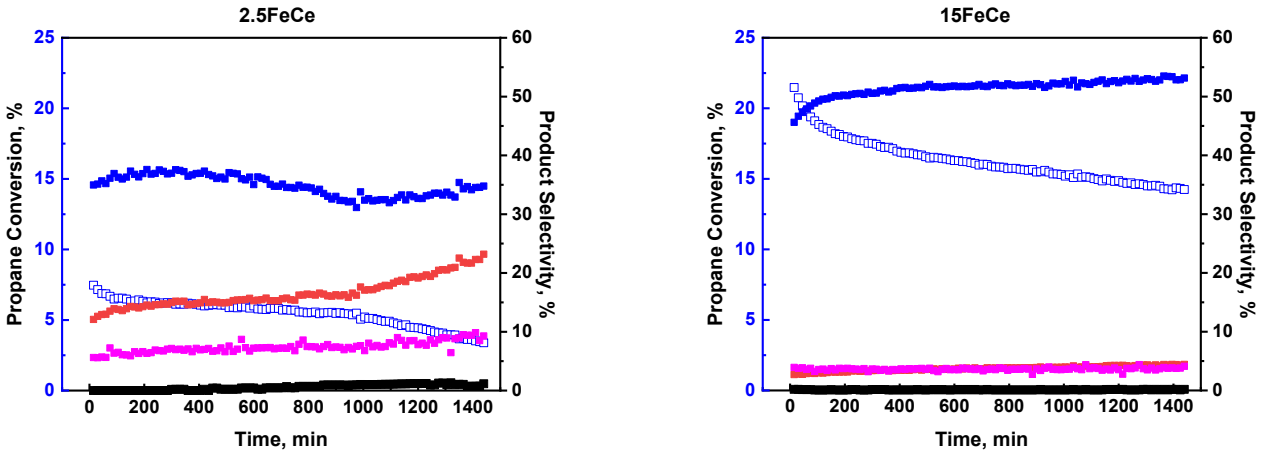

Figure S4: Time-on-stream catalytic performance of 2.5FeCeO2, and 15FeCeO2 catalyst. Data pertain to 20ml/min total flow (w/F=0.6 g.s/cc) and constant temperature at 550°C.

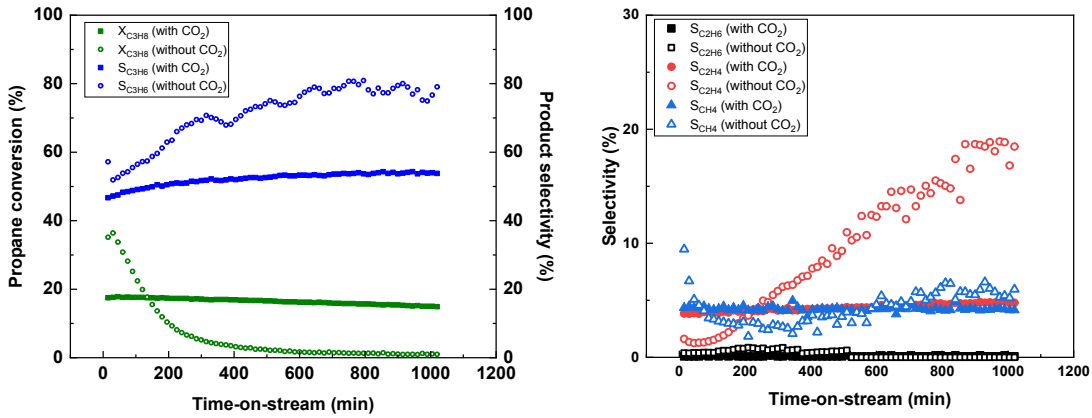

Figure S5: Stability analysis of 10FeCe600 in the absence of CO2 (hollow symbols) as compared to the performance in the presence of CO2 (solid symbols.) Reaction conditions: 200mg catalyst loading, 550oC, 20mL/min total flow. Propane partial pressure: 5%; CO2 partial: 0 or 5%.

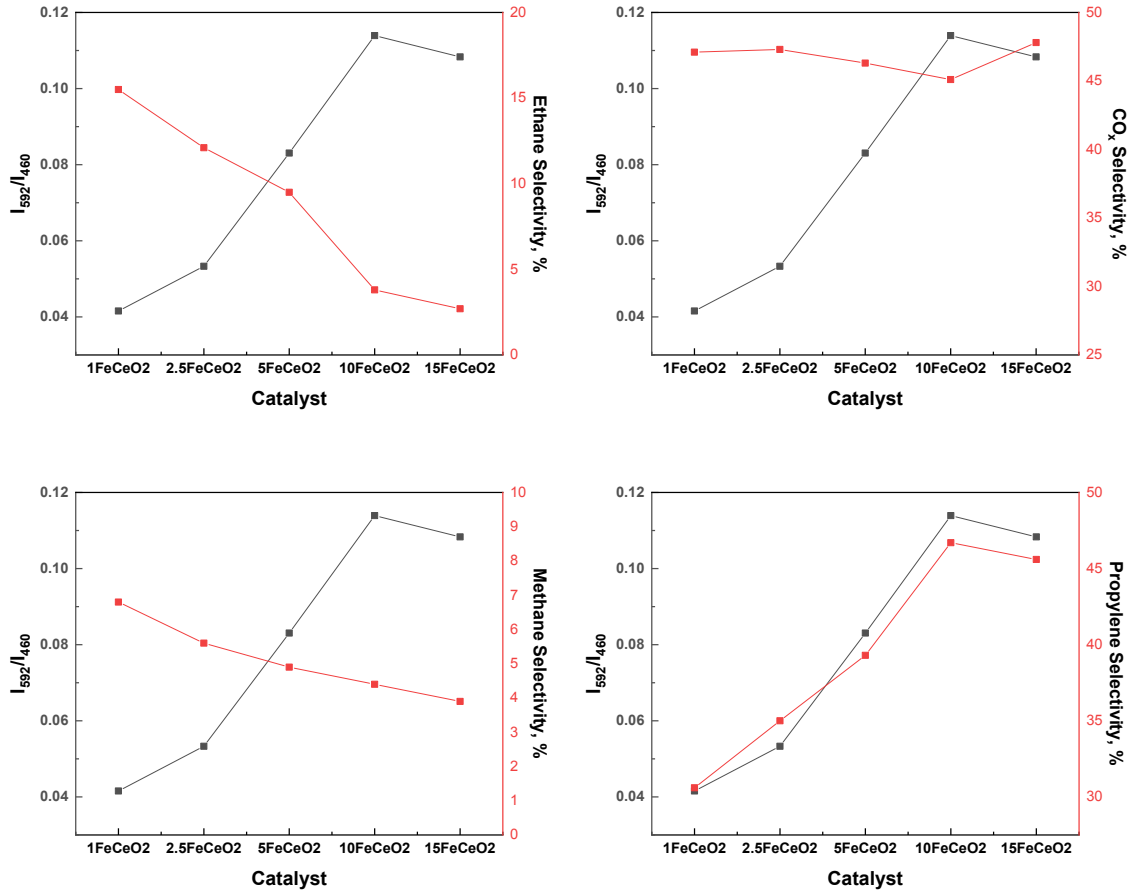

Figure S6: I_{592}/I_{460} as a function of different catalysts and relevant product selectivity

Table S2. XPS analysis and quantification of surface carbon and oxygen atomic percentage and C/O ratio for fresh/spent Fe-doped ceria catalysts.

Fe content	*pre-reaction*			*post-reaction*		
	C atomic %	O atomic %	C/O ratio	C atomic %	O atomic %	C/O ratio
1	11.3	56.9	0.20	28	48.9	0.57
2.5	13.4	57.8	0.23	28.9	46.7	0.62
5	11.7	55.2	0.21	23.1	51.3	0.45
10			16.5	55.3	0.30	14.3	57.2	0.25
15			16.3	52.8	0.31	15.7	54.2	0.29

Table S3. Peak table for carbon chemical state quantification based on deconvolution of XPS C1s scans of spent Fe-doped ceria catalysts. (sp^2: coke/carbon deposition; sp^3: adventitious carbon contamination)

	sp2	Area %	sp3	Area %	C-O	Area %	COO	Area %	carbonate	Area %
1Fe	284.2	41.09	284.6	32.85	286.1	9.75	288.7	8.05	290.3	8.26
2.5Fe	284.2	38.51	284.7	32.37	286.4	9.79	288.6	10.13	290.2	9.2
5Fe	284.1	32.17	284.8	31.84	286.3	11.54	288.6	11.05	290	13.4
10Fe	284.3	27.34	284.9	33.71	286.4	8.48	288.8	17.59	290.2	12.87
15Fe	284.2	28.68	284.7	33.37	286.4	9.67	288.6	13.25	290	15.03

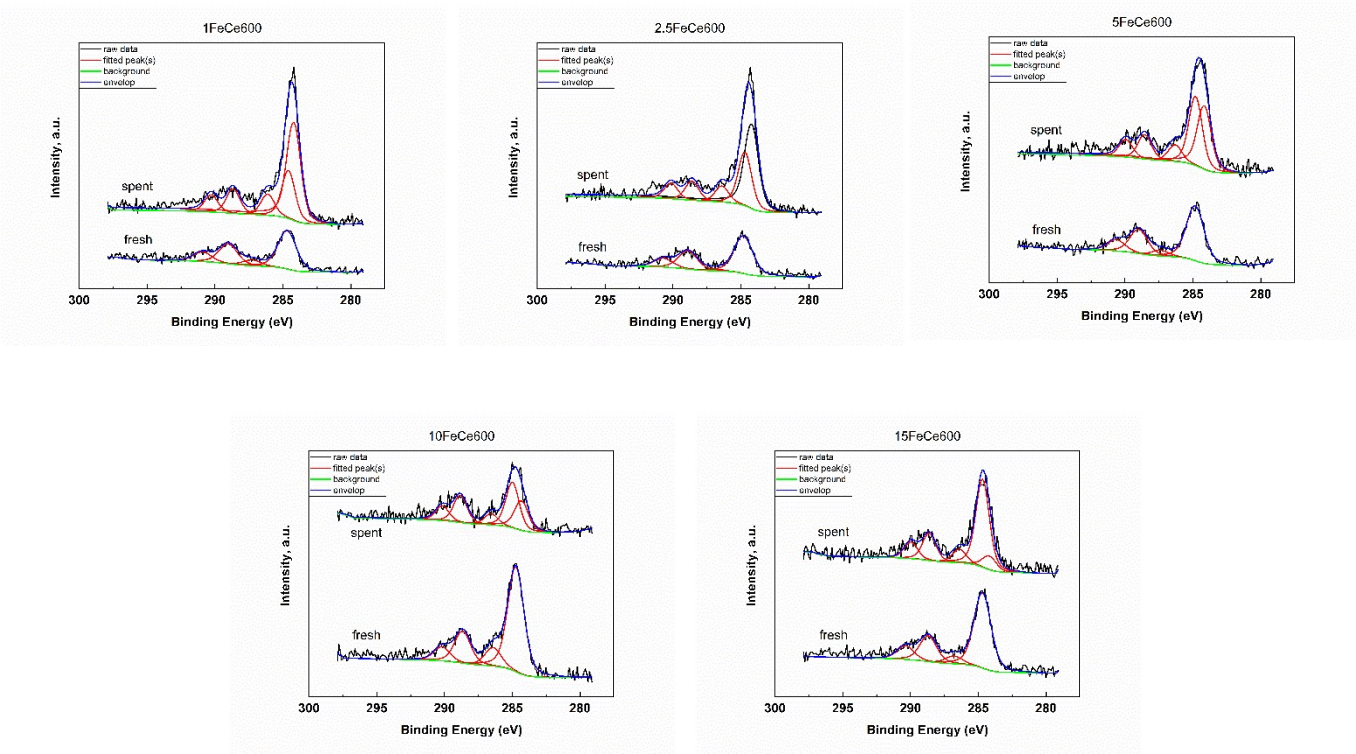

Figure S7: Ex-situ XPS analysis of C1s peak deconvolution for a series of fresh and spent Fe-doped ceria catalysts.