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Dry Reforming of HC_s (Methane, Ethane, and Propane) over a $40Ni_{0.75}(Ce_{1-x}Fe_x)_{0.25}/Al_2O_3$ Catalyst: A comparative study

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Supporting information:

Table S1: The H_2 consumption, CO_2 desorption, and Hydrogen Chemisorption analysis of the synthesized catalysts.

Catalyst	**H_2 –consumption (ml/g_{cat})**	**CO_2 –desorption (ml/g_{cat})**	**H_2-Chemisorption analysis**		
			Metal Dispersion (PD) (%)	**Metallic Surface Area per gram of Metal (SAmetallic) (m^2/g-metal)**	**Active Particle Size (APS) (nm)**
$40Ni_{0.75}Ce_{0.25}/Al_2O_3$	216.8	0.353	24.2	161.2	12.9
$40Ni_{0.75}(Ce_{0.75}Fe_{0.25})_{0.25}/Al_2O_3$	227.4	0.565	24.5	163.2	11.5
$40Ni_{0.75}(Ce_{0.5}Fe_{0.5})_{0.25}/Al_2O_3$	183.1	0.301	23.7	158.3	12.8
$40Ni_{0.75}(Ce_{0.25}Fe_{0.75})_{0.25}/Al_2O_3$	170.4	0.223	23.2	154.5	13.5
$40Ni_{0.75}Fe_{0.25}/Al_2O_3$	158.8	0.175	23	153.6	12.5

Table S2: The % Yield and % conversion of various products during the HC dry reforming reaction, all the reaction performed on 600 °C reaction temperature and 1 atm pressure. Total reactant flow rate was set at 70 ml/min ($HC:CO_2:N_2$ = 1:1:5).

Catalyst	**Reactants**	**% Yield of**			**% Conversion of**		**H_2:CO ratio**
		CH_4	**H_2**	**CO**	**HC**	**CO_2**	
$40Ni_{0.75}Ce_{0.25}/Al_2O_3$	**$CH_4 + CO_2$**	-	60	67	62	69	0.90
$40Ni_{0.75}(Ce_{0.75}Fe_{0.25})_{0.25}/Al_2O_3$		-	66	74	68	76	0.91
$40Ni_{0.75}(Ce_{0.5}Fe_{0.5})_{0.25}/Al_2O_3$		-	59	71	61	74	0.94
$40Ni_{0.75}(Ce_{0.25}Fe_{0.75})_{0.25}/Al_2O_3$		-	56	68	58	70	0.93
$40Ni_{0.75}Fe_{0.25}/Al_2O_3$		-	52	67	54	69	0.90
$40Ni_{0.75}Ce_{0.25}/Al_2O_3$	**$C_2H_6 + CO_2$**	12	69	76	86	81	1.3
$40Ni_{0.75}(Ce_{0.75}Fe_{0.25})_{0.25}/Al_2O_3$		16	73	77	91	85	1.3
$40Ni_{0.75}(Ce_{0.5}Fe_{0.5})_{0.25}/Al_2O_3$		15	68	75	90	83	1.18
$40Ni_{0.75}(Ce_{0.25}Fe_{0.75})_{0.25}/Al_2O_3$		14	67	74	89	79	1.31
$40Ni_{0.75}Fe_{0.25}/Al_2O_3$		13	67	72	84	77	1.4
$40Ni_{0.75}Ce_{0.25}/Al_2O_3$	**$C_3H_8 + CO_2$**	21	70	81	88	86	1.3
$40Ni_{0.75}(Ce_{0.75}Fe_{0.25})_{0.25}/Al_2O_3$		22	80	84	90	88	1.1
$40Ni_{0.75}(Ce_{0.5}Fe_{0.5})_{0.25}/Al_2O_3$		21	69	80	88	85	1.12
$40Ni_{0.75}(Ce_{0.25}Fe_{0.75})_{0.25}/Al_2O_3$		20	69	77	87	84	1.12
$40Ni_{0.75}Fe_{0.25}/Al_2O_3$		19	70	76	86	83	1.13

Table S3: The % Yield and % conversion of various products during the HC dry reforming reaction, at different reaction temperature and 1 atm pressure. Total reactant flow rate was maintained at 70 ml/min (HC:CO_2:N_2 = 1:1:5) over the catalyst $40Ni_{0.75}(Ce_{0.75}Fe_{0.25})_{0.25}/Al_2O_3$.

Reactants	**Reaction Temperature (°C)**	**% Yield of**					**% Conversion of**		**H_2:CO ratio**
		CH_4	**C_2H_4**	**C_3H_6**	**H_2**	**CO**	**HC**	**CO_2**	
CH_4 & CO_2	500	-	-	-	-	-	-	-	-
	550	-	-	-	-	-	-	-	-
	600	-	-	-	66	74	67	75	0.93
	650	-	-	-	68	61	81	86	0.91
	700	-	-	-	77	59	93	100	0.95
	750	-	-	-	87	57	96	100	1
	800	-	-	-	88	54	98	100	1
C_2H_6 & CO_2	500	30	44	-	32	40	78	65	1.47
	550	29	42	-	43	44	87	72	1.38
	600	16	-	-	73	77	91	85	1.3
	650	6	-	-	82	80	96	90	1.35
	700	4	-	-	87	82	100	100	1.34
	750	2	-	-	86	83	100	100	1.25
	800	6	38	-	86	75	99	100	1.04
C_3H_8 & CO_2	500	61	-	-	54	50	88	77	1.1
	550	51	-	-	68	62	89	80	1.19
	600	22	-	-	80	84	90	88	1.1
	650	13	-	-	84	85	91	88	1.1
	700	11	-	3	85	82	93	89	0.99
	750	16	-	14	87	89	94	99	0.93
	800	36	-	26	94	79	99	100	0.68

Table S4: The % Yield and % conversion of various products during the HC dry reforming reaction, where HC (10 ml/min) reactant and N_2 (50 ml/min) flow rate is fixed and CO_2 flow rate varies (10, 15, 20, 25, 30 ml/min) over the catalyst $40Ni_{0.75}(Ce_{0.75}Fe_{0.25})_{0.25}/Al_2O_3$.

Reactant and reaction temperature	**HC:CO_2 ratio**	**% Yield of**					**% Conversion of**		**H_2:CO ratio**
		CH_4	**C_2H_4**	**C_3H_6**	**H_2**	**CO**	**HC**	**CO_2**	
CH_4 & CO_2 700 °C	1:1	-	-	-	77	58	94	100	0.95
	1:1.5	-	-	-	85	72	96	86	0.8
	1:2	-	-	-	78	66	99	76	0.73
	1:2.5	-	-	-	79	65	100	68	0.68
	1:3	-	-	-	76	64	100	56	0.60
C_2H_6 & CO_2 650 °C	1:1	6	0	-	82	80	95	90	1.35
	1:1.5	8	0	-	73	78	97	90	1.25
	1:2	6	27	-	45	61	95	85	1.07
	1:2.5	4	22	-	26	47	90	76	0.91
	1:3	11	32	-	41	53	82	71	0.76
C_3H_8 & CO_2 600 °C	1:1	22	-	-	80	84	90	88	1.1
	1:1.5	33	-	-	79	71	99	90	0.89
	1:2	29	-	-	78	67	95	75	0.80
	1:2.5	18	-	-	75	60	83	68	0.82
	1:3	17	-	-	72	60	69	57	0.75

Table-S5: The detailed percent conversion of various catalysts (reported) and the synthesized catalysts (present study).

Catalysts	**Reaction**	**Temperature (^oC)**	**% Conv. of HC**	**% Conv. of CO_2**	**References**
$15Ni/Al_2O_3$-SiO_2	DRM	700	74	80	8

RuO_2+NiO	DRM	650 800	49.9 87.9	61.1 100	9
Ni-Fe/La-Al	DRM	800	92	98	16
5Ni/0.3Mg-HAP	DRM	700	75	78	21
Ni/La-Al_2O_3	DRE	650	75	63	3
$NdFe_{0.7}Ni_{0.3}O_3$	DRE	600	33	44	10
FeNi/Ce-$Al_{0.5}$	DRE	600	17	41	13
$LaFe_{0.9}Ni_{0.1}O_3$	DRE	600	21.4	49.7	19
NiO(25)-MgO	DRP	600 650 700 800	40 45 80 100	43 62 85 100	14
A-LCO	DRP	550	19	35	15
3wt.%La_2O_3	DRP	750	70	15	20
NiO-CeO_2/Al-F	DRP	650 700 750	64 100 100	46 75 90	31

$40Ni_{0.75}Ce_{0.25}/Al_2O_3$	DRM DRE DRP	700 650 600	93 96 90	100 90 88	Present study

S.1. The % conversion, % yield, deactivation factor, and the H_2:CO ratio were calculated for the DRM, DRE, and DRP reactions.

a) DRM reaction:

$$\% X_{CH_4} = \frac{C_{CH_4\,(in)} - C_{CH_4\,(out)}}{C_{CH_4\,(in)}} * 100$$

$$\% X_{CO_2} = \frac{C_{CO_2\,(in)} - C_{CO_2\,(out)}}{C_{CO_2\,(in)}} * 100$$

$$\% Y_{H_2} = \frac{mole\ of\ H_{2\,(out)}}{2 * mole\ of\ CH_{4\,(in)}} * 100$$

$$\% Y_{CO} = \frac{mole\ of\ CO_{\,(out)}}{mole\ of\ CH_{4\,(in)} + mole\ of\ CO_{2\,(in)}} * 100$$

$$\frac{H_2}{CO} = \frac{mole\ of\ H_2\ produced}{mole\ of\ CO\ produced}$$

$$DF = \frac{Final\ HC\ conversion - Initial\ HC\ conversion}{Initial\ HC\ conversion}$$

DF- Deactivation Factor

b) DRE reaction:

$$\% X_{C_2H_6} = \frac{C_{C_2H_6\,(in)} - C_{C_2H_6\,(out)}}{C_{C_2H_6\,(in)}} * 100$$

$$\% X_{CO_2} = \frac{C_{CO_2\,(in)} - C_{CO_2\,(out)}}{C_{CO_2\,(in)}} * 100$$

$$\% Y_{H_2} = \frac{mole\ of\ H_{2\,(out)}}{3 * mole\ of\ C_2H_{6\,(in)}} * 100$$

$$\% Y_{CO} = \frac{mole\ of\ CO_{(out)}}{mole\ of\ C_2H_{6\,(in)} + mole\ of\ CO_{2\,(in)}} * 100$$

$$\% Y_{CH_4} = \frac{mole\ of\ CH_{4\,(out)}}{2 * mole\ of\ C_2H_{6\,(in)}} * 100$$

$$\% Y_{C_2H_4} = \frac{mole\ of\ C_2H_{4\,(out)}}{mole\ of\ C_2H_{6\,(in)} + mole\ of\ CO_{2\,(in)}} * 100$$

$$\frac{H_2}{CO} = \frac{mole\ of\ H_2\ produced}{mole\ of\ CO\ produced}$$

c) DRP reaction:

$$\% X_{C_3H_8} = \frac{C_{C_3H_8\,(in)} - C_{C_3H_8\,(out)}}{C_{C_3H_8\,(in)}} * 100$$

$$\% X_{CO_2} = \frac{C_{CO_2\,(in)} - C_{CO_2\,(out)}}{C_{CO_2\,(in)}} * 100$$

$$\% Y_{H_2} = \frac{mole\ of\ H_{2\,(out)}}{4 * mole\ of\ C_3H_{8\,(in)}} * 100$$

$$\% \, Y_{CO} = \frac{mole\ of\ CO_{(out)}}{mole\ of\ C_3H_{8\,(in)} + mole\ of\ CO_{2\,(in)}} * 100$$

$$\% \, Y_{CH_4} = \frac{mole\ of\ CH_{4\,(out)}}{3 * mole\ of\ C_3H_{8\,(in)}} * 100$$

$$\% \, Y_{C_3H_6} = \frac{mole\ of\ C_3H_{8\,(out)}}{mole\ of\ C_3H_{8\,(in)} + mole\ of\ CO_{2\,(in)}} * 100$$

$$\frac{H_2}{CO} = \frac{mole\ of\ H_2\ produced}{mole\ of\ CO\ produced}$$