Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Dry reforming activity due to ionic Ru in $La_{1.99}Ru_{0.01}O_3$: Role of specific carbonates

Bhanu P. Gangwar,[a,†] Phanikumar Pentyala,[b,†] Khushbo Tiwari,[c] Krishanu Biswas,[c] Sudhanshu Sharma,[a,*] Parag A. Deshpande[b,*]

[a]Department of Chemistry, Indian Institute of Technology Gandhinagar, Palaj, Gandhinagar, Gujarat 382355, India.

[b]Quantum and Molecular Engineering Laboratory, Department of Chemical Engineering, Indian Institute of Technology Kharagpur, Kharagpur 721302, India.

[c]Department of Materials Science and Engineering, Indian Institute of Technology Kanpur, Kanpur 208016, India.

[*]Corresponding authors: parag@che.iitkgp.ac.in (P. A. Deshpande), Phone: (+91)-3222-283916; ssharma@iitgn.ac.in (S. Sharma), Phone: 9727696682, Fax: +91-79-23972324, 23972583

[†]These authors have contributed equally to the study

Supporting information

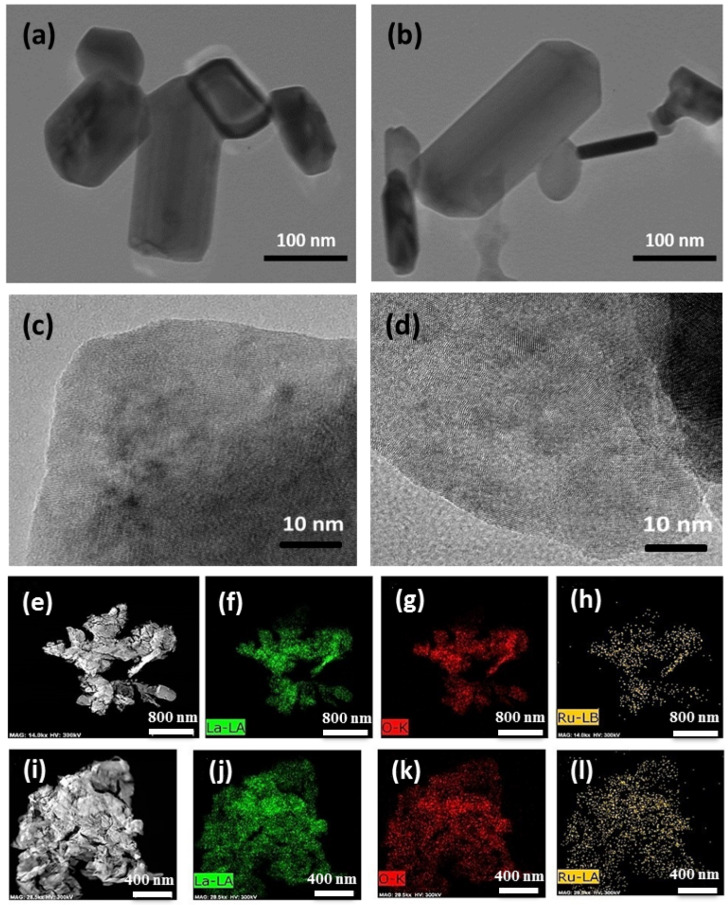

Figure S1: TEM images of as-synthesized (a-b) $La_{1.99}Ru_{0.01}O_3$. HR-TEM images of (c) $La_{1.99}Ru_{0.01}O_3$ and (d) $La_{1.98}Ru_{0.02}O_3$. STEM-HAADF analyses are shown in (e-n).

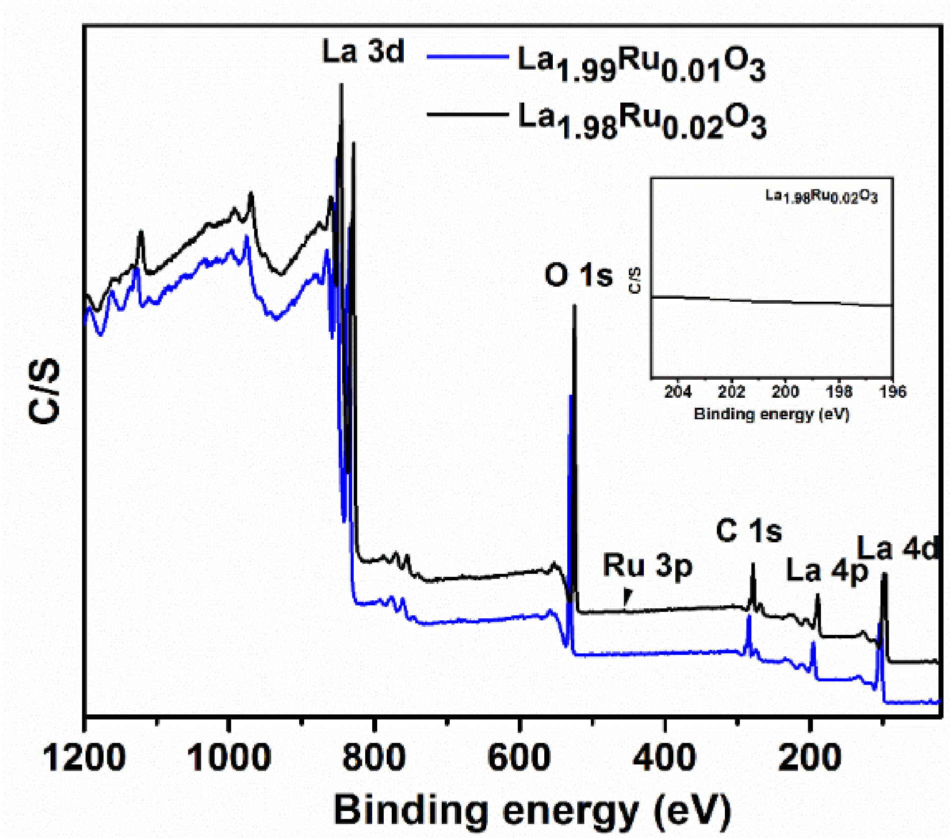

Figure S2: XPS survey scan for $La_{1.99}Ru_{0.01}O_3$ and $La_{1.98}Ru_{0.02}O_3$ catalysts. The inset image show expended region for Cl(2p).

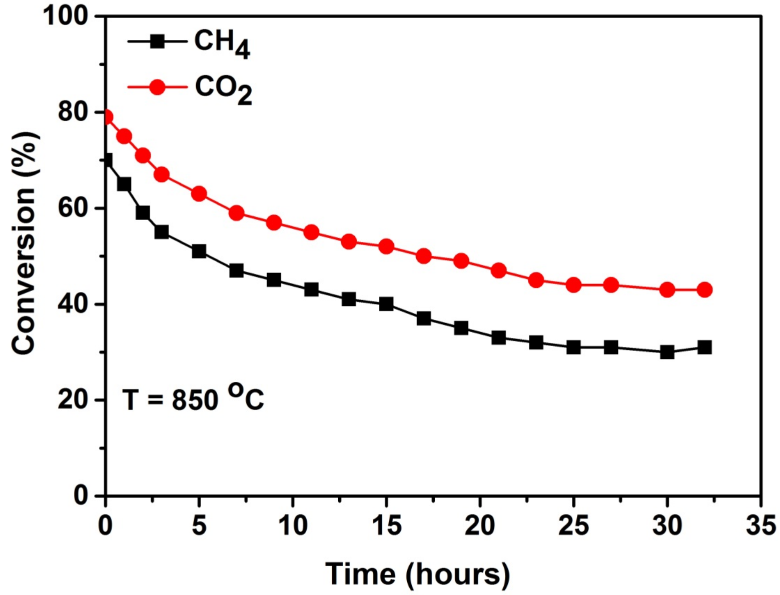

Figure S3: Time-on-stream stability test of $La_{1.99}Ru_{0.01}O_3$ in a fixed-bed reactor at 850 ^{o}C for 32 h. Reaction conditions: CO_2/CH_4 =1, CO_2:CH_4:N_2 = 1:1:18 (total flow rate = 20 sccm), GHSV = 20000 h^{-1}.

Table S1: Elemental compositions of 0.5 atom % Ru doped La_2O_3 ($La_{1.99}Ru_{0.01}O_3$) and 1 atom % Ru doped La_2O_3 ($La_{1.98}Ru_{0.02}O_3$) catalysts obtained by ICP-OES analysis

Catalyst type	La (mg/kg)	La (%) ± error	Ru (mg/kg)	Ru (%) ± error
$La_{1.99}Ru_{0.01}O_3$	1497000	99.75 ± 5	3662.4	0.25 ± 0.013
$La_{1.98}Ru_{0.02}O_3$	1348600	99.47 ± 5	7118.0	0.53 ± 0.027

Table S2: C-O bond lengths (Å) of different carbonates observed on $La_{2-2x}Ru_{2x}O_3$ and $La_{2-2x}Ru_{2x}O_{3-\delta}$

	LR_{C1}	LR_{C2}	LRV_{C1}	LRV_{C2}
C-O1	1.28	1.28	1.28	1.28
C-O2	1.3	1.28	1.29	1.29
C-O3	1.32	1.36	1.33	1.36

Sample calculation for deterination of OSC

No of hydrogen moles through calibration plot

$Y = 2.331*10^7X + 38.942$

Where Y = area, X = moles of H_2 uptake

$193 = 2.331*10^7X + 38.94$

$154.1 = 2.331*10^7X$ (Moles are estimated by running TPR of known amount of CuO)

$X = 66.1089*10^{-7}$ moles

$= 66.1089*10^{-7}$ moles/50 mg (because, 50 mg sample is taken for experiment)

Molecular weight of La_2O_3 = 325.8 moles/g

Oxygen storage capacity (consumed oxygen) = $325.8*1.32*10^{-4} \approx 0.043$

Oxygen atom (O) $= 3-0.043 \approx 2.96$

Hence La_2O_3 after reduction becomes $La_2O_{2.96}$