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

Electronic supporting information

Highly efficient nanosized Mn and Fe codoped ceria-based solid solutions for elemental mercury removal at low flue gas temperatures

Deshetti Jampaiah[a,b], Samuel J. Ippolito[b], Ylias M. Sabri[b], Benjaram M. Reddy[a,*] and Suresh K. Bhargava[b,*]

[a]*RMIT-IICT Joint Research Centre, CSIR-Indian Institute of Chemical Technology, Uppal Road, Hyderabad – 500 007, India*

[b]*Centre for Advanced Materials & Industrial Chemistry (CAMIC), School of Applied Sciences, RMIT University, GPO BOX 2476, Melbourne – 3001, Australia*

*Corresponding Authors

E-mail: bmreddy@iict.res.in; Fax: +91 40 2716 0921; Tel: +91 40 27193510

E-mail: suresh.bhargava@rmit.edu.in; Tel: +61 3 9925 3365

Table S1 The chemical compositions of elements of $Ce_{0.7}Mn_{0.3}O_{2-\delta}$ (CM), $Ce_{0.65}Mn_{0.3}Fe_{0.05}O_{2-\delta}$ (CMF5), $Ce_{0.6}Mn_{0.3}Fe_{0.1}O_{2-\delta}$ (CMF10), $Ce_{0.55}Mn_{0.3}Fe_{0.15}O_{2-\delta}$ (CMF15), and $Ce_{0.5}Mn_{0.3}Fe_{0.2}O_{2-\delta}$ (CMF20) catalysts.

Sample	Nominal values			Actual values from ICP-OES analysis			Chemical formulae
	Ce	Mn	Fe	Ce	Mn	Fe	
CM	0.7	0.3	-	0.69	0.31	-	$Ce_{0.69}Mn_{0.31}O_{2-\delta}$
CMF5	0.65	0.3	0.05	0.61	0.32	0.07	$Ce_{0.61}Mn_{0.32}Fe_{0.07}O_{2-\delta}$
CMF10	0.6	0.3	0.10	0.58	0.34	0.08	$Ce_{0.58}Mn_{0.34}Fe_{0.08}O_{2-\delta}$
CMF15	0.55	0.3	0.15	0.54	0.32	0.13	$Ce_{0.54}Mn_{0.32}Fe_{0.13}O_{2-\delta}$
CMF20	0.50	0.3	0.20	0.51	0.32	0.17	$Ce_{0.51}Mn_{0.32}Fe_{0.17}O_{2-\delta}$

Table S2 The surface atomic concentrations and binding energies of CeO_2, $Ce_{0.7}Mn_{0.3}O_{2-\delta}$ (CM), $Ce_{0.65}Mn_{0.3}Fe_{0.05}O_{2-\delta}$ (CMF5), $Ce_{0.6}Mn_{0.3}Fe_{0.1}O_{2-\delta}$ (CMF10), $Ce_{0.55}Mn_{0.3}Fe_{0.15}O_{2-\delta}$ (CMF15), and $Ce_{0.5}Mn_{0.3}Fe_{0.2}O_{2-\delta}$ (CMF20) catalysts.

Sample	$Ce^{3+}/Ce^{3+}+Ce^{4+}$ (%)	O 1s centre (eV)		
		O_I	O_{II}	O_{III}
CeO_2	12.6	530.4	531.9	-
CM	16.51	529.1	531.4	532.9
CMF5	19.13	529.0	531.4	533.1
CMF10	26.46	528.9	530.6	533.2
CMF15	30.87	528.7	531.3	533.6
CMF20	37.01	528.5	530.4	533.4

O_I = lattice oxygen; O_{II} = surface adsorbed oxygen; O_{III} = chemisorbed water and/or carbonates

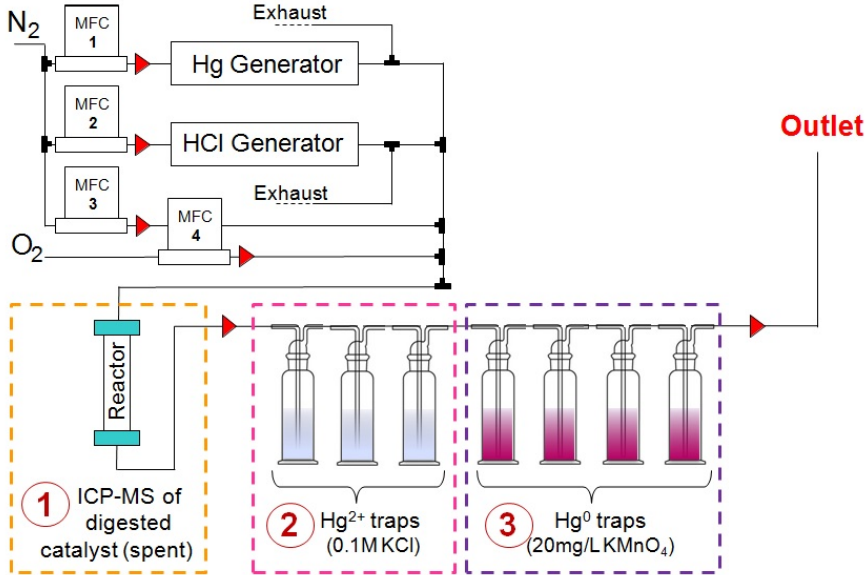

Fig. S1. Schematic experimental diagram set up.

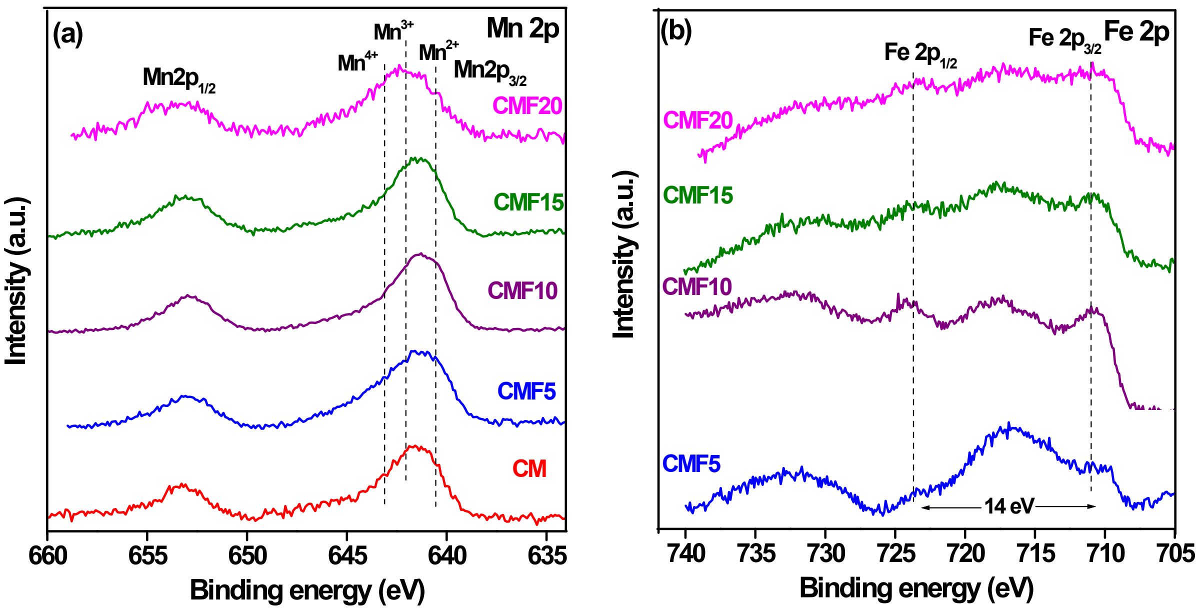

Fig. S2(a) Mn 2p (b) Fe 2p XP spectra of CeO_2, $Ce_{0.7}Mn_{0.3}O_{2-\delta}$ (CM), $Ce_{0.65}Mn_{0.3}Fe_{0.5}O_{2-\delta}$ (CMF5), $Ce_{0.6}Mn_{0.3}Fe_{0.1}O_{2-\delta}$ (CMF10), $Ce_{0.55}Mn_{0.3}Fe_{0.15}O_{2-\delta}$ (CMF15), and $Ce_{0.5}Mn_{0.3}Fe_{0.2}O_{2-\delta}$ (CMF20) catalysts.

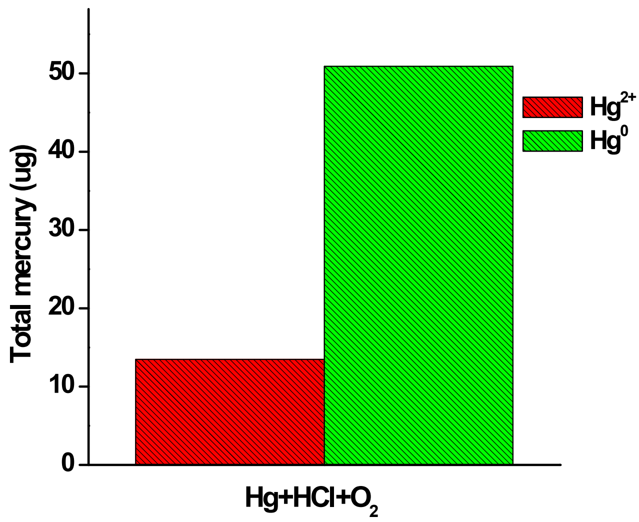

Fig. S3 Mercury speciation in presence of HCl and O_2 gas conditions without catalyst.

It can be observed that ~16 % of the Hg^0 is oxidised without the presence of a catalyst. This may be due to the presence of gas species that promote Hg^0 oxidation, namely HCl and O_2.

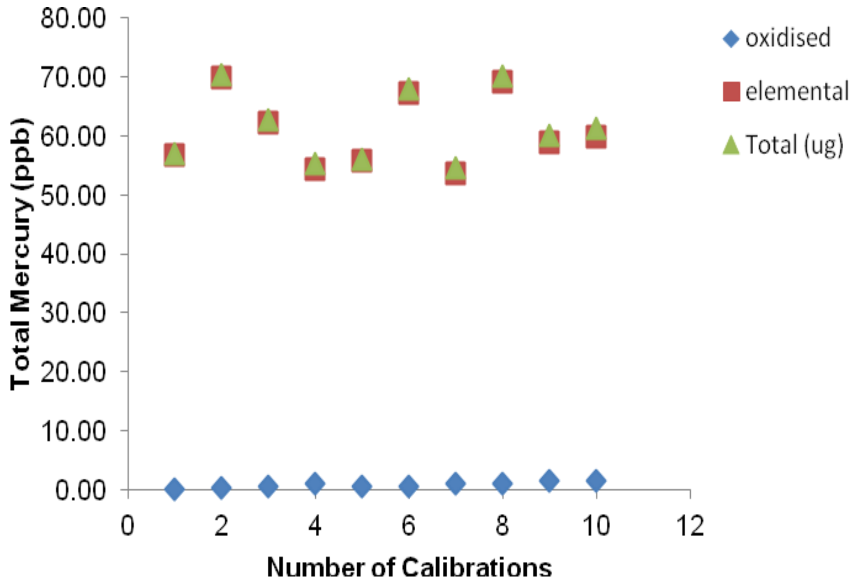

Fig. S4 The calibration experiments for total amount of inlet mercury (Hg^0_{inlet}).

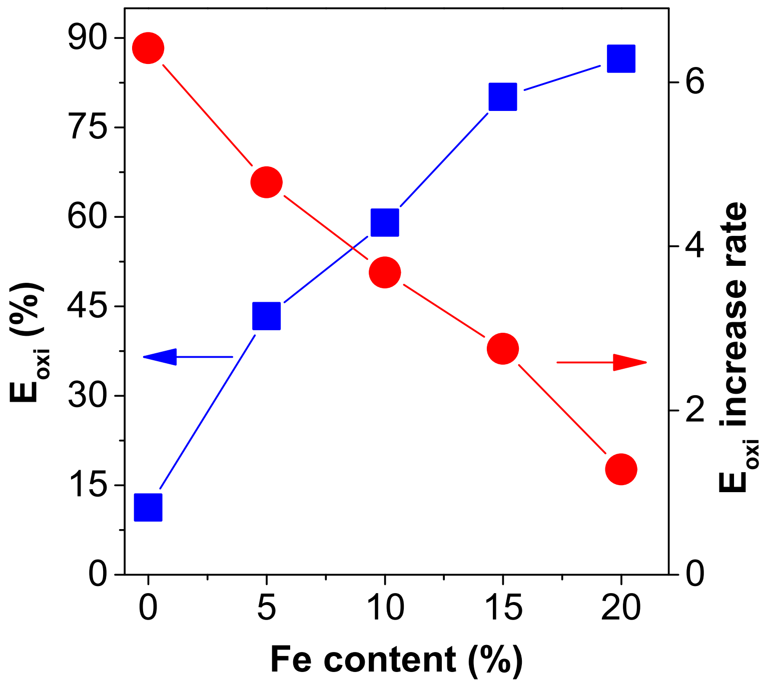

Fig. S5 The relation between E_{oxi} and rate of increase in E_{oxi} with respect to the Fe content in the presence of HCl and Hg^0.