Wednesday, 4th January			
11:00	Registration desk opens at Burleigh Court Hotel		
12:30	Lunch at Holywell Park		
13.50	Welcome – Conference commences at Holywell Park		
	Chair – Prof. Richard Catlow		
14.00	PI 01 – Prof. Martin Schröder *(Turing Lecture Theatre)*		
14.45	Coffee		
	Session A (Turing Lecture Theatre) CatalysisHub session	*Session B (Brunel/Murdoch Lecture Theatre)*	*Session C (Stephenson Lecture Theatre)*
Chair/IT	Artioli/Nayan	Kondrat/ Inns	James/Wagh
15.15	K1 (Crimmin)	O6	O13
15.35		O7	O14
15.55	O1	O8	O15
16.15	O2	O9	K2 (Carravetta)
16.35	O3	O10	
16.55	Coffee		
Chair/IT	Artioli/Pei	Simons/ De-Zanet	Mitchell/ Sabah
17.25	O4	O11	K3 (Buchard)
17.45	O5	O12	
	Chair – Prof. Charlotte Williams		
18.10	PI 02 – Prof. Unni Olsbye *(Turing Lecture Theatre)*		
20.00	Dinner		

Thursday, 5th January			
	Chair – Prof. Graham Hutchings		
9.00	PI 03 – Prof. Javier Pérez-Ramírez *(Turing Lecture Theatre)*		
	Session A (Turing Lecture Theatre)	*Session B (Brunel/Murdoch Lecture Theatre)*	*Session C (Stephenson Lecture Theatre)*
Chair/IT	Paterson/Nayan RSC INTEREST GROUP APPLIED CATALYSIS session	Lennon/ Wallbridge	Muldoon/Nagy
9.50	K4 (Johnston)	O24	O38
10.10		O25	O39
10.30	O16	O26	O40
10.50	Coffee		
Chair/IT	Paterson/Yang	Wells/ Symillidis	Weller/ Mukundan
11.20	K5 (Sunley)	O27	O41
11.40		O28	O42
12.00	O17	O29	O43
12.20	O18	O30	K7 (Muldoon)
12.40	O19	O31	
13.00	Lunch		
	Chair – Prof. Chris Hardacre		
14.00	PI 04 – Prof. Emiel J.M. Hensen *(Turing Lecture Theatre)*		
14.45	Coffee		
	(Turing Lecture Theatre)	*(Brunel/Murdoch Lecture Theatre)*	*(Stephenson Lecture Theatre)*
Chair/IT	Manyar/Isah RSC INTEREST GROUP SURFACE REACTIVITY & CATALYSIS session	Wood/Inns	Beale/Wagh
15.15	K6 (Bruijnincx)	O32	O44
15.35		O33	O45
15.55	O20	O34	O46
16.15	Coffee		

Chair/IT	McGregor/Pei	Lin/ Asad	Wass/ Sabah
16.45	O21	O35	O47
17.05	O22	O36	O48
17.25	O23	O37	O49
17.45	**Poster session**		
20.00	Conference Dinner		

Friday, 6th January

	Session A (Turing Lecture Theatre)	*Session B (Brunel/Murdoch Lecture Theatre)*	*Session C (Stephenson Lecture Theatre)*
Chair/IT	Manyar/ Wallbridge	Dingwall/Nagy	Smyth/Yang
9.00	K8 (Zhou)	O51	O58
9.20		O52	O59
9.40	K9 (Duyar)	O53	O60
10.00		O54	O61
10.20	Coffee		
Chair/IT	Garforth/ Rehman	Whiston/ Symillidis	Reza/ Mukundan
10.50	K10 (Lin)	O55	O62
11.10		O56	O63
11.30	O50	O57	O64
	Chair – Prof. Matthew Davidson		
11.55	PI 05 – Dr. Sofia Diaz-Moreno *(Turing Lecture Theatre)*		
12.40	Closing remarks		

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List of Talks UKCC 2023

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Pl 02	Thermo-catalytic conversion of CO_2 and H_2 to higher hydrocarbons	Unni Olsbye
Pl 03	Catalysis Engineering for Sustainable Development	Javier Pérez-Ramírez
Pl 04	Controlling metal-support interfaces for sustainable catalysis	Emiel J.M. Hensen
Pl 05	X-ray spectroscopy characterisation of catalysts and chemically active systems	Sofia Diaz-Moreno
K 01	Fluoride Metathesis, HF Transfer, and HF Shuttling: New Approaches in the Circular Chemistry of Fluorine	Mark Crimmin
K 02	Applications of solid-state NMR for materials	Marina Carravetta
K 03	Catalysis for More Sustainable Polymers	Antoine Buchard
K 04	Commercialisation of Gold Catalysts for VCM Production	Peter Johnston
K 05	Aromatic and digital notes in zeolite catalysed methanol dehydration to dimethyl ether	Glenn Sunley
K 06	Catalysts, Conversion Routes and Analytics for Circular Chemicals and Materials	Pieter Bruijnincx
K 07	Developing Sustainable Palladium Catalysis for Wacker-Type Oxidation Reactions	Mark J. Muldoon
K 08	In Situ and Operando Gas and Heating TEM on Catalysis Materials	Dan Zhou
K 09	Dual function materials for CO_2 capture and utilisation	Melis Duyar
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Samarium doped Ceria as an active catalyst for emission control

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Introduction

The introduction of the Euro 7 standards for tailpipe emissions of light-duty vehicles (cars and vans) presents the need for further optimisation of the existing after-treatment technologies. New rules propose a 35% reduction for NOx emissions from these vehicle types compared to Euro 6 standards [1]. Lean NOx Trap (LNT) catalysts are a commonly used for NOx emission control in lean-burn engines, however, their function during cold-start engine operation is a target area for improvement. They consist of PGM(s) supported on ceria or other mixed oxides. Ceria's redox property allows it to store NOx at low temperatures (<300˚C), independently from exhaust gas conditions. The NOx storage and reduction properties of ceria can be further enhanced using dopants. [2] Rare earth (RE) elements such as Samarium are commonly used in these systems to their reported increase in oxygen vacancies and defect densities as well an altered Pt reducibility and Pt-ceria interaction. These in turn allow for higher NOx storage capacity during lean operation as well as enhanced activation during rich purge. Sm doped catalysts (10 wt.%) were synthesised on a range of ceria and alumina-based catalysts with increasing loadings of Pt (0-1 wt.%). The objective of this study was to investigate the effect that doping had on the catalyst structure and how this in turn affected the performance of the catalyst in realistic conditions. Morphological changes were observed, using many characterisation techniques (H_2-TPR, XPS, EELS & Raman Spectroscopy), and oxidation and storage activities were measured in cold-start conditions (150-300˚C).

Materials and Methods

NOx Storage Capacity (NSC) experiments were performed in the range 150 to 300˚C in a fixed bed reactor using 40 mg of catalyst. Lean, dry conditions consisted of 5% O_2, 400 ppm NO and an Ar balance to 200 Ncc/min. On-line measurements were taken using an Bruker Matrix MG5 FTIR gas analyser. The initial activation and cleaning cycle ran from RT to 450˚C, with a 10 minute dwell at 450˚C, in 0.4% H_2/Ar. XPS data was acquired using a Kratos Axis SUPRA using monochromated Al kα (1486.69 eV) X-rays at 15 mA emission and 12 kV HT (180W) and a spot size/analysis area of 700 x 300 µm.

Results and Discussion

NOx Storage Capacity (NSC) experiments were performed to assess the storage capabilities of the catalysts to adsorb NOx between 150-300˚C. NSC was measured as the cumulative NO stored during a one hour isothermal hold in oxidising conditions. The results are reported as Figure 1. It was observed that upon Sm addition, the NSC of the catalysts with the highest Pt loading (1 wt.%) increases by circa 100 μmol NO_X/g catalyst at all temperatures. This is a NSC increase of 52% at the lowest temperature (150˚C). The highest NSC is observed on the doped sample at the highest metal loading. This observation, therefore, was indicative of significant chemistry changes due to doping. To better understand the storage changes observed, as well as potential differences in catalytic and redox activity, of the doped catalysts, XPS was carried out on the same sample set. In particular, the Pt and Ce oxidation states were measured and are reported in Table 1. The increase in oxidised Pt and Ce, evidenced in Table 1, was observed to be in line with the increased NOx storage capacity of the doped samples. The higher surface oxygen content can potentially be related to the increase in the rate of NO oxidation to NO_2, as well as to the formation mechanisms of the nitrate and nitrite species, proposed by Filtschew et al. [3]. This increased oxygen content was confirmed, as the Ce^{4+}/Ce^{3+} and Pt^{4+}/Pt^{2+} ratios both increased when Sm was present on the support (at all Pt loadings). XPS also indicated that this increase to higher oxidation states changes the relative percentage of surface to lattice oxygen; to favour surface oxides. According to literature [4], a greater oxygen content on the surface of the catalyst promotes oxygen donation, therefore potentially increasing the rate of the NOx storage mechanisms [3]. Further characterisations such as H_2-TPR show changes in both, overall reducibility, and contributions from spillover mechanisms due to changing Pt-Ce interactions. Raman spectroscopy illustrated increases in defect densities on Sm doped catalysts. Further, cyclic performance testing, designed to test catalyst efficiency in lean and rich conditions, also indicated an increase in lean phase NOx storage as well as greater HC oxidation.

Metal	Pt Ion (%)		Ce Ion (%)	
Valance	**Pt2+**	**Pt4+**	**Ce3+**	**Ce4+**
Ce	--	--	19.6	80.4
Sm-Ce	--	--	13.9	86.1
0.25Pt-Ce	88.1	11.9	14.5	85.5
0.25Pt-Sm-Ce	63.6	36.4	10.6	89.4
1Pt-Ce	87	13	12.5	87.5
1Pt-Sm-Ce	59.7	40.3	9.47	90.5

Table 1. Cerium and Platinum cations, relative percentage differences in oxidation state.

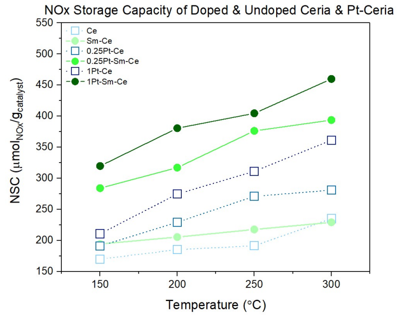

Figure 1. NOx storage capacity experiments. *(Ce = Ceria)

As the NOx storage capabilities of the catalyst improve with doping in both static dry conditions, and in lean/rich cyclic conditions containing CO_2 and H_2O (data not presented), this linked effect was confirmed. It was also crucial to note that the relative selectivity to by-products (N_2O and NH_3) was not adversely affected in the presence of the dopant, even with higher levels of NOx being stored on the surface.

Significance

Performance testing shows that the presence of Samarium, on Ceria and Pt-Ceria increases the NOx storage capacity of the catalyst at low temperatures (150-300˚C) and subsequently decreases the temperature needed for NOx reduction. This is important for the application of these catalysts to reduce NOx emissions during cold start operation. Changes in catalyst structure and morphology caused by Sm addition have been examined using a multitude of characterisations. Changes in oxygen content, defect structure and metal-support interactions have all been observed and related to performance changes. This work can help improve catalyst development for emission control solutions in a wide range of chemical engineering disciplines.

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