Supplementary Material (ESI) for PCCP

Supporting Information for

Highly active ceria-supported gold clusters for 1,3-butadiene hydrogenation

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Results

Table S1. Catalytic performance in 1,3-butadiene hydrogenation, structural parameters from fitted EXAFS spectra and estimate of the fraction of cationic gold from XANES for Au/CeO_2 and Au/CeO_2-CN as a function of the gas treatment and for a Au foil.

Sample	Treatment	r (mmol/g_{Au}.s)	f_{Au3+}[a] (%)	EXAFS analysis[b]							TOF[d] (s^{-1})
				Shell	R (Å)	CN	$\Delta\sigma^2$ ($Å^2$)	E_0 (eV)	F (%)	D (%)[c]	
Au foil	-	-	0	Au Au	2.87 4.06	12 4	0.009 0.012	-7.2	22	-	
Au/CeO_2	He, 393 K	0.31	55	O Au	1.96 2.84	0.4 7.8	0.001 0.013	-7.3	41	37	0.17
	H_2, 393 K	0.35	7				n.d.[e]		n.d.	37[f]	0.19
	H_2, 423 K	0.40	0				n.d.		n.d.	37[f]	0.21
	H_2, 473 K	0.70	0				n.d.		n.d.	37[f]	0.37
	H_2, 523 K	3.3	0	Au	2.81	7.1	0.010	-5.8	36	45	1.5
	H_2, 623 K	1.1	0	Au	2.82	7.0	0.009	-7.2	37	47	0.47
	H_2, 773 K	0.22	0	Au	2.83	7.0	0.011	-7.4	40	47	0.09
Au/CeO_2-CN	He, 393 K	2.7 (12)[g]	100	O Ce	1.97 3.23	3.1 4.2	0.003 0.013	-8.2	36	100	0.4 (0.7)[g]
	H_2, 393 K	14	72				n.d.		n.d.	100	2.7
	H_2, 423 K	42	40				n.d.		n.d.	100[f]	8.2
	H_2, 473 K	91	20				n.d.		n.d.	100[f]	18
	H_2, 523 K	94	18	O Au	2.01 2.73	0.4 3.7	0.001 0.013	-3.1	46	100[f]	19
	H_2, 623 K	94	17				n.d.		n.d.	100[f]	19
	H_2, 773 K	5.3	8	O Au	2.11 2.78	0.2 5.9	0.001 0.013	-5.6	36	65	1.6

[a] estimated fraction of Au^{3+} from fitting of whiteline of near-edge spectra [b] fitting of k^3-weighted EXAFS spectra; Δk=2.8-11.0 $Å^{-1}$ for Au/CeO_2; Δk=2.8-10.3 $Å^{-1}$ for Au/CeO_2-CN; estimated error in R ±0.02 Å, N ±20%, $\Delta\sigma^2$ ±10%; F is the normalized residual [c] dispersion from Au-Au coordination number according to Ref. 22 [d] turnover frequency computed from D [e] not determined [f] assumed equal to dispersion of previous treatment [g] after 12 h time on stream.

EXAFS analysis - EXAFS functions of the k^3-weighted data and corresponding fits are given below for Au/CeO_2 and Au/CeO_2-CN pre-treated under varying conditions.

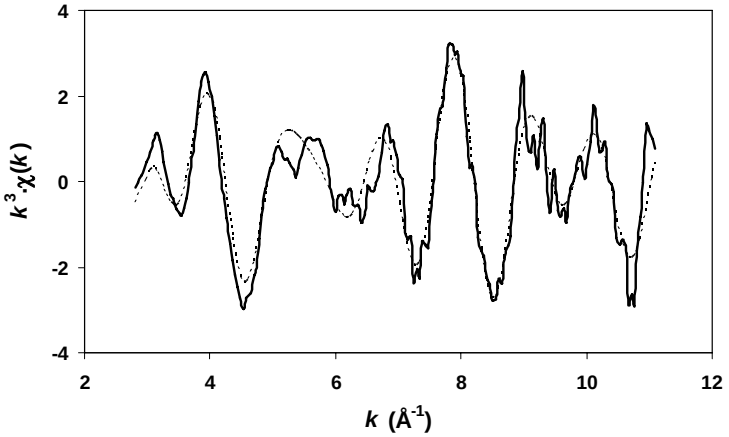

Figure S1. Experimental k^3-weighted EXAFS function (solid line) and fit (dashed line) for Au/CeO_2 dried at 393K.

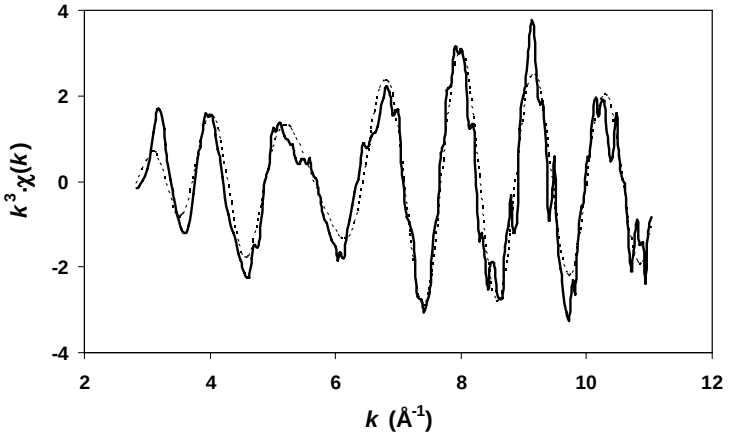

Figure S2. Experimental k^3-weighted EXAFS function (solid line) and fit (dashed line) for Au/CeO_2 reduced at 523 K.

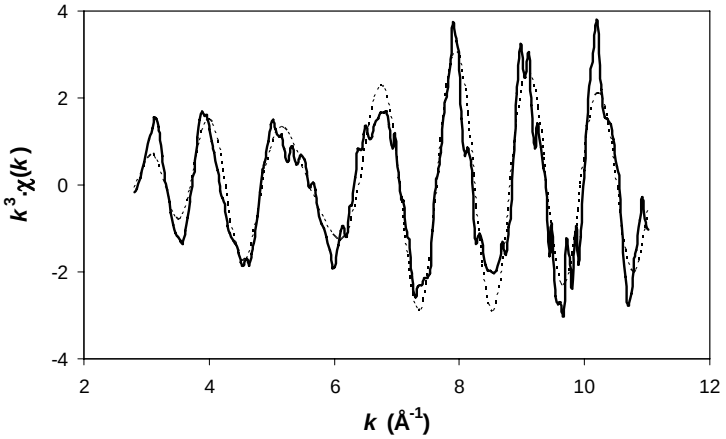

Figure S3. Experimental k^3-weighted EXAFS function (solid line) and fit (dashed line) for Au/CeO_2 reduced at 623 K.

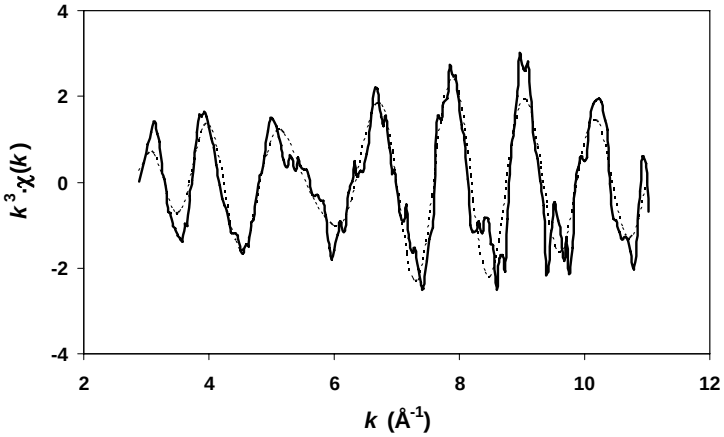

Figure S4. Experimental k^3-weighted EXAFS function (solid line) and fit (dashed line) for Au/CeO_2 reduced at 773 K.

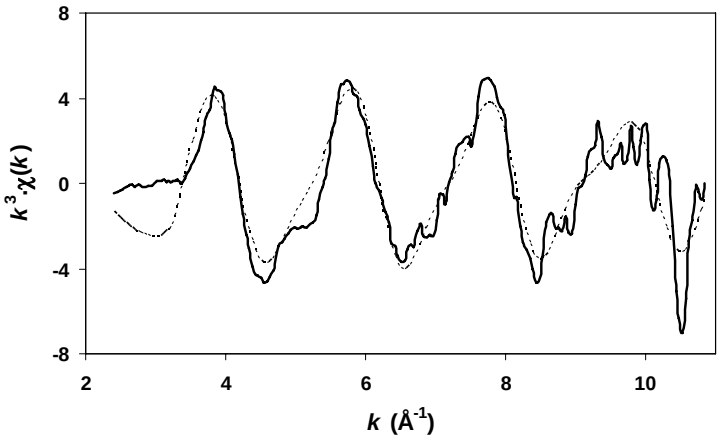

Figure S5. Experimental k^3-weighted EXAFS function (solid line) and fit (dashed line) for Au/CeO_2-CN dried at 393K.

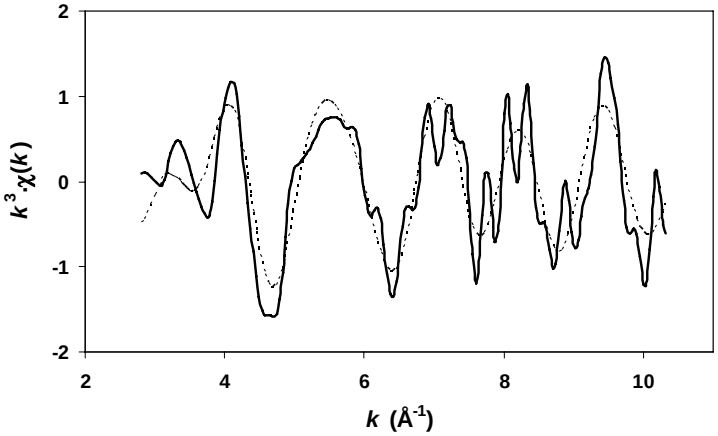

Figure S6. Experimental k^3-weighted EXAFS function (solid line) and fit (dashed line) for Au/CeO_2-CN reduced at 523K.

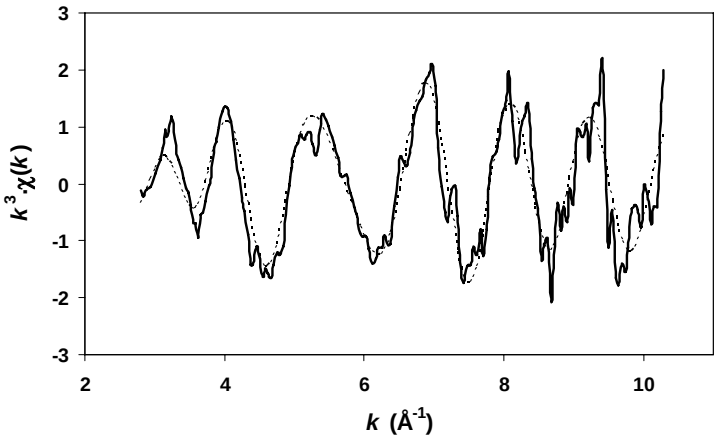

Figure S7. Experimental k^3-weighted EXAFS function (solid line) and fit (dashed line) for Au/CeO_2-CN reduced at 773K.