Electronic Supplementary Information

Nanostructured terbium-doped ceria spheres: Effect of dopant on physical and chemical properties under reducing and oxidizing conditions

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Table 1. Structural parameters and standard Rietveld agreement factor for nanostructured TbDC10 spheres (HMW).

Atmosphere	Air	5%H_2/He	5%H_2/He	21%O_2/ N_2	21%O_2/ N_2
T (ºC)	25	300	500	500	25
a (Å)	5.4069(6)	5.4223(9)	5.4472(8)	5.4347(8)	5.4038(8)
V (Å^3)	158.077(3)	159.422(5)	161.629(4)	160.525(4)	157.798(4)
R_p	3.22	3.55	3.64	3.64	3.20
R_{wp}	3.84	4.24	4.33	4.29	3.93
R_e	2.29	2.25	2.33	2.33	2.22
χ^2	2.80	3.53	3.46	3.40	3.14

Table 2. Structural parameters and standard Rietveld agreement factor for nanostructured TbDC20 spheres (HMW).

Atmosphere	Air	5%H_2/He	5%H_2/He	21%O_2/ N_2	21%O_2/ N_2
T (ºC)	25	300	500	500	25
a (Å)	5.4049(6)	5.4213(9)	5.4479(8)	5.4291(8)	5.3992(8)
V (Å^3)	157.896(3)	159.337(5)	161.699(4)	160.025(4)	157.399(4)
R_p	3.06	3.04	3.59	3.35	3.34
R_{wp}	3.73	3.68	4.19	4.07	4.06
R_e	2.45	2.33	2.40	2.43	2.46
χ^2	2.32	2.50	3.04	2.80	2.72

Table 3. Structural parameters and standard Rietveld agreement factor for nanostructured TbDC10 powder (CC).

Atmosphere	Air	5%H_2/He	5%H_2/He	21%O_2/ N_2	21%O_2/ N_2
T (ºC)	25	300	500	500	25
a (Å)	5.4032(6)	5.4261(9)	5.4474(8)	5.4346(8)	5.4036(8)
V (Å^3)	157.750(3)	159.761(5)	161.647(4)	160.511(4)	157.780(4)
R_p	2.39	2.90	3.37	3.16	2.50
R_{wp}	2.95	3.45	3.89	3.70	3.08
R_e	2.25	2.24	2.29	2.32	2.27
χ^2	1.72	2.39	2.89	2.55	1.84

Table 4. Structural parameters and standard Rietveld agreement factor for nanostructured TbDC20 powder (CC).

Atmosphere	Air	5%H_2/He	5%H_2/He	21%O_2/ N_2	21%O_2/ N_2
T (ºC)	25	300	500	500	25
a (Å)	5.3931(6)	5.4118(9)	5.4484(8)	5.4219(8)	5.3891(8)
V (Å^3)	156.862(3)	158.499(5)	161.736(4)	159.388(4)	156.516(4)
R_p	2.49	2.61	3.14	3.00	2.48
R_{wp}	3.06	3.28	3.79	3.68	3.21
R_e	2.44	2.33	2.44	2.48	2.47
χ^2	1.57	1.98	2.40	2.20	1.39

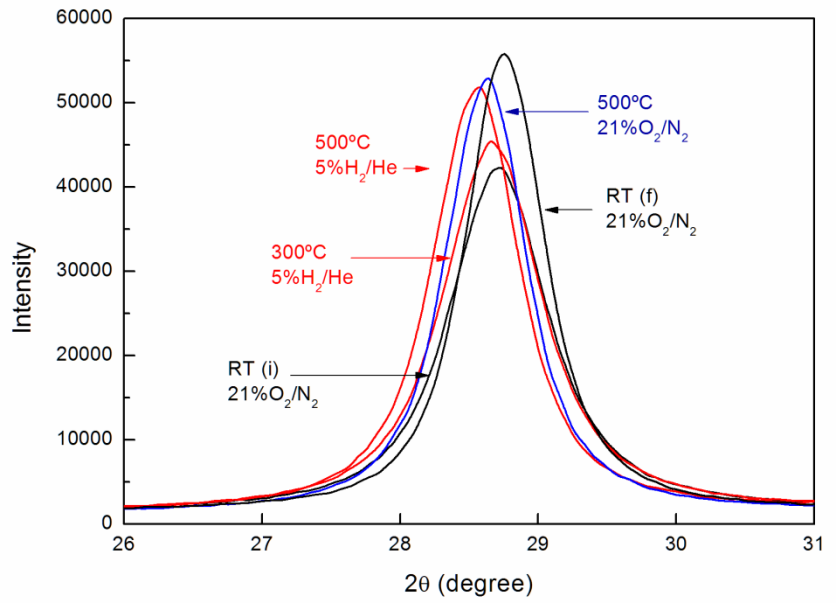

Figure S1. SR-XRD patterns in the vicinity of the 111 reflection for nanostructured TbDC10 spheres (HMW). RT (i) and (f) indicate the initial state (fresh sample) and final state (after exposure to the different redox conditions described in the text) of the sample, respectively.

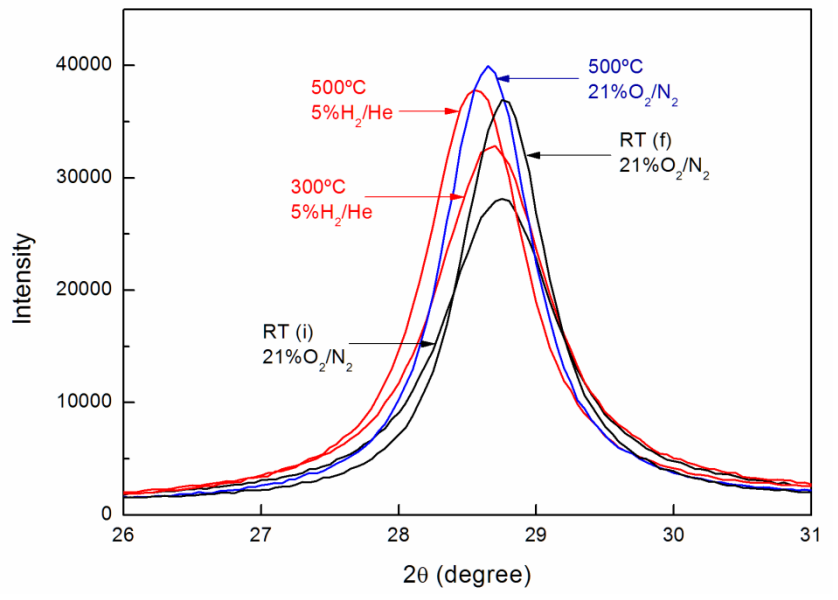

Figure S2. SR-XRD pattern in the vicinity of the 111 reflection for nanostructured TbDC20 spheres (HMW). RT (i) and (f) indicate the initial state (fresh sample) and final state (after exposure to the different redox conditions described in the text) of the sample, respectively.

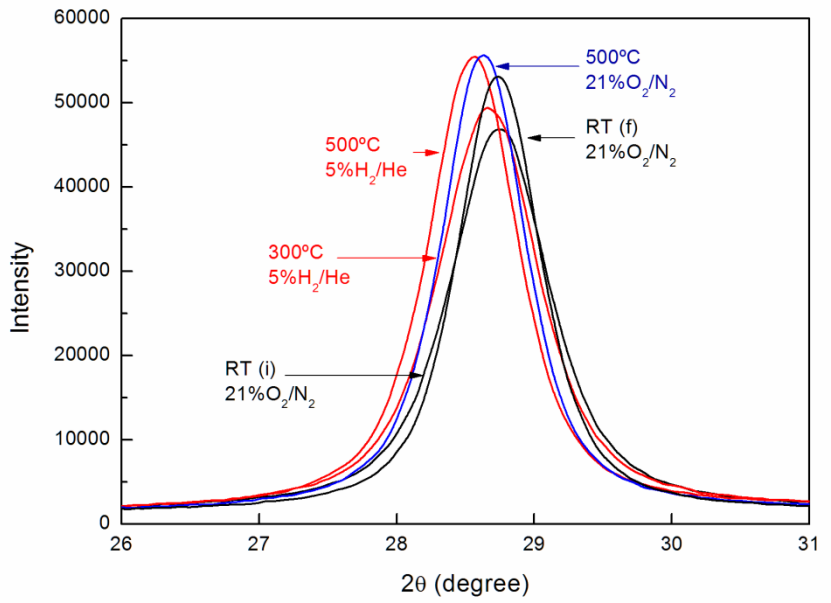

Figure S3. SR-XRD pattern in the vicinity of the 111 reflection for nanostructured TbDC10 powders (CC). RT (i) and (f) indicate the initial state (fresh sample) and final state (after exposure to the different redox conditions described in the text) of the sample, respectively.

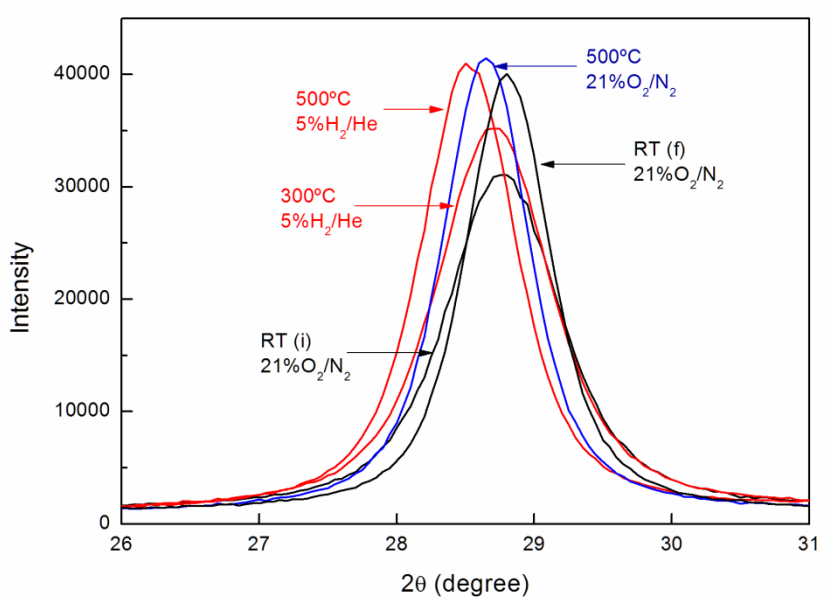

Figure S4. SR-XRD pattern in the vicinity of the 111 reflection for nanostructured TbDC20 powders (CC). RT (i) and (f) indicate the initial state (fresh sample) and final state (after exposure to the different redox conditions described in the text) of the sample, respectively.

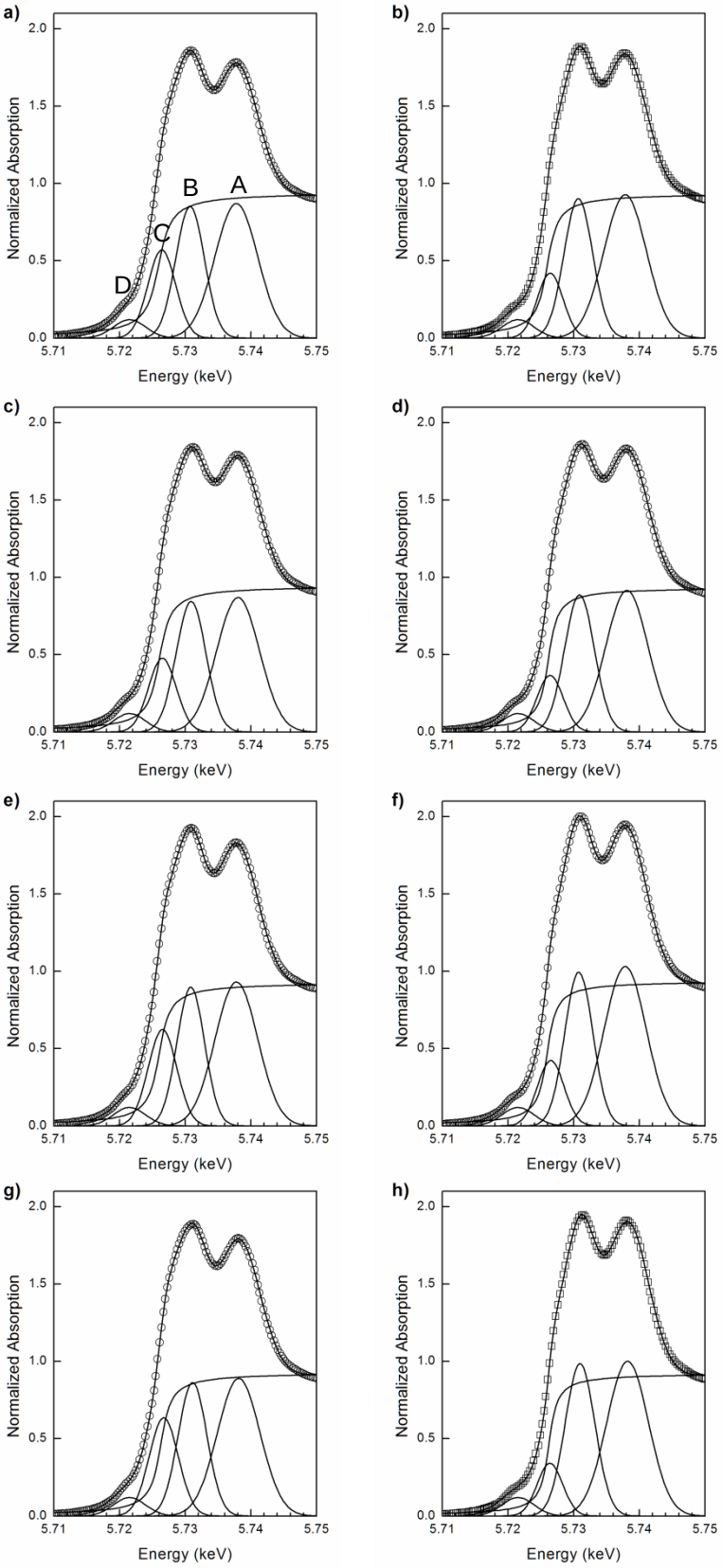

Figure S5. Normalized XANES spectra at the Ce L_3-edge for TbDC10-HMW, TbDC20-HMW, TbDC10-CC and TbDC20-CC at 500 ºC under (a, c, e and g) reducing and (b, d, f and h) oxidizing conditions, respectively, showing the experimental data (empty circles), four Gaussian peaks (A–D), one arctangent function obtained by least-squares fitting and the sum of all five functions (continuous line).