

Supplementary Materials: Effect of the (Nd,Dy)-Double Doping on the Structural Properties of Ceria

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Table 1. Hybrid structural model compared to the F structure typical of CeO₂ and the C structure typical of sesquioxides of heavy rare earths, such as Dy₂O₃; data of Dy₂O₃ are taken from M. Chandrasekar *et al.*, *Mater. Res. Bull.* **2014**, *55*, 237-245.

CeO ₂ F structure <i>cF12 Fm-3m Z = 4</i> <i>a = 5.4097(1) Å [8]</i>			Ce _{1-x} (Nd _{0.63} Dy _{0.37}) _x O _{2-x/2} Hybrid model for Rietveld refinement of samples with <i>x = 0.5</i> and <i>0.6</i> <i>cI96 Ia-3 Z = 32</i>			Dy ₂ O ₃ C structure <i>cI80 Ia-3 Z = 16</i> <i>a=10.684 Å</i>		
Atom	Wyckoff site	Coordinates	Atom	Wyckoff site	Coordinates	Atom	Wyckoff site	Coordinates
Ce	4 <i>a</i>	0, 0, 0	Ce/Nd/Dy1	24 <i>d</i>	<i>x</i> , 0, 1/4 <i>x = 0.25</i>	Dy1	24 <i>d</i>	<i>x</i> , 0, 1/4 <i>x = 0.2761</i>
			Ce/Nd/Dy2	8 <i>a</i>	0, 0, 0	Dy2	8 <i>a</i>	0, 0, 0
O	8 <i>c</i>	1/4, 1/4, 1/4	O1	48 <i>e</i>	<i>x</i> , <i>y</i> , <i>z</i> <i>x = 0.125</i> <i>y = 0.375</i> <i>z = 0.125</i>	O	48 <i>e</i>	<i>x</i> , <i>y</i> , <i>z</i> <i>x = 0.1039</i> <i>y = 0.359</i> <i>z = 0.1489</i>
			O2	16 <i>c</i>	<i>x</i> , <i>x</i> , <i>x</i> <i>x = 0.125</i>			