

High Pressure X-ray Diffraction as a Tool for Designing Doped Ceria Thin Films Electrolytes

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Table S1. Hybrid structural model compared to the F model typical of CeO₂ and the C model typical of sesquioxides of heavy rare earths, such as Tm₂O₃. Data of CeO₂ are taken from C. Artini et al. [1]; data of Tm₂O₃ are taken from J.L. Blanus et al. [2].

CeO ₂ F structure <i>cF12 Fm-3m Z=4</i> <i>a=5.4097(1) Å</i>			Ce _{1-x} RE _x O _{2-x/2} Hybrid Model for Rietveld Refinement of Sample with <i>x=0.6</i> <i>cI96 Ia-3 Z=32</i>			RE ₂ O ₃ C Structure <i>cI80 Ia-3 Z=16</i> for RE ≡ Tm, <i>a=10.4908(1) Å</i>		
Atom	Wyckoff site	Coordinates	Atom	Wyckoff site	Coordinates	Atom	Wyckoff site	Coordinates
Ce	4 <i>a</i>	0, 0, 0	RE1	24 <i>d</i>	<i>x</i> , 0, 1/4 <i>x</i> = 0.25	RE1	24 <i>d</i>	<i>x</i> , 0, 1/4 <i>x</i> = 0.2839
			RE2	8 <i>a</i>	0, 0, 0	RE2	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</i> = 0.125 <i>y</i> = 0.375	O	48 <i>e</i>	<i>x</i> , <i>y</i> , <i>z</i> <i>x</i> = 0.096 <i>y</i> = 0.361
					<i>z</i> = 0.125			<i>z</i> = 0.129
			O2	16 <i>c</i>	<i>x</i> , <i>x</i> , <i>x</i> <i>x</i> = 0.125	-	-	-

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