Insights into the Fe^{3+}-doping effects on the structure and electron distribution of Cr_2O_3 nanoparticles

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Table S1: Crystal data and refined parameters for $Cr_{2-x}Fe_xO_3$ ($0.0 \leq x \leq 0.18$) nanoparticles obtained from X-ray diffraction.

Parameters	$Cr_{2-x}Fe_xO_3$			
	x = 0.0	**x = 0.06**	**x = 0.12**	**x = 0.18**
Crystal system	Rhombohedral	Rhombohedral	Rhombohedral	Rhombohedral
Space group	R -3c (167)	R -3c (167)	R -3c (167)	R -3c (167)
Lattice parameters				
a = b (Å)	4.957243	4.957635	4.959920	4.960923
c (Å)	13.594714	13.595851	13.599133	13.598163
c/a	2.742394	2.742407	2.741805	2.741055
$\alpha = \beta$ (°)	90.00	90.00	90.00	90.00
γ(°)	120.0	120.00	120.00	120.00
Unit cell volume (Å^3)	289.322	289.392	289.729	289.825
X-ray density (g/cm^3)	5.245	5.253	5.261	5.269
Atomic coordinates				
Cr^{3+}/Fe^{3+}				
x	0	0	0	0
y	0	0	0	0
z	0.34765	0.34702	0.34783	0.34780
Biso	1.82691	2.04750	2.24590	1.81561
Occupancy	0.35246/0	0.33757/0.02426	0.32969/0.03638	0.31478/0.04148
Wyckoff notations	12c	12c	12c	12c
O^{2-}				
x	0.31465	0.31061	0.30636	0.30669
y	0.00000	0.00000	0.00000	0.00000
z	1/4	1/4	1/4	1/4
Biso	0.0	0.0	0.0	0.0
Occupancy	0.51913	0.51427	0.51639	0.51148
Wyckoff notations	18e	18e	18e	18e
Microstructure				
Average crystallite size (nm)	22.9 ± 2.8	33.5 ± 4.3	43.2 ± 3.0	75.5 ± 7.7
Crystallite Apparent size 010 (nm)	22.9	31.0	43.5	77.3
Crystallite Apparent size 001 (nm)	25.1	43.5	47.4	87.5
Crystallite Apparent size 100 (nm)	18.1	29.2	41.4	68.2
Microstrain $\langle\varepsilon\rangle \times 10^{-4}$	11.2 ± 2.5	5.2 ± 1.7	5.8 ± 1.4	1.4 ± 0.8
Bond Valence Sum				
Cr^{3+}	2.903	3.014	3.102	3.345
Fe^{3+}	-	3.609	3.519	3.126
O^{2-}	1.935	1.992	2.084	1.972
Refinement parameters				
R_P	6.20	6.14	5.59	5.40
R_{WP}	7.90	7.83	7.15	6.82
R_{Exp}	6.82	6.98	6.62	6.19
χ^2	1.34	1.26	1.16	1.21
R_d (%)	100	99.59	98.89	94.85

Bond lengths (Å)				
(Cr/Fe)-O1	2.047(9)	2.033(7)	2.024(6)	2.036(7)
(Cr/Fe)-O2	1.943(2)	1.952(2)	1.958(3)	1.945(8)
<Cr/Fe-O>	1.995(6)	1.992(9)	1.991(5)	1.991(3)
Angles (degree)				
(Cr/Fe)-O-(Cr/Fe)	80.3(4)	80.8(3)	82.5(4)	82.9(1)