Supporting information for

The Local and Electronic Structure Study of $Lu_xGd_{1-x}VO_4$ ($0 \leq x \leq 1$) Solid Solution Nanocrystals

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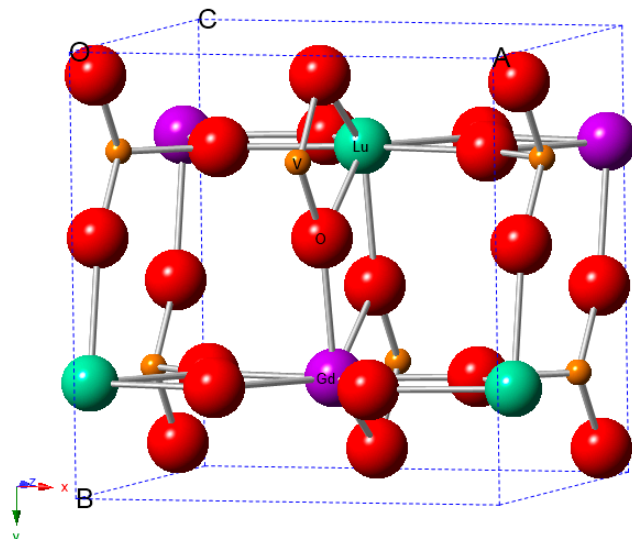
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Figure S1. Unit cell model of $Lu_{0.5}Gd_{0.5}VO_4$.

Table S1. Rietveld refined cell parameters and R factors for $Lu_xGd_{1-x}VO_4$ solid solutions.

x_{calc}	a (Å)	c (Å)	V (Å^3)	Bragg R-factor (%)	Rp (%)	Rwp (%)
0	7.21287	6.35552	330.649	5.25	5.29	6.64
0.1	7.19318	6.34168	328.130	3.48	4.84	6.18
0.3	7.15467	6.31936	323.484	8.87	5.68	7.24
0.5	7.12131	6.29779	319.380	3.40	5.91	7.47
0.7	7.08135	6.27193	314.509	3.39	6.03	7.81
0.9	7.04636	6.25044	310.342	4.85	7.54	9.53
1	7.02852	6.23600	308.059	8.11	9.85	12.8

Table S2. Fitting results of the nearest and next nearest neighbor coordination shells of the FT-EXAFS spectra of $Lu_xGd_{1-x}VO_4$ at the Gd L$_3$-edge, the coordination number (N) was fixed.

x	Gd⋯O1.1			Gd⋯O1.2		Gd⋯O	Gd⋯V			S_0^2	R-factor (%)
	R(Å)	σ^2(Å^2)	ΔE_0(eV)	R(Å)	σ^2(Å^2)	R(Å)	R(Å)	ΔE_0(eV)	σ^2(Å^2)		
0	2.339±0.025	0.0054	3.6	2.457±0.029	0.0069	2.398±0.027	3.201±0.013	7.2	0.0035	1.0	0.83
0.1	2.328±0.017	0.0045	3.2	2.455±0.021	0.0057	2.392±0.019	3.197±0.012	7.0	0.0035	1.0	0.70
0.3	2.326±0.015	0.0044	3.4	2.454±0.021	0.0060	2.390±0.018	3.200±0.012	8.4	0.0036	1.0	0.83
0.5	2.301±0.014	0.0036	2.1	2.444±0.016	0.0040	2.372±0.015	3.187±0.012	6.3	0.0034	1.0	0.82
0.7	2.318±0.015	0.0034	3.8	2.458±0.022	0.0050	2.388±0.018	3.181±0.014	6.6	0.0033	1.0	1.3
0.9	2.280±0.020	0.0028	1.4	2.434±0.022	0.0020	2.357±0.021	3.173±0.023	4.9	0.0030	1.0	1.7

Table S3. Fitting results of the nearest and next nearest neighbor coordination shells of the FT-EXAFS spectra of $Lu_xGd_{1-x}VO_4$ at the Lu L$_3$-edges, the coordination number (N) was fixed.

x	Lu⋯O1.1			Lu⋯O1.2		Lu⋯O	Lu⋯V			S_0^2	R-factor (%)
	R(Å)	σ^2(Å^2)	ΔE_0(eV)	R(Å)	σ^2(Å^2)	R(Å)	R(Å)	ΔE_0(eV)	σ^2(Å^2)		
0.1	2.296±0.015	0.0032	8.1	2.417±0.039	0.0093	2.356±0.027	3.135±0.012	5.1	0.0022	0.91	2.1
0.3	2.266±0.017	0.0048	6.0	2.396±0.025	0.0079	2.331±0.021	3.152±0.012	7.8	0.0040	0.89	0.85
0.5	2.263±0.010	0.0049	5.8	2.397±0.018	0.0087	2.330±0.014	3.153±0.008	8.5	0.0039	0.93	0.77
0.7	2.251±0.008	0.0045	5.3	2.394±0.013	0.0076	2.322±0.011	3.149±0.008	8.7	0.0042	0.94	0.61
0.9	2.244±0.009	0.0048	5.1	2.386±0.016	0.0077	2.315±0.012	3.136±0.008	7.5	0.0040	0.92	0.77
1	2.242±0.006	0.0045	5.0	2.386±0.012	0.0076	2.314±0.009	3.134±0.006	7.7	0.0036	0.91	0.42

Table S4. Average distances from the dodecahedron central atoms to the first and second coordination shells and the dodecahedron distortion indexes for $Lu_xGd_{1-x}VO_4$ solid solutions.

x	Average distances		Dodecahedron distortion index	
	RE···O (Å)	**RE···V (Å)**	**GdO$_8$**	**LuO$_8$**
0	2.398±0.027	3.201±0.013	0.0246	
0.1	2.388±0.020	3.191±0.012	0.0266	0.0257
0.3	2.372±0.019	3.186±0.012	0.0268	0.0279
0.5	2.351±0.014	3.170±0.010	0.0301	0.0288
0.7	2.342±0.013	3.159±0.010	0.0293	0.0308
0.9	2.319±0.013	3.140±0.010	0.0327	0.0307
1	2.314±0.009	3.134±0.006		0.0311

The polyhedral distortion index was calculated by $D = \frac{1}{n}\sum_{i=1}^{n} \frac{|l_i - l_{av}|}{l_{av}}$ [1].

Table S5. Binding energies of characteristic peaks of all component elements and binding energy differences (ΔBE) between metal and oxygen characteristic peak of $Lu_xGd_{1-x}VO_4$ solid solutions.

x	0	0.2	0.4	0.5	0.6	0.8	1
O 1s (eV)	530.12	530.22	530.00	529.95	530.03	529.92	529.87
V^{5+} 2$p_{3/2}$ (eV)	517.32	517.40	517.18	517.14	517.22	517.11	517.07
ΔBE (O-V) (eV)	12.80	12.82	12.82	12.81	12.81	12.81	12.80
Lu 4$d_{5/2}$ (eV)	-	196.76	196.41	196.40	196.36	196.24	196.13
ΔBE (O-Lu) (eV)	-	333.46	333.59	333.55	333.67	333.68	333.74
ΔBE (Lu 4d$_{3/2}$-4d$_{5/2}$) (eV)		9.89	9.92	9.84	9.93	9.93	9.93
Gd 4d (eV)	141.66	141.79	141.47	141.55	141.50	141.48	-
ΔBE (O-Gd) (eV)	388.46	388.43	388.53	388.40	388.53	388.44	-

1. Baur, W.H. The geometry of polyhedral distortions. Predictive relationships for the phosphate group. *Acta Crystallogr. Sect. B* **1974**, *30*, 1195-1215.