

## Supplementary Information

# Investigation of crystal field effects for the spectral broadening of Yb<sup>3+</sup>-doped Lu<sub>x</sub>Y<sub>2-x</sub>O<sub>3</sub> sesquioxide crystals

Ruiqi Guo,<sup>1</sup> Dapeng Huang,<sup>1</sup> Dazhi Lu,<sup>1</sup> Fei Liang,<sup>1</sup> Qingli Zhang,<sup>2</sup> Haohai Yu,<sup>1</sup> Huaijin Zhang<sup>1</sup>

<sup>1</sup>State Key Laboratory of Crystal Materials and Institute of Crystal Materials, Shandong University, Jinan 250100, China

<sup>2</sup>Anhui Institute of Optics and Fine Mechanics, Chinese Academy of Sciences, Hefei 230031, China

**Table S1.** Lattice parameters of the Yb:Lu<sub>x</sub>Y<sub>2-x</sub>O<sub>3</sub> series crystals

<i>x</i>	0	0.79	0.99	1.19	1.39	2.00
<i>a</i> (Å)	10.3776	10.462	10.4796	10.494	10.5218	10.6056

**Table S2.** Crystal field parameters obtained by SM fitting as initial parameters of CFPfit (unit: cm<sup>-1</sup>).

<i>x</i>	$B_0^2(0)$	$B_2^2(0)$	$B_0^4(0)$	$B_2^4(0)$	$B_4^4(0)$
0	-98.67	129.95+316.65i	-1224.47	36.87+1351.2i	-1140.53-269i
0.79	-175.1	121.37+395.6i	-1179.04	14.33+1294.9i	-1134.49-264.08i
0.99	-151.22	115.31+353.03i	-1202.01	16.2+1335.9i	-1159.46-274.12i
1.19	-185.64	154.26+439.09i	-1153.11	19.36+1281.36i	-1112.39-263.76i
1.39	-135.08	134.63+376.5i	-1214.65	27.66+1347.57i	-1147.49-268.81i
2.00	-135.25	84.05+378.37i	-1256.62	13.7+1374.51i	-1163.36-258.5i
<i>x</i>	$B_0^6(0)$	$B_2^6(0)$	$B_4^6(0)$	$B_6^6(0)$	
0	133.58	11.31+32.82i	-484.89-15.05i	-68.08+59.45i	
0.79	193.03	16.12+29.76i	-622-35.73i	-73.96+82.52i	
0.99	190.77	17.08+35.09i	-641.5-34.83i	-79.91+86.6i	
1.19	206.85	17.85+39.89i	-694.97-34.98i	-90.16+93.25i	

1.39	186.29	17.64+35.43i	-654.81-26.52i	-84.66+82.52i
2.00	195.37	22.17+13.03i	-666.56-36.22i	-63.23+78.12i

**Table S3.** Experimental and calculated energy levels in unit  $\text{cm}^{-1}$  and calculational accuracy of CFPFit\*.

$x$		E(1)	E(2)	E(3)	E(4)	E(5)	E(6)	E(7)	$R$ (%)	$\sigma$ ( $\text{cm}^{-1}$ )
	$E_{\text{Exp}}$	0	422.72	532.45	943.58	10245.9	10548.52	11013.22		
0	$E_{\text{Cal}}$	-0.17	422.85	532.7	944.28	10246.01	10548.35	11012.38	0.0063	0.9469
	$\Delta_E$	0.17	-0.13	-0.25	-0.7	-0.11	0.17	0.84		
	$E_{\text{Exp}}$	0	448.64	555.21	956.68	10256.41	10559.66	11025.36		
0.79	$E_{\text{Cal}}$	0	448.65	555.23	956.73	10256.41	10559.64	11025.3	0.0005	0.0683
	$\Delta_E$	0	-0.01	-0.02	-0.05	0	0.02	0.06		
	$E_{\text{Exp}}$	0	452.49	558.97	960.14	10256.41	10565.24	11031.44		
0.99	$E_{\text{Cal}}$	-0.01	452.5	558.99	960.2	10256.42	10565.23	11031.37	0.0005	0.0787
	$\Delta_E$	0.01	-0.01	-0.02	-0.06	-0.01	0.01	0.07		
	$E_{\text{Exp}}$	0	463.51	565.17	967.99	10261.67	10570.82	11037.53		
1.19	$E_{\text{Cal}}$	0	463.54	565.2	968.06	10261.66	10570.79	11037.45	0.0006	0.097
	$\Delta_E$	0	-0.03	-0.03	-0.07	0.01	0.03	0.08		
	$E_{\text{Exp}}$	0	467.35	565.17	972.31	10261.67	10576.41	11043.62		
1.39	$E_{\text{Cal}}$	-0.01	467.37	565.19	972.37	10261.66	10576.38	11043.54	0.0006	0.0891
	$\Delta_E$	0.01	-0.02	-0.02	-0.06	0.01	0.03	0.08		
	$E_{\text{Exp}}$	0	482.2	577.02	992.22	10266.94	10587.61	11049.72		
2.00	$E_{\text{Cal}}$	0.52	483.05	577.93	993.56	10266.07	10586.41	11048.2	0.0154	2.3272
	$\Delta_E$	-0.52	-0.85	-0.91	-1.34	0.87	1.2	1.52		

$$*\Delta_E = E_{\text{Exp}} - E_{\text{Cal}}, R = \sqrt{\frac{\sum_{i=1}^{14} (E_i^{\text{exp}} - E_i^{\text{cal}})^2}{\sum_{i=1}^{14} (E_i^{\text{exp}})^2}}, \sigma = \sqrt{\frac{\sum_{i=1}^{14} (E_i^{\text{exp}} - E_i^{\text{cal}})^2}{3}}$$