

*Supporting Information for:*

## **Color-Tunable and Single-Band Red Upconversion Luminescence form Rare-Earth Doped Vernier Phase Ytterbium Oxyfluoride Nanoparticles**

*Ting Wen, Yannan Zhou, Yanzhen Guo, Chunmei Zhao, Baocheng Yang and Yonggang Wang\**

Institute of Nanostructured Functional Materials, Huanghe Science and Technology College, Zhengzhou, Henan 450006, China

### ***Supporting figures:***

**Figure S1.** Schematic representation of Yb-Yb distances in the Yb sublattice in *V*-YbOF exhibiting 2D layered structural feature.

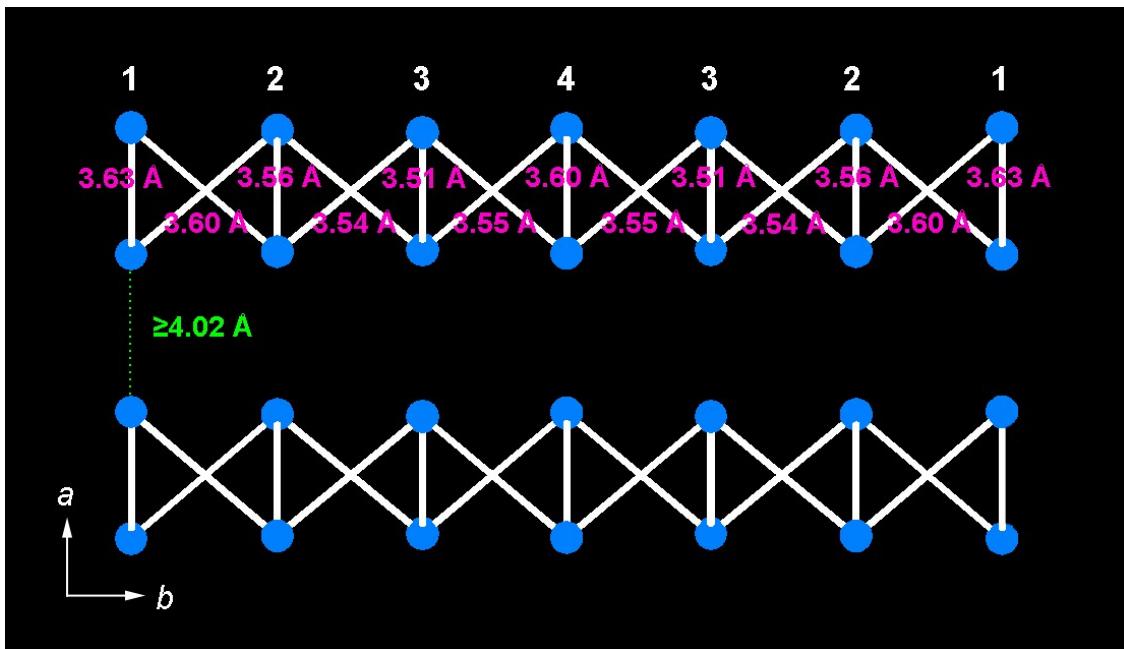
**Figure S2.** CIE chromaticity diagram of UC PL from *V*-YbOF:Ho (0.2-6 mol%) nanoparticles under 980 nm irradiation.

### ***Supporting tables:***

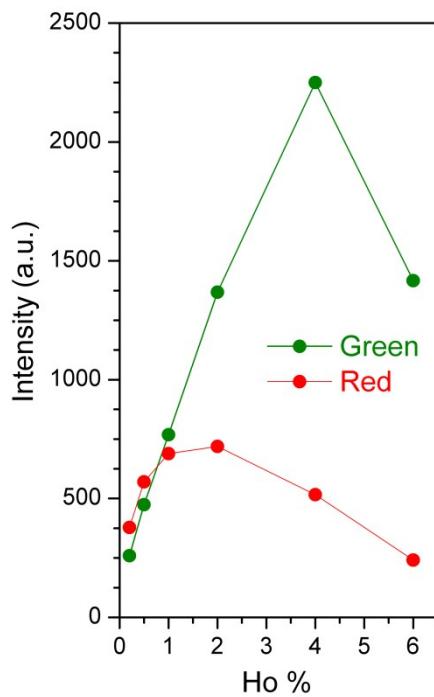
**Table S1.** EDX results of individual undoped *V*-YbOF particles.

**Table S2.** Refined crystal structure of Vernier phase  $\text{Yb}_6\text{O}_5\text{F}_8$  from powder X-ray diffraction data at room temperature.

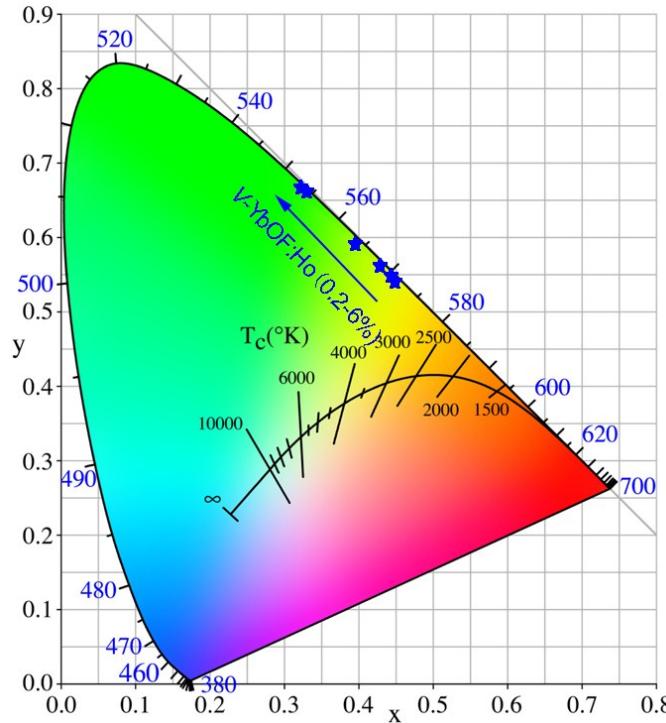
**Table S3.** Measured lifetimes of the green and red UC emissions for  $x\%\text{Ho}^{3+}$  doped *V*-YbOF ( $x = 0.5, 1, 2, 5$ ).



**Figure S1.** Schematic representation of Yb-Yb distances in the Yb sublattice in  $V$ -YbOF exhibiting 2D layered structural feature.



**Figure S2.** UC PL intensities of the two peaks of  $\text{Ho}^{3+}$ -doped  $V$ -YbOF as a function of the  $\text{Ho}^{3+}$  doping concentration.



**Figure S3.** CIE chromaticity diagram of UC PL from  $V\text{-YbOF:Ho}$  (0.2-6 mol%) nanoparticles under 980 nm irradiation.

**Table S1.** EDX results of individual undoped  $V\text{-YbOF}$  particles.

Particles	1	2	3	4	5	6	7	8	average
Yb/O/F	1.15/1/1.78	1.17/1/1.58	1.24/1/1.71	1.26/1/1.63	1.13/1/1.74	1.14/1/1.58	1.21/1/1.62	1.13/1/1.72	1.18/1/1.67

**Table S2.** Refined crystal structure of Vernier phase  $\text{Yb}_6\text{O}_5\text{F}_8$  from powder X-ray diffraction data at room temperature.<sup>a</sup>

Atom	Site	<i>x</i>	<i>y</i>	<i>z</i>	Occ.	BVS
Yb1	4 <i>c</i>	0.69434	0.00000	0.25000	1	+2.85
Yb2	8 <i>e</i>	0.28382	0.08387	0.28268	1	+2.81
Yb3	8 <i>e</i>	0.71056	0.16358	0.23121	1	+2.75
Yb4	4 <i>c</i>	0.28908	0.25000	0.29836	1	+2.79
O1	8 <i>e</i>	0.42560	0.04754	0.04139	1	
O2	8 <i>e</i>	0.51792	0.12288	0.47124	1	
O3	8 <i>e</i>	0.49454	0.20387	0.00112	0.5	
F1	8 <i>e</i>	0.49454	0.20387	0.00112	0.5	
F2	8 <i>e</i>	0.00605	0.03542	0.41742	1	
F3	8 <i>e</i>	0.93895	0.10649	0.11570	1	
F4	8 <i>e</i>	0.09279	0.17882	0.34194	1	
F5	4 <i>c</i>	0.18913	0.25000	0.17351	1	

<sup>a</sup>Space group:  $Pcmb$ ,  $a = 5.3323(7)$  Å,  $b = 6 \times 5.4581(5)$  Å, and  $c = 5.4676 (8)$  Å,  $R_p = 3.98\%$ ,  $R_{wp} = 5.32\%$ .

**Table S3.** Measured lifetimes of the green and red UC emissions for  $x\%$ Ho<sup>3+</sup> doped  $V$ -YbOF ( $x = 0.5, 1, 2, 4$ ).

$x$ in $x\%$ Ho: $V$ -YbOF	0.5%	1.0%	2.0%	4.0%
545 nm	4.8 $\mu$ s	5.4 $\mu$ s	5.6 $\mu$ s	7.2 $\mu$ s
660 nm	5.4 $\mu$ s	6.3 $\mu$ s	6.8 $\mu$ s	11.5 $\mu$ s