

Supporting Information

Design and synthesis of a novel blue-emitting **CaNaSb₂O₆F:Bi³⁺ phosphor for optical temperature sensing**

Xuexia Chen,^{a,b} Ran Pang,^a Shangwei Wang,^a Jiangyue Su,^{a,b} Weihong Yuan,^{a,b}
Shengjian Jiao,^{a,b} Haiyan Wu,^{a,b} Da Li, *^a Chengyu Li^{a,b} and Hongjie Zhang^{a,c}

^a State key Laboratory of Rare Earth Resource Utilization, Changchun Institute of Applied Chemistry, Chinese Academy of Sciences, Changchun 130022, P. R. China

^b School of Applied Chemistry and Engineering, University of Science and Technology of China, Hefei 230026, China

^c The GBA National Institute for Nanotechnology Innovation, Guangzhou 510535, China

* Corresponding author: Tel: +86-0431-85262258

E-mail address: cyli@ciac.ac.cn and pangran@ciac.ac.cn

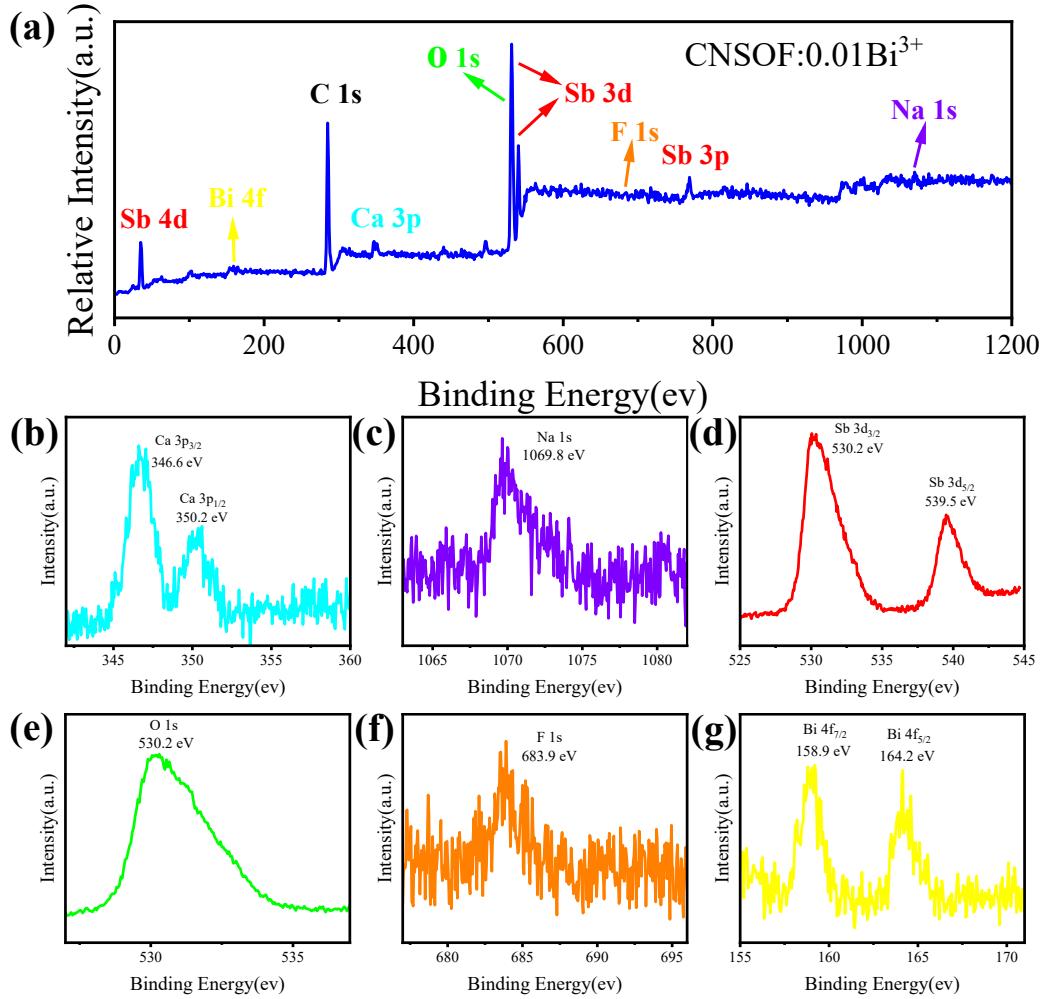


Fig. S1 XPS spectrogram of the CNSOF:Bi³⁺ phosphor. (a) Survey spectrum, (b) Ca-3p, (c) Na-1s, (d) Sb-3d, (e) O-1s, (f) F-1s and (g) Bi-4f.

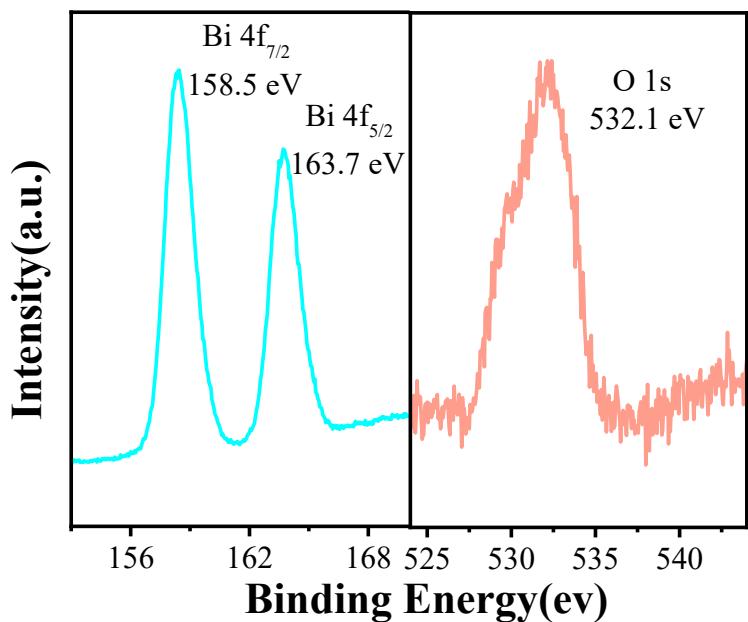


Fig. S2 XPS survey spectrum of the Bi_2O_3 .

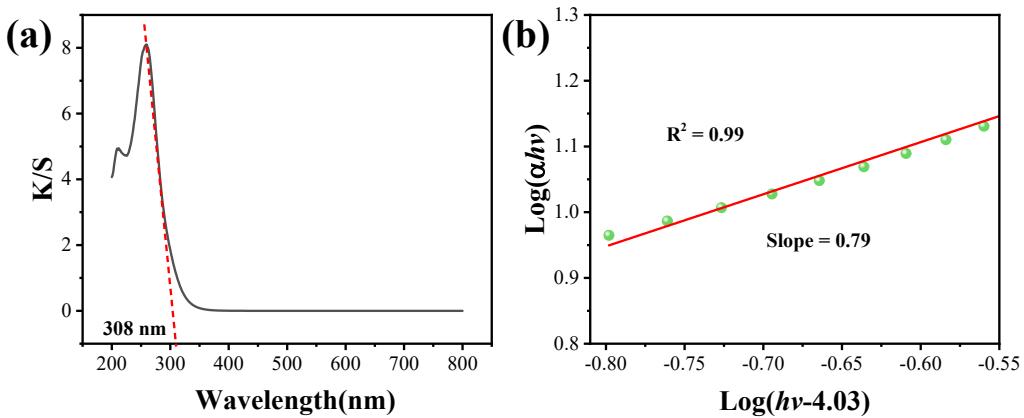


Fig. S3 Determination of the band gap of $\text{CaNaSb}_2\text{O}_6\text{F}$.

The band gap of $\text{CaNaSb}_2\text{O}_6\text{F}$ can be estimated according to equation (E1).

$$\alpha h\nu = A(h\nu - E_g)^{m/2} \quad (\text{E1})$$

Where $h\nu$ is the photon energy; E_g is the value of the band gap; $m = 1$ for a direct band-gap; $m = 4$ for an indirect band-gap. This equation can be derived as:

$$\text{Log}(ahv) = (m/2) \text{log}(h\nu - E_g) + \text{log}(A) \quad (\text{E2})$$

A spectrum shown in Figure S3a similar to the absorption spectrum is converted from the DRS spectrum. An approximate E_g is estimated as 4.03 eV. According to the derived formula, the slope of $\text{Log}(ahv)$ vs. $\text{Log}(h\nu - E_g)$ is fitted with a liner equation to give the value of m . As shown in Figure S3b, m value is calculated to be 1. Thus, $\text{CaNaSb}_2\text{O}_6\text{F}$ has a direct band gap.

Table S1 Structure Refinement Parameters Obtained through Rietveld Refinement of Powder Diffraction Data of CNSOF.

Formula	CNSOF
Space group	<i>Fd-3m</i> (277)
$a = b = c$ (Å)	10.2850
$\alpha = \beta = \gamma$ (°)	90
Units, Z	8
V (Å ³)	1087.97
R_p (%)	5.47
R_{wp} (%)	8.08
χ^2	9.52

Table S2 Atomic coordinates of the CNSOF.

atom	site	x	y	z	Occupancy
Na1	16d	0.625000	0.625000	0.625000	0.5000
Ca1	16d	0.625000	0.625000	0.625000	0.5000
Sb1	16c	0.125000	0.125000	0.125000	1.0000
O1	48f	0.200000	0.000000	0.000000	1.0000
F1	8b	0.500000	0.500000	0.500000	1.0000

Table S3 The realistic possible error of the decay time of Bi³⁺ ion content in the range of 0.2-3 mol%.

x (mol%)	τ (ns)	ε (ns)
0.002	536.562	2.55
0.004	527.245	2.29
0.006	508.842	2.07
0.008	469.995	1.74
0.01	438.663	1.43
0.02	372.639	0.92
0.03	334.227	0.61