

## Supporting Information

### UNRAVELING THE PHOTOLUMINESCENCE PROPERTIES OF THE Sr<sub>10</sub>V<sub>6</sub>O<sub>25</sub> STRUCTURE THROUGH EXPERIMENTAL AND THEORETICAL ANALYSES

Mayara Mondego Teixeira<sup>1\*</sup>, Amanda Fernandes Gouveia<sup>2\*</sup>, Aleksandro Gama de Sousa Gama<sup>3</sup>, Luís Fernando da Silva<sup>4</sup>, Regiane Cristina de Oliveira<sup>5</sup>, Miguel A. San-Miguel<sup>2</sup>, Máximo Siu Li<sup>6</sup> and Elson Longo<sup>1\*</sup>.

<sup>1</sup>CDMF-UFSCar, Universidade Federal de São Carlos, P.O. Box 676, 13565-905, São Carlos, São Paulo, Brazil.

<sup>2</sup>Institute of Chemistry, State University of Campinas, 13083-970, Campinas, São Paulo, Brazil.

<sup>3</sup>UESB, Universidade Estadual do Sudeste da Bahia, 45700-000, Campus Itapetinga, Bahia, Brazil.

<sup>4</sup>Departamento de Física, Universidade Federal de São Carlos, Rod. Washington Luiz, km 235, P.O. Box 676, 13565-905, São Carlos, São Paulo, Brazil.

<sup>5</sup>Grupo de Modelagem e Simulações Moleculares, Universidade Estadual Paulista Júlio de Mesquita Filho, Faculdade de Ciências, P. O. Box 473, 17033-360, Bauru, São Paulo, Brazil.

<sup>6</sup>IFSC-Universidade de São Paulo, P.O. Box 369, 13560-970, São Carlos, São Paulo, Brazil.

**\*Corresponding authors:** elson.liec@gmail.com; mayaramondego.ufma@gmail.com; amandafernandes.gouveia@gmail.com

#### Supporting Information Details:

Number of pages: 4

Number of Figures: 3

Number of Tables: 2

#### Tables

**Table SI - 1.** Bond distance and bond angles in the [VO<sub>4</sub>], [Sr(1)O<sub>6</sub>], and [Sr(5)O<sub>7</sub>] clusters of the Sr<sub>10</sub>V<sub>6</sub>O<sub>25</sub> structure obtained by the MAH method with variation in the synthesis times. ....S2

**Table SI - 2.** CIE chromaticity coordinates (x, y), obtained from Fig. SI-3, for Sr<sub>10</sub>V<sub>6</sub>O<sub>25</sub> obtained by the MAH method.....S4

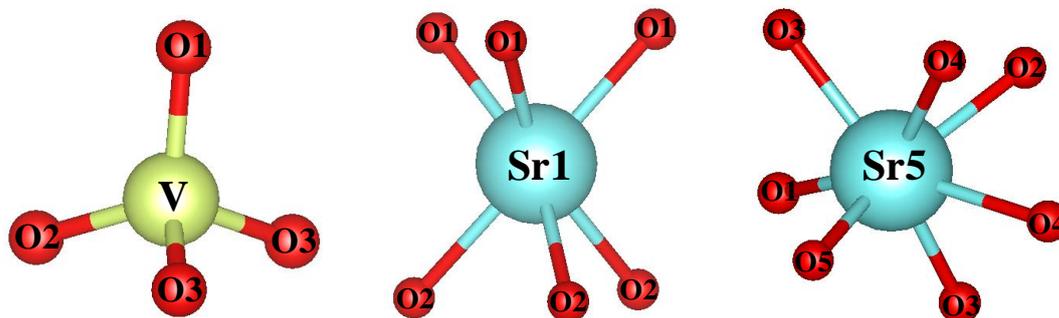
#### Figures

**Figure SI - 1.** FTIR spectra of the Sr<sub>10</sub>V<sub>6</sub>O<sub>25</sub> samples obtained by the MAH method at 120 °C by using different synthesis times. ....S3

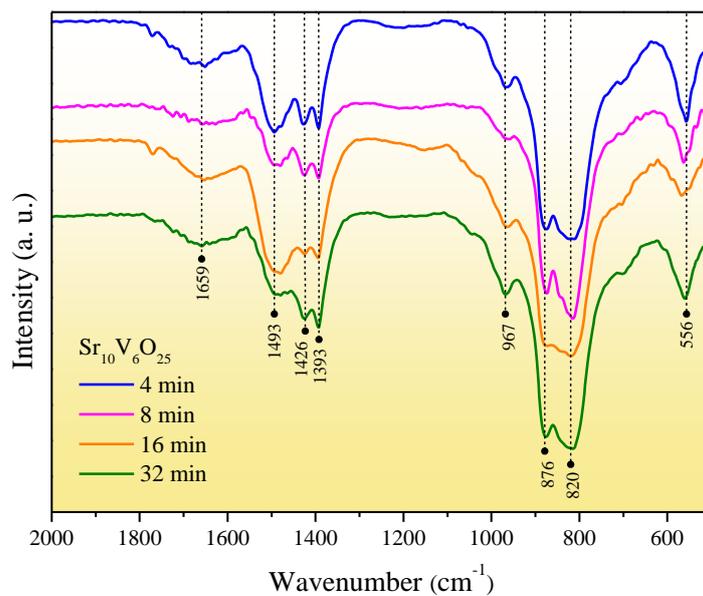
**Figure SI - 2.** High-resolution XPS spectra of (a) C 1s, and (b) O 1s for the Sr<sub>10</sub>V<sub>6</sub>O<sub>25</sub> samples obtained by the MAH method at 120 °C.....S3

**Figure SI - 3.** (a) PL spectra at room temperature ( $\lambda_{\text{ex}} = 350$  nm), and (b) CIE chromaticity diagram for the Sr<sub>10</sub>V<sub>6</sub>O<sub>25</sub> samples obtained by MAH using different synthesis times. ....S4

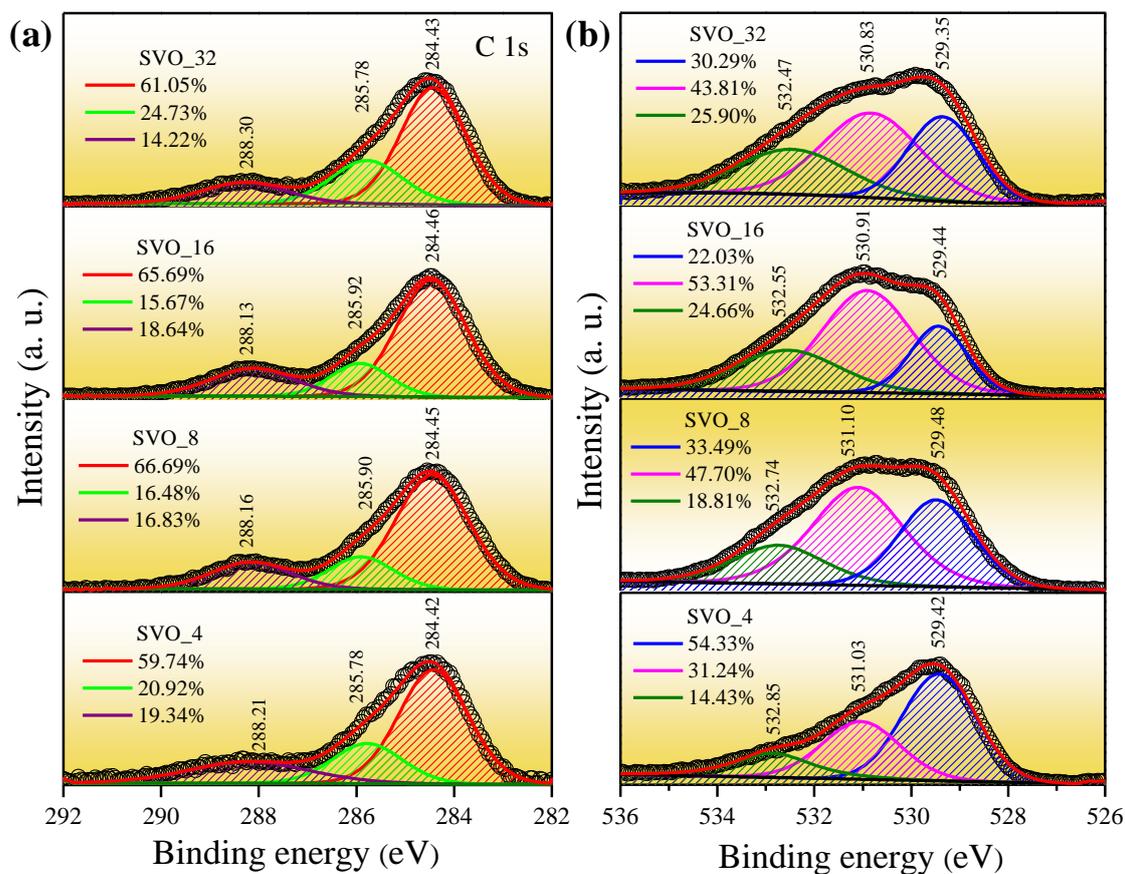
**Table SI - 1.** Bond distance and bond angles in the [VO<sub>4</sub>], [Sr(1)O<sub>6</sub>], and [Sr(5)O<sub>7</sub>] clusters of the Sr<sub>10</sub>V<sub>6</sub>O<sub>25</sub> structure obtained by the MAH method with variation in the synthesis times.



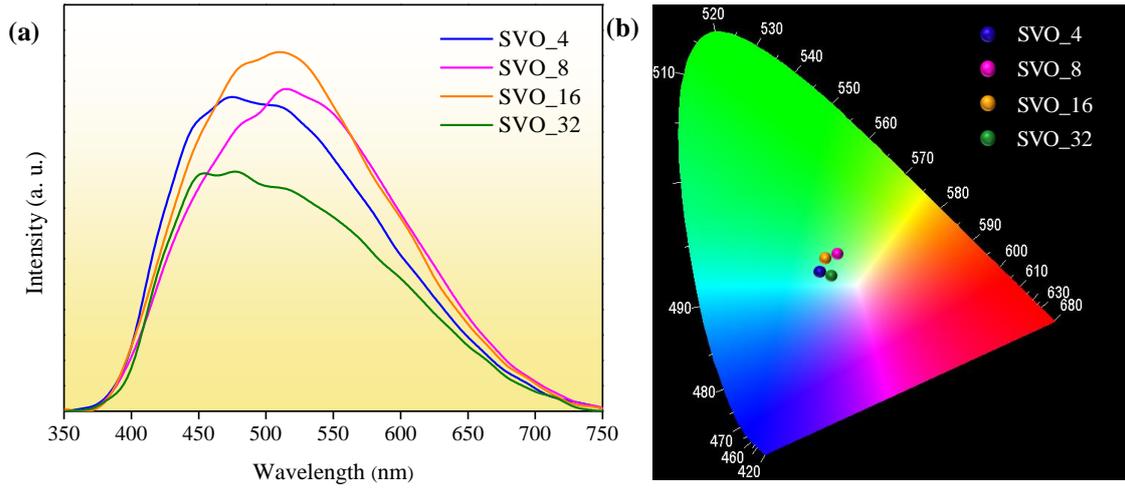
Cluster	Bond	Sr <sub>10</sub> V <sub>6</sub> O <sub>25</sub>			
		4 min	8 min	16 min	32 min
[VO <sub>4</sub> ]	V–O1 (Å)	1.67578(0)	1.65711(0)	1.65751(2)	1.71346(0)
	V–O2 (Å)	1.70371(0)	1.70348(3)	1.63370(0)	1.66805(0)
	V–O3 (x2) (Å)	1.72068(0)	1.74541(0)	1.76254(3)	1.67586(3)
	O1–V–O2 (°)	112.7752(0)	113.1613(0)	113.6263(0)	111.5897(0)
	O1–V–O3 (°)	110.0825(0)	108.4343(0)	108.1811(0)	109.3687(0)
	O2–V–O3 (°)	108.7250(0)	109.7463(0)	108.4651(0)	108.9033(0)
	O3–V–O3 (°)	106.2243(0)	107.1273(0)	109.8929(0)	108.6560(0)
[Sr(1)O <sub>6</sub> ]	Sr–O1 (x3) (Å)	2.57875(2)	2.61103(3)	2.63547(3)	2.57951(4)
	Sr–O2 (x3) (Å)	2.65012(0)	2.65715(3)	2.64750(3)	2.64663(4)
	O1–Sr–O2 (°)	93.2400(0)	92.5141(0)	92.4458(0)	93.4204(0)
[Sr(5)O <sub>7</sub> ]	Sr–O1 (Å)	2.76249(3)	2.73373(0)	2.74165(3)	2.77492(3)
	Sr–O2 (Å)	2.49460(0)	2.48283(0)	2.51946(0)	2.50881(0)
	Sr–O3 (x2) (Å)	2.48253(3)	2.44947(4)	2.43991(5)	2.51033(6)
	Sr–O4 (x2) (Å)	2.67321(3)	2.67571(0)	2.69275(3)	2.67502(3)
	Sr–O5 (Å)	2.49397(3)	2.48919(0)	2.48628(3)	2.48869(3)
	O1–Sr–O2 (°)	102.6186(0)	102.8531(0)	103.1716(0)	102.1875(0)
	O1–Sr–O3 (°)	71.9087(0)	72.0808(0)	70.4609(0)	71.3923(0)
	O1–Sr–O4 (°)	148.4082(0)	147.9503(0)	147.0741(0)	148.6430(0)
O1–Sr–O5 (°)	107.4956(0)	106.7532(0)	105.8066(0)	107.1700(0)	



**Figure SI - 1.** FTIR spectra of the  $\text{Sr}_{10}\text{V}_6\text{O}_{25}$  samples obtained by the MAH method at 120 °C by using different synthesis times.



**Figure SI - 2.** High-resolution XPS spectra of (a) C 1s, and (b) O 1s for the  $\text{Sr}_{10}\text{V}_6\text{O}_{25}$  samples obtained by the MAH method at 120 °C.



**Figure SI - 3.** (a) PL spectra at room temperature ( $\lambda_{\text{ex}} = 350 \text{ nm}$ ), and (b) CIE chromaticity diagram for the  $\text{Sr}_{10}\text{V}_6\text{O}_{25}$  samples obtained by MAH using different synthesis times.

**Table SI - 2.** CIE chromaticity coordinates (x, y), obtained from Figure SI-3, for  $\text{Sr}_{10}\text{V}_6\text{O}_{25}$  obtained by the MAH method.

$\text{Sr}_{10}\text{V}_6\text{O}_{25}$	CIE coordinates X	CIE coordinates Y
4 min	0.28	0.36
8 min	0.31	0.40
16 min	0.29	0.39
32 min	0.30	0.35
Pure White light	0.33	0.33