

# **ZnWO<sub>4</sub> nanocrystals: Synthesis, morphology, and photoluminescence and photocatalytic properties**

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## **Electronic Supplementary Information (ESI)**

## FIGURES

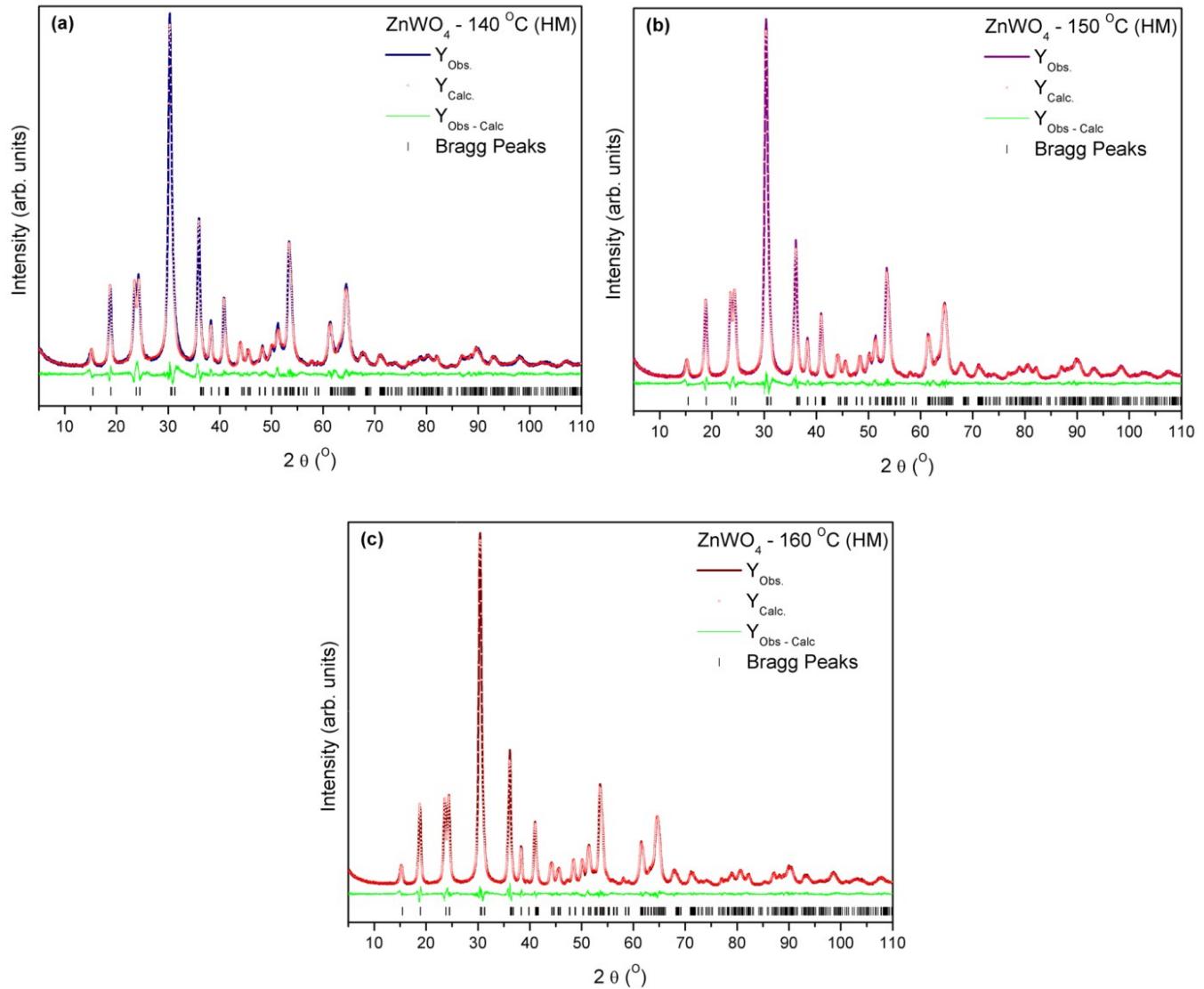


Fig. ESI-1 Rietveld refinement plot of  $ZnWO_4$  obtained by the MH method at 140, 150, and 160 °C for 1 hour.

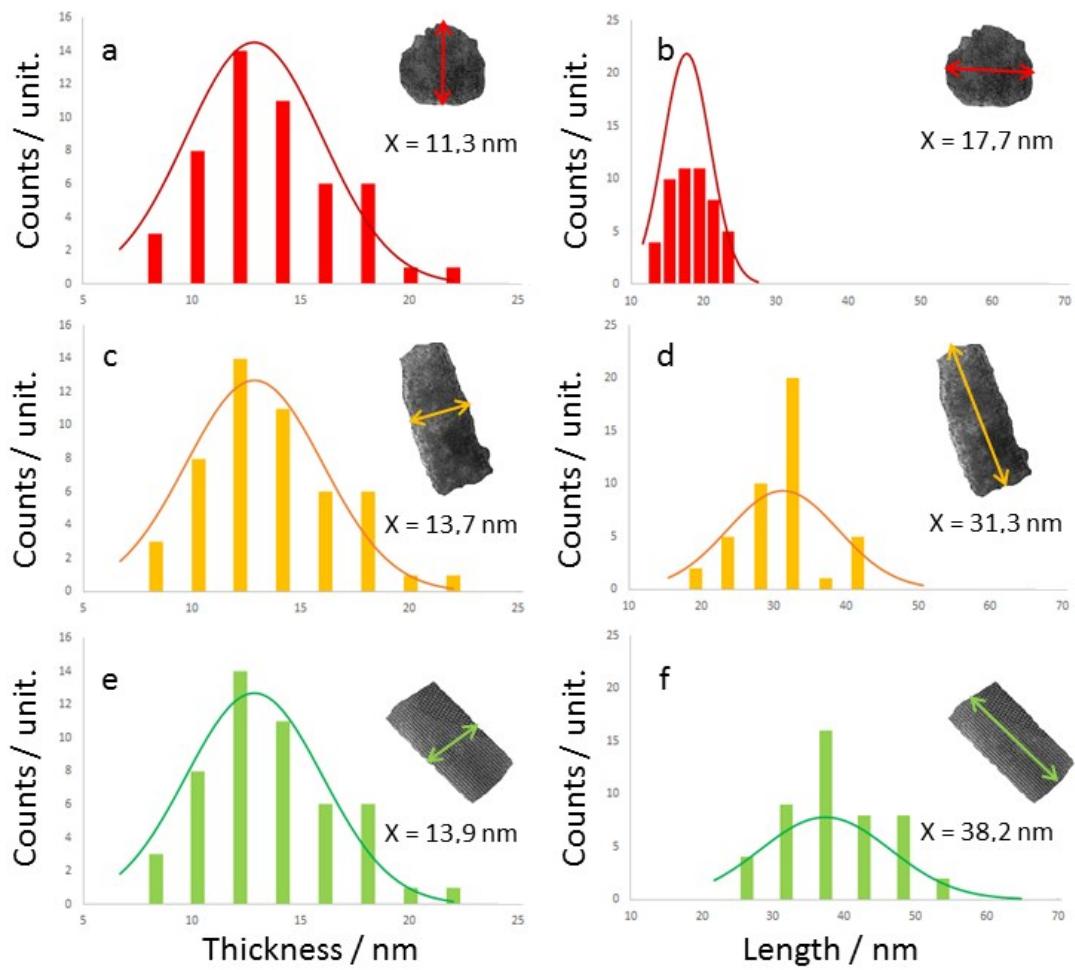


Fig. ESI-2 Size distributions of  $\text{ZnWO}_4$  nanocrystals obtained by the MH method at (a, b) 140, (c, d) 150 and (e, f) 160 °C for 1 h.

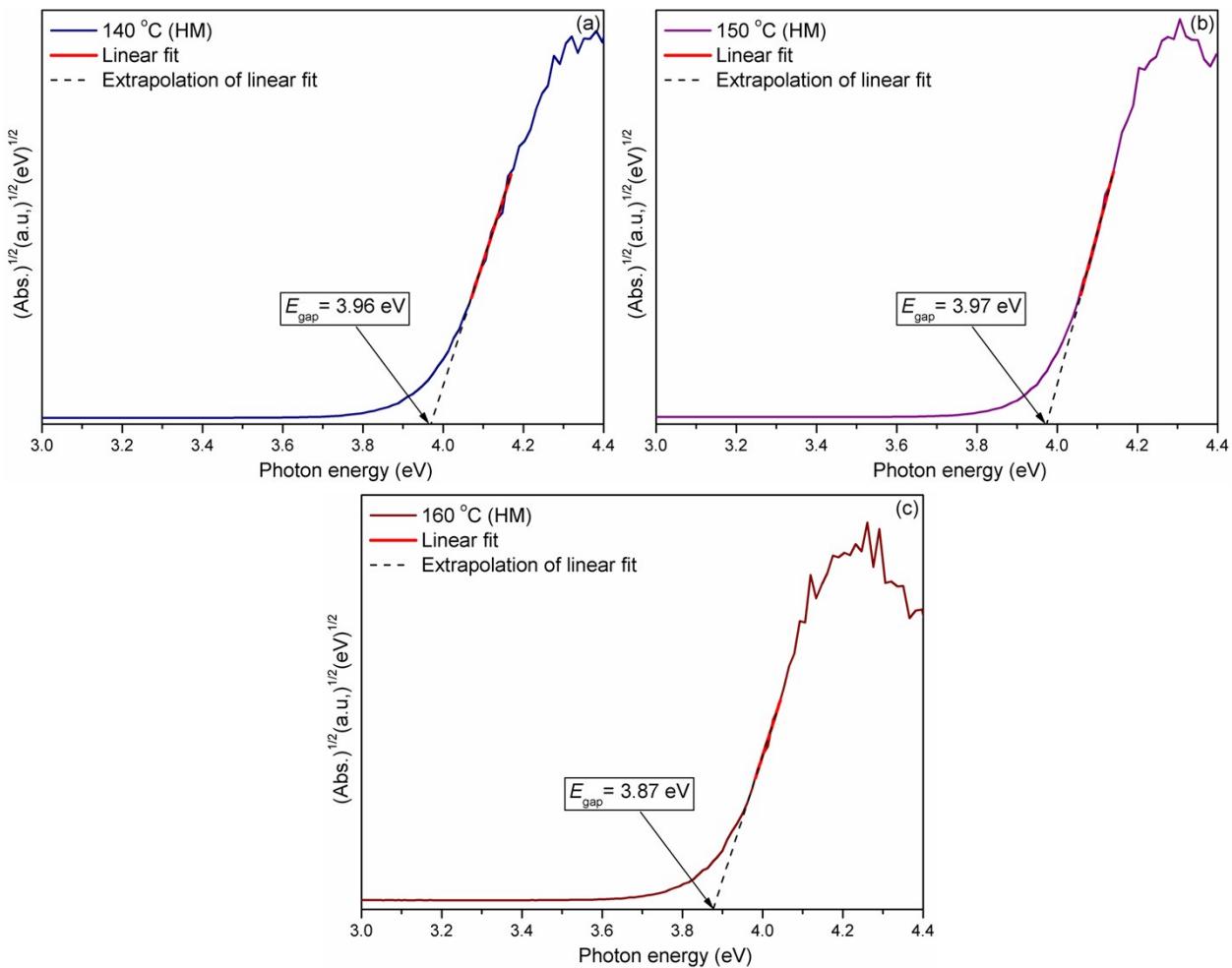


Fig. ESI-3 UV-Vis spectra for  $\text{ZnWO}_4$  nanocrystals obtained by the MH method at (a) 140, (b) 150, and (c) 160 °C for 1 h.

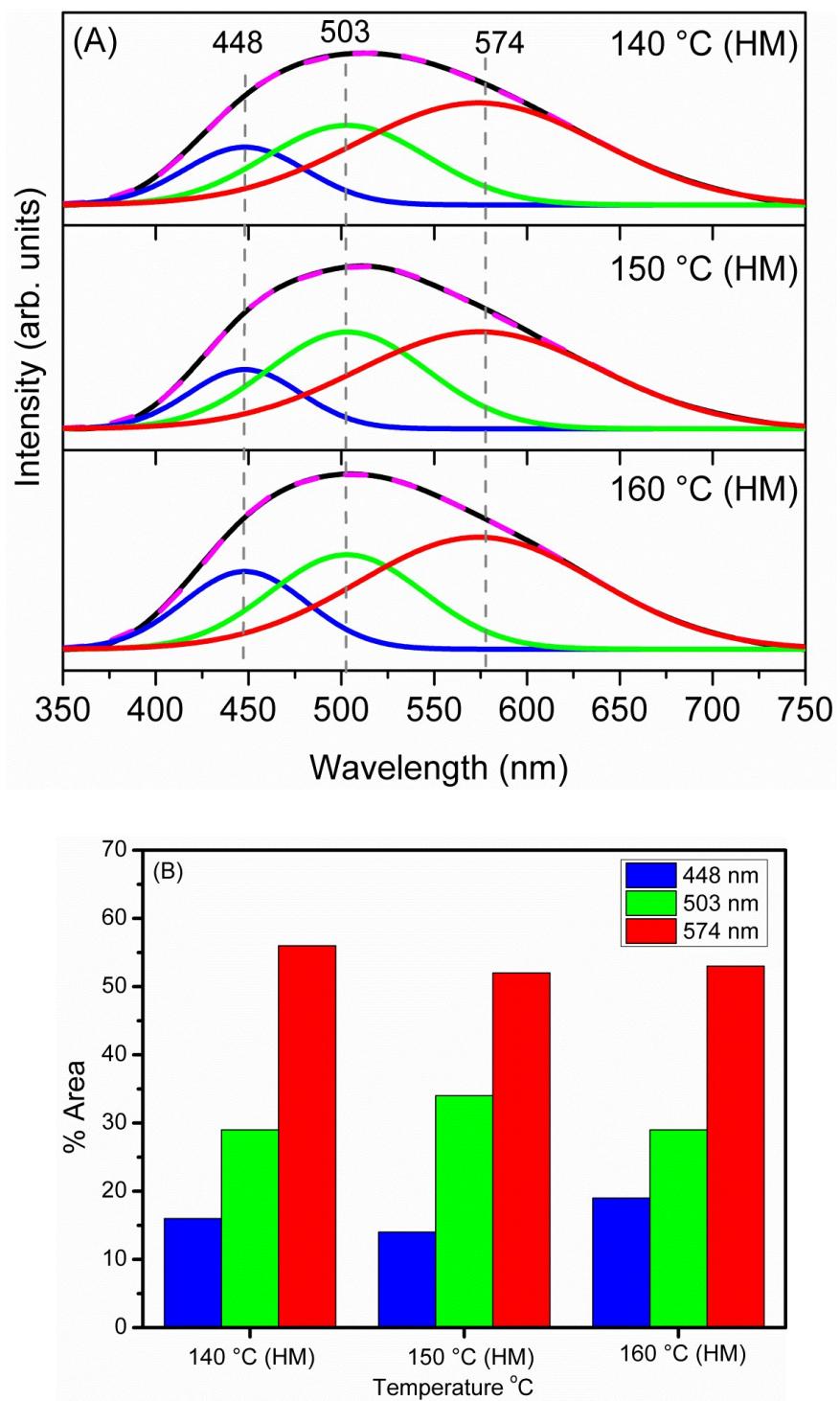


Fig. ESI-4 (A) Deconvolution of PL spectra of  $\text{ZnWO}_4$  nanocrystals obtained by the MH method at 140, 150 and 160 °C for 1 h. (B) Area percentage of each color component corresponding to the emission peak.

## TABLES

Table ESI-1 Raman modes (in  $\text{cm}^{-1}$ ) of  $\text{ZnWO}_4$  nanoparticles obtained by the MH method at 140, 150, and 160 °C for 1 hour, and compared to the literature.

Raman Modes	Raman Shift ( $\text{cm}^{-1}$ )				
	Ede et al. <sup>94</sup>	Dai et al. <sup>95</sup>	Theoretical*	Theoretical*	MH
			PBE	HSE06	method*
$\text{B}_g$	—	—	68	76	—
$\text{A}_g$	—	120	109	119	123
$\text{B}_g$	—	—	123	134	—
$\text{A}_g$	—	—	144	161	—
$\text{B}_g$	167	161	153	167	163
$\text{B}_g$	—	—	174	189	—
$\text{A}_g$	198	192	232	—	192
$\text{A}_g$	276	271		251	273
$\text{A}_g$	316	311		—	314
$\text{B}_g$	—	—	296	305	—
$\text{B}_g$			310	326	
$\text{A}_g$	344	339	350	370	344
$\text{B}_g$	—	—	356	376	—
$\text{A}_g$	411	404	421	444	406
$\text{B}_g$	516	512	457	493	512
$\text{A}_g$	549	542	531	562	544
$\text{B}_g$	680	676	609	649	675
$\text{A}_g$	711	706	662	695	707
$\text{B}_g$	788	784	664	702	783
$\text{A}_g$	909	904	817	878	905

\*This work

Table ESI-2 FWHM, intensities and positions of the Raman peaks of ZnWO<sub>4</sub> nanoparticles synthesized by MH method at 140, 150 and 160 °C for 1 hour.

Methods	FWHM	Intensities	Positions
<b>140 °C</b>	15.787	0.5064	903.51
<b>150 °C</b>	13.422	0.7145	904.06
<b>160 °C</b>	11.879	0.7964	904.32

Table ESI-3 FT-IR modes of  $\text{ZnWO}_4$  nanoparticles obtained by the MH method at 140, 150 and 160 °C for 1 hour, and compared to the literature.

Vibrational Modes	Wavenumber ( $\text{cm}^{-1}$ )				
	Zhou et al. <sup>103</sup>	Yan et al. <sup>104</sup>	Theoretical*	Theoretical*	MH
	PBE	HSE06	method*		
$\text{B}_\text{u}$	-	-	80	96	-
$\text{A}_\text{u}$	-	-	125	134	-
$\text{B}_\text{u}$	-	-	159	176	-
$\text{B}_\text{u}$	-	-	213	231	-
$\text{B}_\text{u}$	-	-	248	266	255
$\text{A}_\text{u}$	-	-	267	292	-
$\text{B}_\text{u}$	-	-	281	294	306
$\text{B}_\text{u}$	-	-	-	-	-
$\text{A}_\text{u}$	-	-	356	376	368
$\text{A}_\text{u}$	426	-	419	444	430
$\text{B}_\text{u}$	466	463	426	457	470
$\text{A}_\text{u}$	-	-	482	515	529
$\text{B}_\text{u}$	578	585	493	521	600
$\text{A}_\text{u}$	714	702	585	616	716
$\text{B}_\text{u}$	826	827	634	672	821
$\text{A}_\text{u}$	880	872	795	851	884

\*This work

Table ESI-4 Surfaces energy value ( $E_{\text{surf}}$ ) using DFT method to  $\text{ZnWO}_4$  faces.

<b>Surface</b>	<b>Surface energy (eV)</b>
(010)	0.26
(110)	0.54
(011)	0.58
(001)	0.84
(111)	1.23
(101)	1.43
(100)	2.63