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Synthesis and characterisation of spherical core-shell Ag/ZnO nanocomposites using single and two - steps ultrasonic spray pyrolysis (USP)

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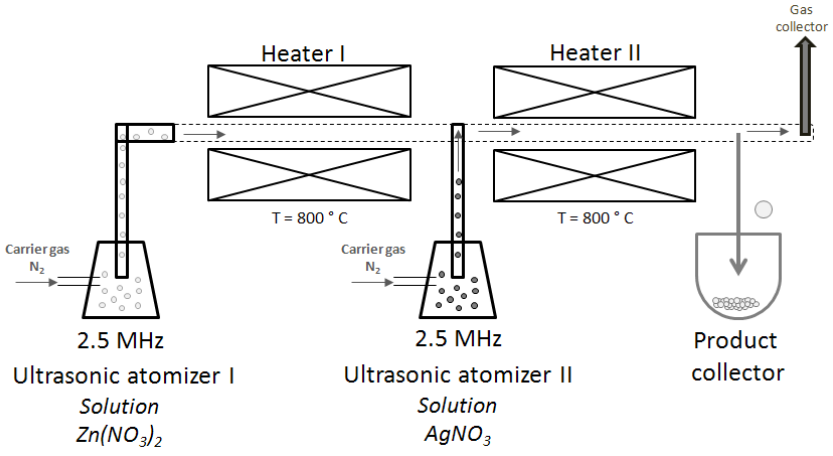
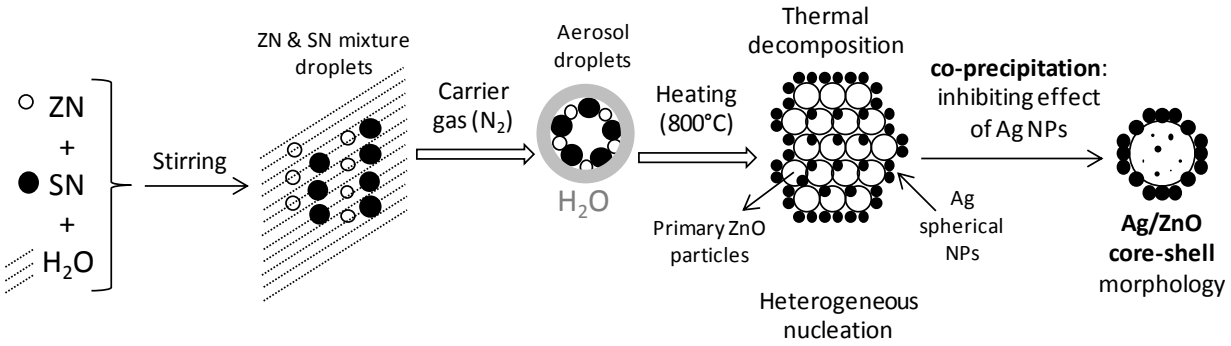


Figure S1: Schematic shown of modified two-step USP equipment (2 steps).

Single step



Two steps

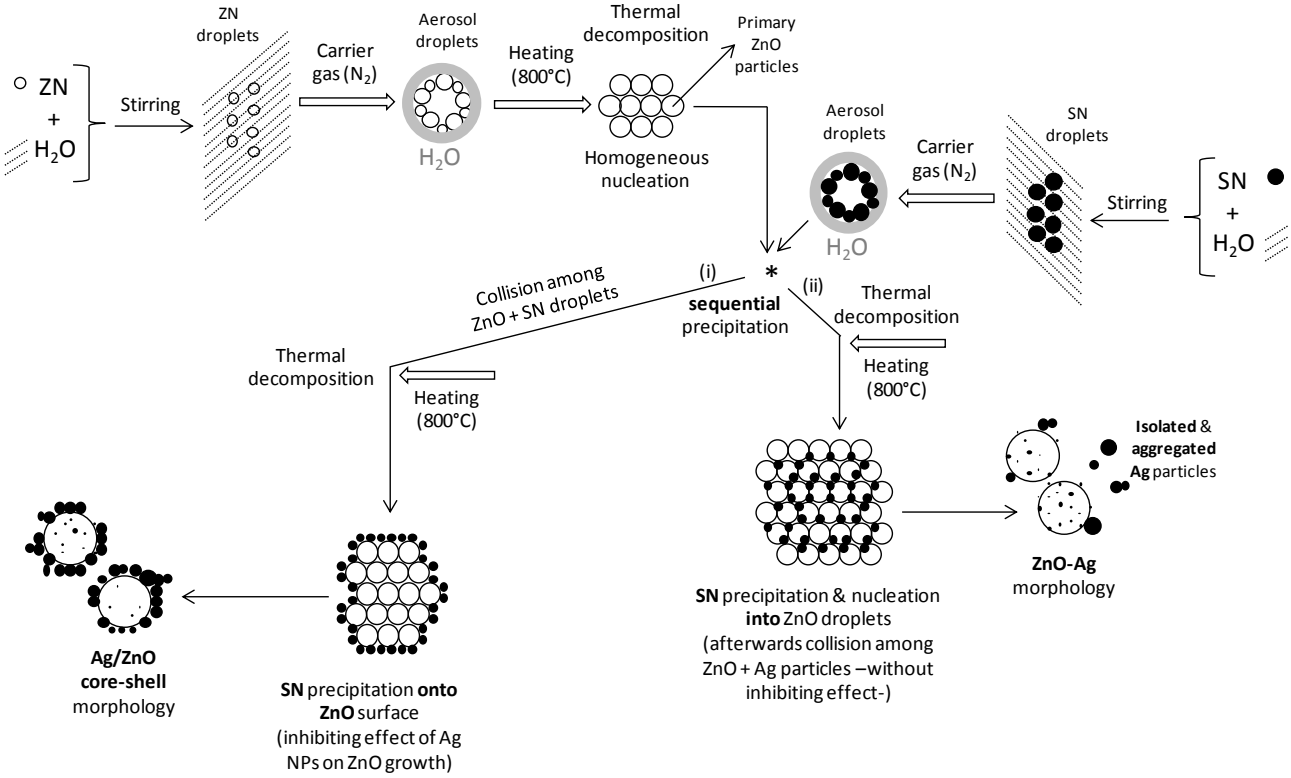


Figure S2. The growth mechanism of Ag/ZnO nanocomposite systems synthesised by USP in single and two steps.

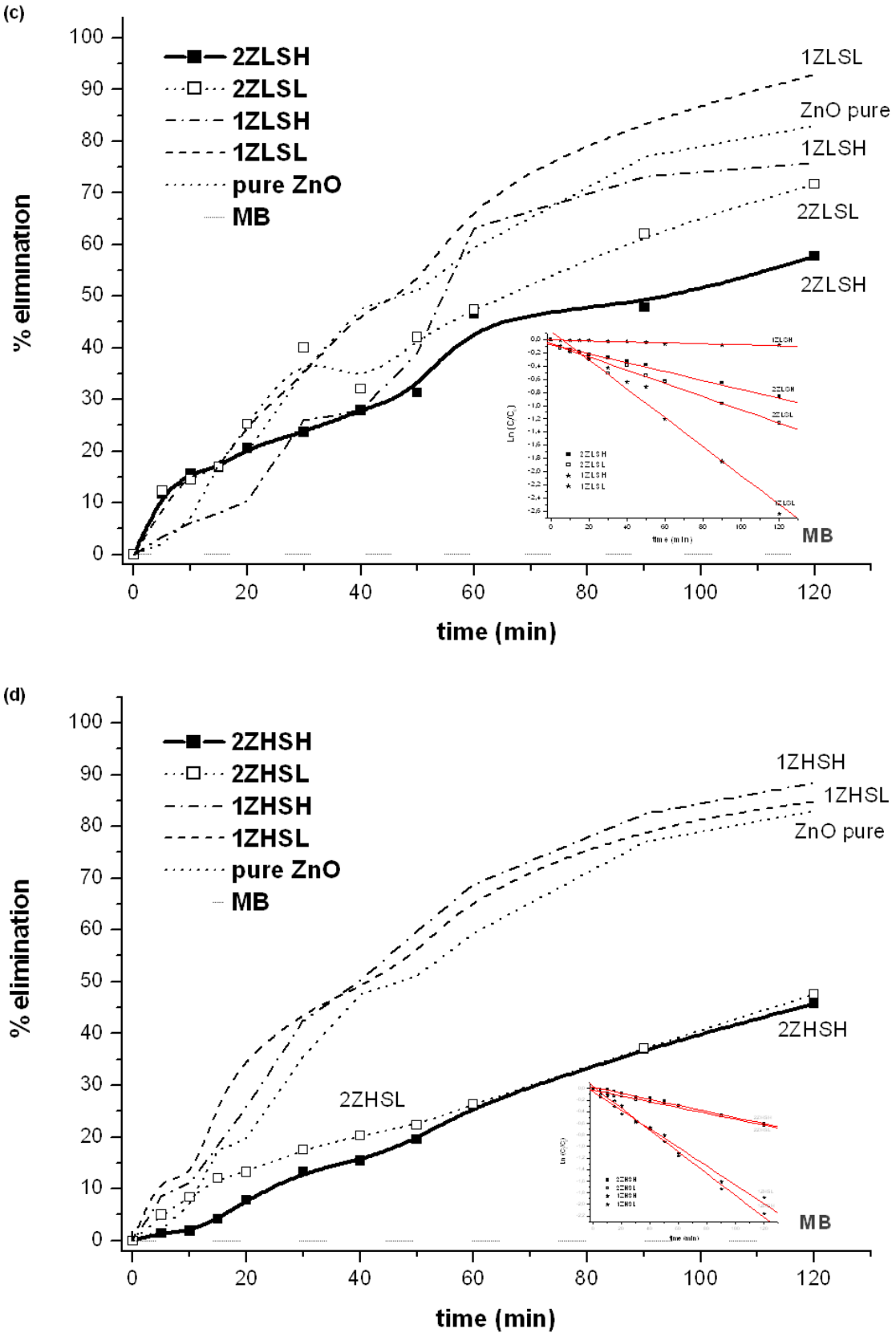


Figure S3. Enlarged figures 4.c and 4.d (photocatalytic activity of Ag/ZnO systems by % elimination of methylene blue (MB) solution under UV irradiation).

Table S1. Synthesis conditions of Ag/ZnO systems obtained by USP at 800 °C.

Sample name [1]	**[Zn^{2+}] (M)**	**[Ag^{+}] (M)**	**USP method**	**Gas flow rate (L/min)**	**Residence time (s)** [2]
1ZLSL	$1.875 \cdot 10^{-2}$	$3.75 \cdot 10^{-3}$	Single step	1.5	3.30
1ZLSH		$7.5 \cdot 10^{-3}$			
1ZHSL	$3.75 \cdot 10^{-2}$	$3.75 \cdot 10^{-3}$			
1ZHSH		$7.5 \cdot 10^{-3}$			
2ZLSL	$1.875 \cdot 10^{-2}$	$3.75 \cdot 10^{-3}$	Two steps	1.5 (1st furnace) 2.5 (2nd furnace)	1.96 (ZnO) 0.86 (Ag)
2ZLSH		$7.5 \cdot 10^{-3}$			
2ZHSL	$3.75 \cdot 10^{-2}$	$3.75 \cdot 10^{-3}$			
2ZHSH		$7.5 \cdot 10^{-3}$			

[1] **samples nomenclature:**

1, 2: samples synthesised in single or two steps USP, respectively.

Z, S: zinc or silver presence, respectively.

L, H: low or high concentration of precursor, respectively.

[2] **residence time estimation (s)** [1]**:**

$$t_{residence} = \frac{V_r \cdot T_{room}}{r_F \cdot T_r},$$

where, V_r = reactor volume (L), T_{room}= room temperature (K), r_F= flow rate (L/s) & T_r= reaction temperature (K).

Table S2. Synthesised sample crystallite sizes, particle sizes, gap values, BET surface areas and photocatalytic activity.

Sample name (Ag^{+}/Zn^{2+} molar)	Crystallite size[1] (nm)		Particle size[2] (µm)	GAP[3] (ev)	BET area[4] (m^2/g)	PCA[5] (% elimination)
	ZnO	Ag				
1ZLSL (r=0.2)	41.2	22.2	427 ± 83	3.27	21.8	93
1ZLSH (r=0.4)	40.6	21.7	709 ± 128	3.24	8.8	76
1ZHSL (r=0.1)	42.3	20.6	673 ± 206	3.24	12.5	85
1ZHSH (r=0.2)	34.9	29.3	878 ± 99	3.24	13.8	88
2ZLSL (r=0.2)	68.1	30.9	698 ± 98	3.24	6.5	72
2ZLSH (r=0.4)	65.2	26.4	761 ± 65	3.24	4.2	58
2ZHSL (r=0.1)	68.8	23.1	667 ± 181	3.23	2.7	48
2ZHSH (r=0.2)	48.9	32.1	947 ± 104	3.24	2.3	46

[1] Results obtained by the Scherrer's formula ($D=K\lambda/\beta\cos\theta$).

[2] Results determined by micrograph analyses (determined from SEM and TEM images).

[3] Band gap calculated from the Kubelka-Munk equation and by UV-vis DRS of synthesised samples. Theoretical E_g=3.37 eV.

[4] The Brunauer–Emmett–Teller (BET) specific surface areas of the samples were obtained by N_2 adsorption/desorption.

[5] Values obtained from % efficiency of elimination after 2 hours of photocatalytic reaction, calculated by [2]:

where C_0 is the initial MB concentration after the equilibrium adsorption and C_t is MB concentration during photoreaction at time ‘‘t”.

PCA (pure ZnO) = 82 %.

Table S3. Synthesised samples elemental composition (weight %).

Sample name (Ag^{+}/Zn^{2+}molar)	Elemental composition* (Wt %)		
	Zn	**O**	**Ag**
1ZLSL (r=0.2)	69.59	18.21	12.20
1ZLSH (r=0.4)	68.86	12.07	19.07
1ZHSL (r=0.1)	79.51	10.05	10.44
1ZHSH (r=0.2)	71.63	11.10	17.27
2ZLSL (r=0.2)	73.92	14.29	11.79
2ZLSH (r=0.4)	70.23	12.44	17.33
2ZHSL (r=0.1)	83.13	9.22	7.65
2ZHSH (r=0.2)	72.65	12.43	14.92

* Values obtained by using the EDX semi-quantitative analysis.

Reference

[1] T.T. Kodas, M.J. Hampden-Smith, Aerosol processing of materials, first ed., Wiley-Vch, USA, 1999.

[2] L. Muñoz-Fernandez, A. Sierra-Fernandez, G. Flores-Carrasco, O. Milošević, M.E. Rabanal, Advanced Powder Technology, 28 (2016), p. 83.