Supporting information for

Structural, morphological, dielectric and semiconducting properties of ZnO nanoparticles calcined at 500 °C

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Table S1. Experimental and standard diffraction angles of calcined (at 500 °C) and standard ZnO.

Sr. No.	Miller indices (*hkl*)	Experimental diffraction angles (*2θ°*)	Standard diffraction angles (*2θ°*) (Ref: JCPDS file No. 036-1451).
01	100	31.778	31.770
02	002	34.400	34.422
03	101	36.231	36.253
04	102	47.562	47.539
05	110	56.600	56.603
06	103	62.898	62.864
07	200	66.324	66.380
08	112	67.931	67.963
09	201	69.183	69.100
10	004	72.503	72.562
11	202	76.969	76.955

Table S2. Ratio between the intensity of the diffraction peaksof standard and calcined ZnO at 500 °C.

Sr. No.	Experimental Diffraction ratio	Standard value (Ref: JCPDS file No. 036-1451).	Calcined ZnO value
01	(100) and (101)	0.57	0.64
02	(002) and (101)	0.44	0.53
03	(101) and (101)	1.00	1.00
04	(102) and (101)	0.23	0.17
05	(110) and (101)	0.32	0.28
06	(103) and (101)	0.29	0.21
07	(200) and (101)	0.04	0.04
08	(112) and (101)	0.23	0.18
09	(201) and (101)	0.11	0.09
10	(004) and (101)	0.02	0.02
11	(202) and (101)	0.04	0.03

Table S3. Lattice Parameters (*a, b and c*), bond angle, bond lengthand unit cell volume (*V*) of standard and calcined ZnO at 500 °C.[S1]

Sr. No.	Lattice parameter[1]	Standard value (Å) (Ref: JCPDS file No. 036-1451).	Calcined ZnO value (Å)
01	***a***	3.2498	3.2494
02	***b***	3.2498	3.2494
03	**c**	5.2066	5.2108
04	**α**	90˚	90˚
05	**β**	90˚	90˚
06	**γ**	120˚	120˚
08	**bond length**		1.9781
08	***V***	47.62 (Å)^3	47.64 (Å)^3

Table S4. Data of Crystallite Diameter Size (*D*), and Interplanar Spacing (*d*) of calcined ZnO at 500 °C.

S. No.	*2θ* of the intense peak (˚)	Miller indices (*hkl*)	FWHM *β* (˚)	Crystallite Diameter *D* (Å)	Interplanar Spacing *d* (Å)
01	31.778	100	0.37822	215.9581	2.814146
02	34.400	002	0.34438	238.7960	2.605411
03	36.231	101	0.42321	195.3067	2.477830
04	47.562	102	0.62619	137.0932	1.910607
05	56.600	110	0.54941	162.3925	1.625084
06	62.898	103	0.66746	137.9581	1.476658
07	66.324	200	1.27334	73.69460	1.408441
08	67.931	112	0.69735	135.8215	1.378981
09	69.183	201	0.60708	157.1833	1.357051
10	72.503	004	0.76253	127.7443	1.302867
11	76.969	202	0.66160	151.6790	1.238019
	average values (nm)			157.6025	1.781372

Table S5. Williamson−Hall Plotting Data of calcined ZnO at 500 °C.[S2-3]

2θ of the intense peak (˚)	FWHM β (˚)	FWHM β (radians)	$cos\theta$	$\beta\ cos\theta$	$4\ sin\theta$	Diameter Size D (Å)	Lattice strain É›
31.778	0.37822	0.0066011843	0.961808	0.006349	1.094897024		
34.400	0.34438	0.0060105649	0.955295	0.005742	1.182615803		
36.231	0.42321	0.0073864079	0.950450	0.007020	1.243507471		
47.562	0.62619	0.0109290772	0.915125	0.010001	1.612680838		
56.600	0.54941	0.0095890134	0.880522	0.008443	1.896024662		
62.898	0.66746	0.0116493746	0.853159	0.009939	2.086604275	535.59	3.71×10^{-3}
66.324	1.27334	0.0222239755	0.837187	0.018606	2.187666935		
67.931	0.69735	0.0121710535	0.829437	0.010095	2.234403410		
69.183	0.60708	0.0105955448	0.823285	0.008723	2.270511445		
72.503	0.76253	0.0133086591	0.806500	0.010733	2.364938009		
76.969	0.66160	0.0115470983	0.782855	0.009040	2.488814826		

Table S6. Electrochemical Impedance Spectroscopy (EIS) fitting parameters for calcined ZnO NPs at 500 °C obtained from ZSimpWin data analysis software.

Temperature	Resistance (ohm)/R_1	CPE/ Yo ($S.s^n$)	Resistance (ohm)/R_2
170 K	7.53×10^7	4.33×10^{-6}	1.36×10^6
180 K	7.53×10^7	4.33×10^{-6}	1.36×10^6
190 K	6.46×10^7	2.76×10^{-7}	2.64×10^8
200 K	5.99×10^7	5.27×10^{-7}	4.72×10^6
210 K	5.73×10^7	8.22×10^{-7}	3.71×10^6
220 K	6.51×10^7	8.09×10^{-7}	5.28×10^6
230 K	5.20×10^7	2.02×10^{-5}	2.03×10^3
240 K	4.86×10^7	2.08×10^{-5}	2.14×10^3
250 K	4.43×10^7	1.68×10^{-6}	3.43×10^3
260 K	3.91×10^7	2.30×10^{-5}	2.21×10^3
270 K	3.42×10^7	2.15×10^{-5}	2.15×10^3
280 K	3.05×10^7	2.30×10^{-5}	1.95×10^3
290 K	2.98×10^7	7.75×10^{-7}	3.92×10^6
300 K	2.68×10^7	7.21×10^{-7}	1.76×10^6
310 K	1.62×10^7	3.04×10^{-7}	7.10×10^7
320 K	1.15×10^7	2.29×10^{-5}	3.69×10^3
330 K	1.15×10^7	2.29×10^{-5}	3.69×10^3
340 K	5.51×10^6	3.82×10^{-7}	2.19×10^7
350 K	4.64×10^6	9.94×10^{-7}	1.00×10^6

Table S7. Comparative study of the properties of the ZnO NPs calcined at a temperature of 100–1400 °C.

Calcination temperature (°C)	**Crystalline size (nm)**	**SEM, particle size (nm)**	**Shape**	κ	tan δ	σ_{AC} **(S/cm)**	E_g **(eV)**	**Ref.**
100 (6 h)	7–24	n.r	n.r	n.r	n.r	n.r	3.42	S4
100 (2 h)	~19	n.r	Spherical	25.59	0.809	11.9×10^{-5}	n.r	S5
200 (6 h)	200–400	n.r	Polyhedron	n.r	n.r	n.r	n.r	S6
200 (12 h)	16–24	n.r	n.r	n.r	n.r	n.r	n.r	S4
300 (2 h)	64	n.r	n.r	n.r	n.r	n.r	3.30	S7
400 (12 h)	29.6–33.6	n.r	n.r	n.r	n.r	n.r	3.29	S8
500 (2 h)	46.2	500–1000	Rods	n.r	n.r	n.r	3.12	S9
500 (6 h)	7–24	27–181	Polyhedron to spherical	97.74	0.96	5.03×10^{-5}	3.16	This Work
600 (2 h)	23.0	n.r	spherical	n.r	n.r	n.r	3.57	S10
700 (3 h)	~50	n.r	n.r	n.r	n.r	1×10^{-8}	n.r	S11
700 (2 h)	131	n.r	n.r	n.r	n.r	n.r	3.27	S7
800 (2 h)	90	n.r	n.r	n.r	n.r	n.r	n.r	S12
900 (3 h)	187	n.r	n.r	n.r	n.r	n.r	n.r	S7
1000 (4 h)	n.r	n.r	Elliptical	1.9×10^5	$\sim 10^2$	1.24×10^{-5}	n.r	S13
1200 (10 h)	n.r	1000–10,000	Wurtzite	1.9×10^4	9.2	n.r	n.r	S14
1300 (10 h)	n.r	3,000–15,000	Wurtzite	2.5×10^3	2.0	n.r	n.r	S14
1400 (10 h)	n.r	3,000–20,000	Wurtzite	3.5×10^3	1.6	n.r	n.r	S14

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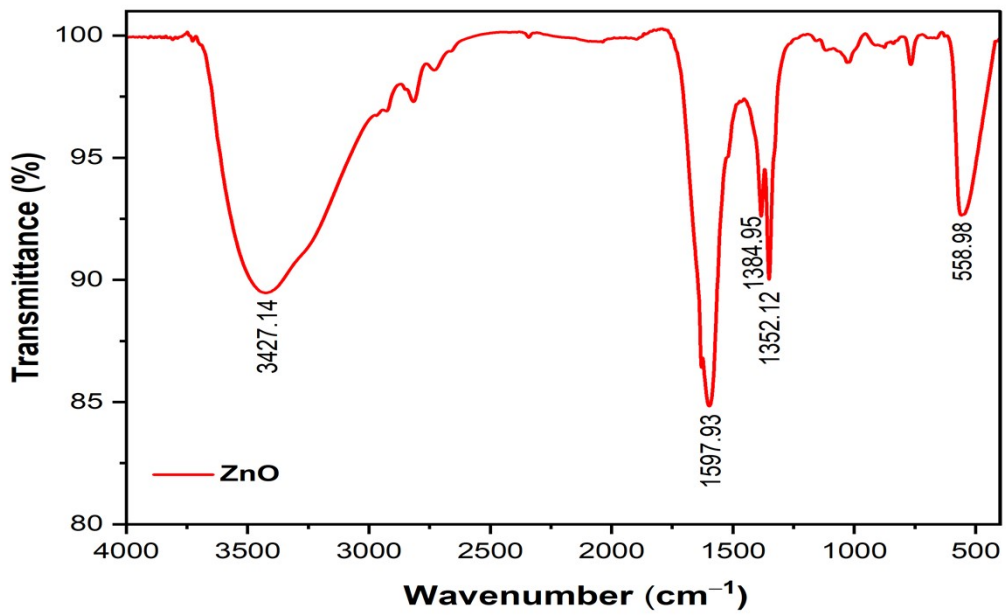

Figure S1. FTIR spectrum of the synthesized ZnO NPs calcined at 500 °C.

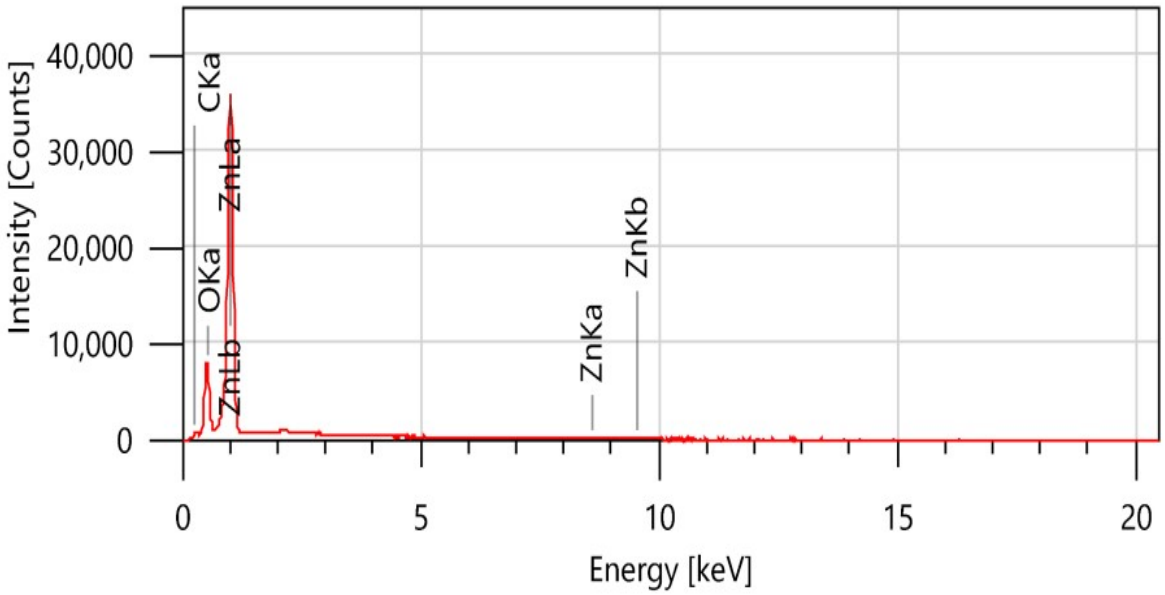

Figure S2. EDX spectrum of the ZnO NPs calcined at 500 °C.

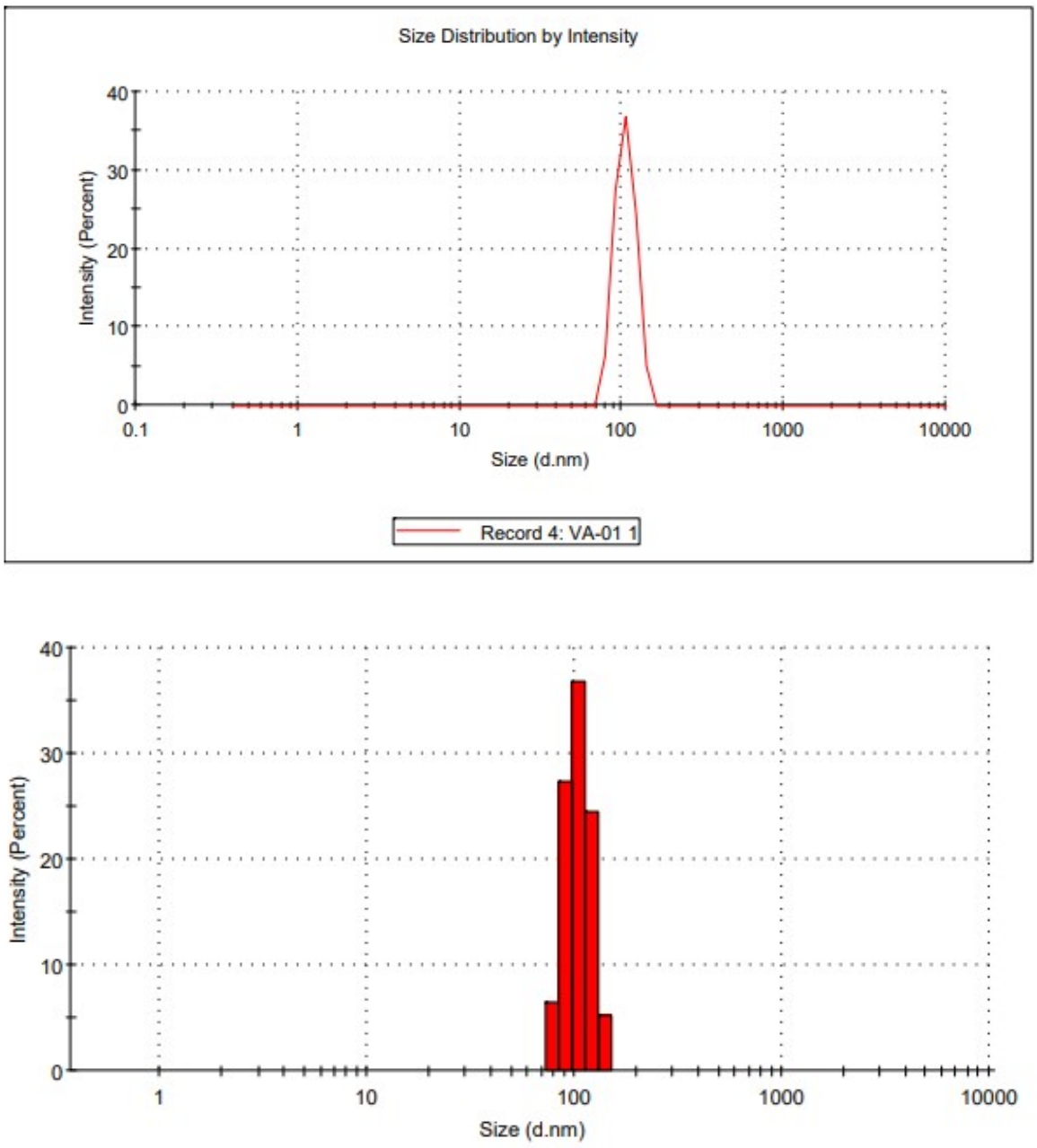

Figure S3. Particles size distribution of the ZnO NPs calcined at 500 °C.

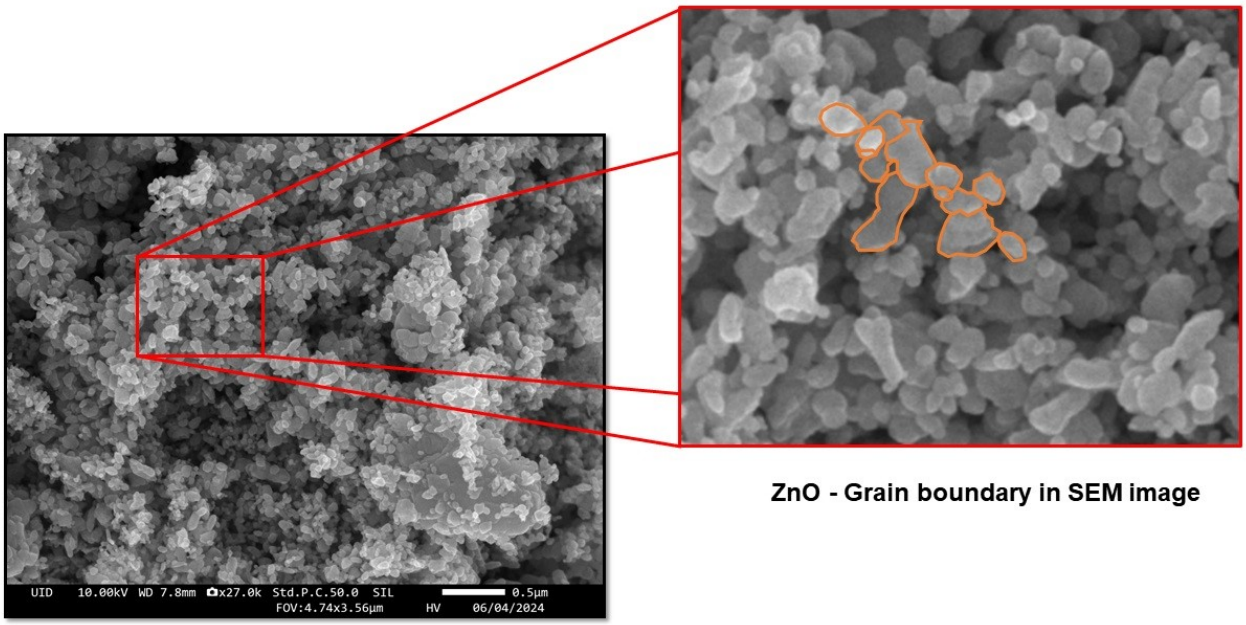

Figure S4. SEM image of ZnO NPs calcined at 500 °C showing a low-magnification view of aggregated nanoparticles, with the red rectangle highlighting the grain boundaries.

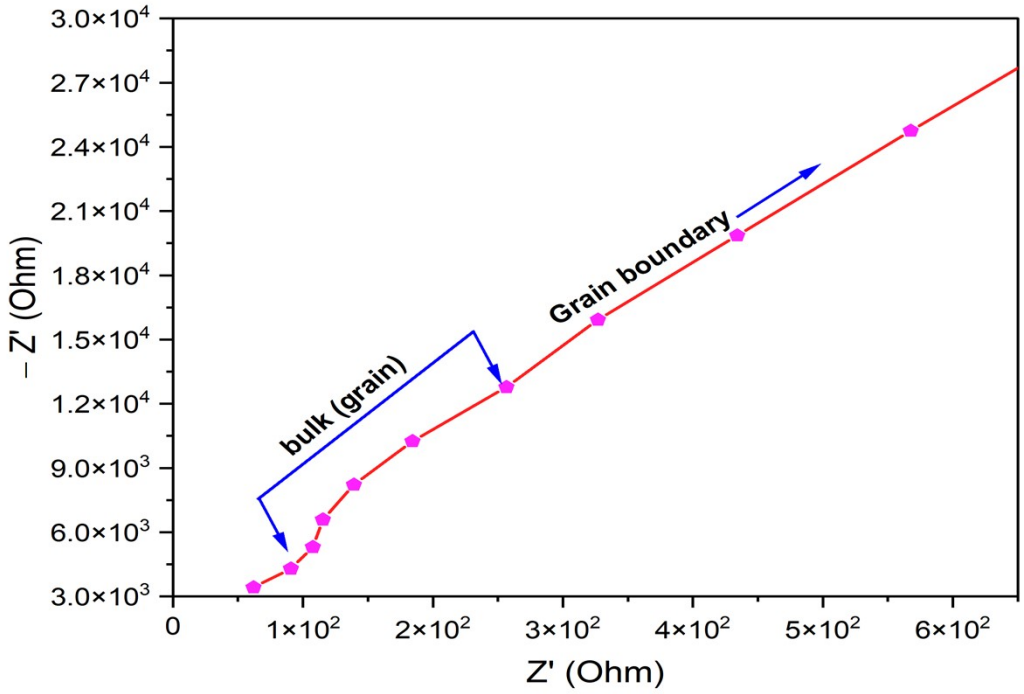

Figure S5. Nyquist plot showing two distinct semicircles: the high-frequency arc corresponds to the grain (bulk) resistance, while the low-frequency arc represents the grain-boundary resistance.