

Rational Synthesis and Characterization of Temperature Switching ZnFe₂O₄/ZnO Nanocomposite Used for Anti-bacterial, Anti-oxidant and Seed Germination Properties

Shatarupa Basak^a, Suranjan Sikdar^b, Salim Ali^a, Modhusudan Mondal^a, Md Salman Haydar^c, Kushankur Sarkar^c, Monoranjan Chowdhury^c, Mahendra Nath Roy^{a,d*}

^aDepartment of Chemistry, University of North Bengal, Darjeeling-734013, West Bengal, India.

^bDepartment of Chemistry, Ghani Khan Choudhury Institute of Engineering and Technology (GKCIET), Malda-732141, West Bengal, India.

^cDepartment of Botany, University of North Bengal, Darjeeling-734013, West Bengal, India.

***Corresponding Author:**

Mahendra Nath Roy: mahendraroy2002@yahoo.co.in, vcapduniversity@gmail.com.

Number of Pages: 05

Number of Tables: 07

Number of Figures: 01

Number of Equations: 05

Table S1: Size and other lattice parameters of the IZ 1 nanocomposites

2θ (degree)	FWHM (degree)	Crystalline size (nm)	Average Crystalline size (nm)	Micro-strain ($\epsilon \times 10^{-3}$)	Dislocation Density ($\delta \times 10^{-3}$) (nm⁻²)
12.2773	1.1003	7.178711934	13.98634295	4.773436	19.40470064
14.1196	1.0747	7.336055375		4.653711	18.58124451
18.1113	0.9468	8.286090904		4.079703	14.56466879
19.058	0.40013	19.58031943		1.721806	2.608317499
28.1672	0.43342	17.77836104		1.834307	3.163854894
29.7281	0.82905	9.261746655		3.496364	11.65773572
32.1589	0.48456	15.75346077		2.031578	4.029471129
32.8242	0.47423	16.06940432		1.984907	3.872580407
35.0503	0.66908	11.32234375		2.783907	7.800587769
36.5344	0.4606	16.3785001		1.908466	3.727792624
42.6242	0.64052	11.55469741		2.603672	7.490017739
52.6034	0.64836	10.9843958		2.536127	8.287960135

56.3136	0.88369	7.926034979		3.399525	15.91798279
58.4374	0.43512	15.93463863		1.657001	3.938361363
61.8149	0.85138	8.006043214		3.187331	15.60142042
73.0479	0.36041	17.71342472		1.263742	3.187094408
85.5602	0.14168	41.15497229		0.453734	0.590412268
88.554	0.59653	9.534971817		1.863573	10.99920186

Table S2: Size and other lattice parameters of the IZ 2 nanocomposites

2θ (degree)	FWHM (degree)	Crystalline size (nm)	Average Crystalline size (nm)	Micro-strain ($\epsilon \times 10^{-3}$)	Dislocation Density ($\delta \times 10^{-3}$) (nm⁻²)
12.6272	1.2794	6.17172577	16.20837843	5.548577	26.25347273
18.1285	0.76278	10.28485684		3.286693	9.45373661
19.0241	0.16525	47.41338539		0.711125	0.444834097
28.0309	0.90404	8.525940391		3.827189	13.75673642
29.8732	0.58693	13.07798958		2.474434	5.846797146
31.7923	0.85689	8.916543717		3.595912	12.57786455
32.7391	0.25331	30.09063377		1.06047	1.1044278
32.9438	0.4094	18.60832131		1.713031	2.887922985
35.1699	0.71095	10.65201893		2.957143	8.813251045
38.6242	0.17664	42.44380013		0.727369	0.555100321
42.7438	0.64146	11.53306087		2.60643	7.518147326
52.9533	0.64073	11.09837408		2.502487	8.118602576
56.51	0.83035	8.427437162		3.191393	14.08020423
58.429	0.41174	16.84015207		1.56803	3.526208454
59.6316	0.62739	10.98629331		2.375137	8.285097454
61.9601	0.78492	8.677328935		2.936292	13.28091137
67.8964	1.46933	4.485124285		5.318333	49.71083247
73.3466	0.64689	9.849818663		2.26387	10.30726709
85.731	0.14571	39.96148321		0.465997	0.626205391
88.8783	0.92633	6.123280201		2.885878	26.67053537

Table S3: Size and other lattice parameters of the IZ 3 nanocomposites

2θ (degree)	FWHM (degree)	Crystalline size (nm)	Average Crystalline size (nm)	Micro-strain ($\epsilon \times 10^{-3}$)	Dislocation Density ($\delta \times 10^{-3}$) (nm⁻²)
12.2434	0.8444	9.35455674	17.97674481	3.66338	11.42756165
14.0601	0.9979	7.901157057		4.321426	16.01838068
18.1285	0.46987	16.69628429		2.024592	3.587239212
21.2502	0.3152	24.77183234		1.351739	1.629610206
22.6064	0.17526	44.44938552		0.749883	0.506137455
28.0309	0.33031	23.3350221		1.398344	1.836468852

29.9244	0.38445	19.96345106	1.620607	2.509162342
31.7667	0.41659	18.34173421	1.748318	2.972481828
32.7646	0.30379	25.08891017	1.271719	1.588679923
34.4278	0.49569	15.30883669	2.065974	4.266930999
35.1955	0.40734	18.59016172	1.69418	2.893567811
36.2446	0.53141	14.20788187	2.203693	4.953832578
36.8843	0.40784	18.47856634	1.688147	2.928622894
42.7694	0.43992	16.81521703	1.787361	3.536674132
47.6311	0.54146	13.42266039	2.161393	5.550380996
53.158	0.44254	16.05441984	1.726879	3.879812766
56.5611	0.50278	13.91472352	1.931937	5.164768225
62.1648	0.54677	12.44342845	2.043204	6.458324913
68.0244	0.32155	20.47945268	1.162995	2.384313228
68.8176	0.86402	7.585762683	3.110349	17.37806816
70.5831	0.21663	29.93264946	0.771516	1.116116891
73.5769	0.47871	13.29030229	1.672793	5.661483962
74.3957	0.22383	28.27165307	0.777947	1.251116047
86.0125	0.54737	10.61346828	1.746553	8.877390983
89.1086	0.5601	10.10710244	1.741487	9.789187901

Table S4: Size and other lattice parameters of the IZ 4 nanocomposites

2θ (degree)	FWHM (degree)	Crystalline size (nm)	Average Crystalline size (nm)	Micro-strain ($\epsilon \times 10^{-3}$)	Dislocation Density ($\delta \times 10^{-3}$) (nm⁻²)
15.0324	0.9467	8.319458135	26.2305043	4.095266	14.44807271
18.2309	0.40053	19.58395517		1.725571	2.607349126
19.0753	0.16694	46.92988244		0.718344	0.454047269
21.2758	0.17873	43.68463114		0.766454	0.524013715
22.5808	0.16235	47.98612238		0.694676	0.434278856
25.1395	0.67965	11.40863486		2.894454	7.683031945
26.163	0.51522	15.01907448		2.189732	4.433162571
28.0309	0.21198	36.36093571		0.897402	0.756362343
29.0289	0.22317	34.46136474		0.942685	0.842044523
29.95	0.29591	25.93521799		1.247302	1.486689228
31.7923	0.23907	31.95924685		1.00325	0.979054634
32.125	0.20082	38.01487674		0.842034	0.691978859
32.7902	0.27352	27.86362702		1.144928	1.288026219
34.479	0.44967	16.87323159		1.873909	3.51239593
35.2211	0.33149	22.84225682		1.378613	1.916558058
36.2446	0.28652	26.35142575		1.188164	1.440097063
36.8075	0.31184	24.17259215		1.291068	1.711407974
38.5986	0.28979	25.87342423		1.193392	1.493799058
42.8462	0.33968	21.77168871		1.379731	2.109676026
47.6055	0.34695	20.94984913		1.385087	2.278443168

48.7569	0.15538	46.56949441	0.617524	0.461101945
53.0556	0.38945	18.25111432	1.52039	3.002072865
56.6379	0.4269	16.38210475	1.639775	3.726152306
58.429	0.24443	28.36707528	0.930863	1.242713103
59.4781	0.35448	19.45942102	1.342999	2.640828334
62.1904	0.45668	14.89615692	1.70632	4.506626051
62.8557	0.46991	14.42582949	1.749575	4.805276816
66.3356	0.2814	23.63163175	1.02779	1.790657719
67.922	0.45033	14.63179533	1.629753	4.67094512
69.1247	0.63959	10.22873423	2.298199	9.557761982
70.6087	0.45993	14.09624147	1.637756	5.032610724
73.5257	0.49059	12.97279941	1.714879	5.941999269
74.5492	0.2648	23.87312987	0.919407	1.754612741
77.1848	0.10967	56.61787064	0.374017	0.311955708
78.3874	0.06675	92.23872719	0.225724	0.117536674
81.5602	0.27236	22.08690728	0.899879	2.049888239
86.0892	0.49248	11.78903907	1.570428	7.195205235
89.0574	0.57325	9.879594973	1.783157	10.24523015

Table S5: Antibacterial efficacy of various concentrations of IZ 3 against different gram-positive and negative bacteria. Results are presented as mean \pm standard deviation

Tested concentrations of IZ 3	Zone of Inhibition (in mm) against studied microorganism				
	<i>B. subtilis</i>	<i>B. megaterium</i>	<i>S. flexneri</i>	<i>S. typhimurium</i>	<i>E. coli</i>
300 $\mu\text{g/mL}$	21.667 \pm 0.577	12.667 \pm 1.528	19.667 \pm 0.577	11.333 \pm 1.155	22.333 \pm 0.577
200 $\mu\text{g/mL}$	13 \pm 1	8 \pm 1	16.667 \pm 1.155	5.333 \pm 0.577	18.667 \pm 1.155
100 $\mu\text{g/mL}$	8.333 \pm 0.577	0	9.667 \pm 0.577	0	10 \pm 1

Table S6: Antioxidant activity of different grade $\text{ZnFe}_2\text{O}_4/\text{ZnO}$ nanocomposites. Data are presented as mean \pm standard deviation (n=3). Different letters (a, b, c, etc.) represented that they are statistically different at $p \leq 0.05$ following Tukey's HSD test.

Sample Name	Antioxidant activity (IC 50 Value in $\mu\text{g/mL}$)			
	ABTS	DPPH	SUPEROXIDE	NITRIC OXIDE
IZ 1	34.245 \pm 0.279 ^a	40.756 \pm 0.721 ^a	65.327 \pm 1.742 ^a	70.128 \pm 4.214 ^a
IZ 2	34.974 \pm 0.579 ^a	40.997 \pm 1.586 ^a	71.137 \pm 2.147 ^b	74.456 \pm 5.124 ^a
IZ 3	59.341 \pm 1.987 ^b	48.121 \pm 0.629 ^b	73.721 \pm 2.245 ^b	75.321 \pm 5.187 ^a

IZ 4	64.297 ±1.734 ^c	55.817±2.421 ^c	79.321±3.141 ^c	133.217±10.427 ^b
------	----------------------------	---------------------------	---------------------------	-----------------------------

Table S7: Various biochemical attributes of treated and control wheat seedlings. Results were presented as mean ± standard deviation, whereas the ‘*’ symbol indicated that they are statistically significant from their respective control at 95% confidence level as observed through two-tailed t-test

Treatments	Chlorophyll (mg/g FWT)	Protein (µg/mg FWT)	Sugar (µg/mg FWT)	Phenol (µg/mg FWT)
IZ 1	3.040 ±0.089*	15.74 ±0.531*	12.489 ±0.531*	0.923 ±0.045
Con	2.453 ±0.067	11.56 ±0.166	9.633 ±0.273	0.893 ±0.035

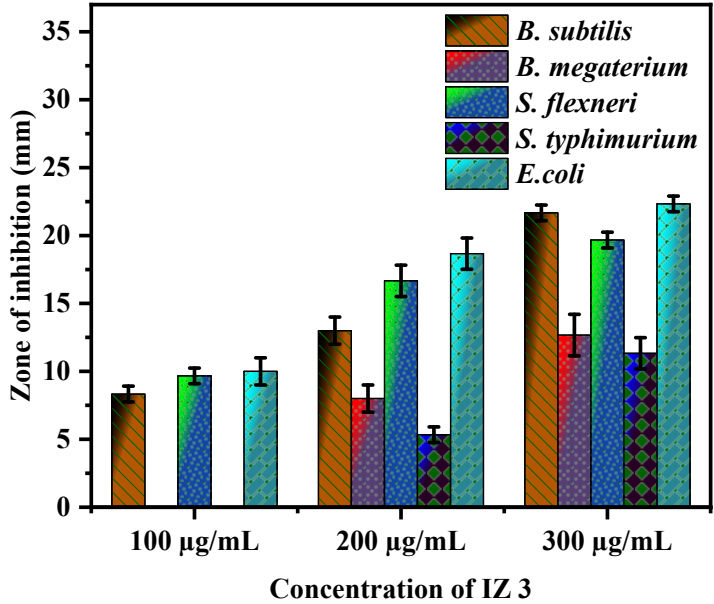


Figure S1 Zone of inhibition (mm) IZ 3 against different bacterial strain at different concentration.

Equations:

$$\text{Inhibition Percentage} = \frac{A_c - A_s}{A_c} \times 100\% \quad (\text{S1})$$

Where, A_c and A_s are the absorbance of control and sample respectively.

$$D = \frac{0.9\lambda}{\beta \cos\theta} \quad (\text{S2})$$

Where, D is the average crystallite size, θ is the angle of diffraction, β is the full width at half maximum intensity and λ is the wavelength of the radiation (1.54 Å).

$$\text{Crystallinity} = \frac{\text{area of the crystalline peaks}}{\text{area of all peaks (crystalline + amorphous)}} \times 100 \quad (\text{S3})$$

$$\varepsilon = \frac{\beta \cos\theta}{4} \quad (\text{S4})$$

$$\delta = \frac{1}{D^2} \quad (\text{S5})$$

Where, ε is the micro-strain and δ is the dislocation density.