

## **Ce-Doping-Induced Burstein–Moss Shift in Biogenically Synthesized ZnO for Multifunctional Gas Sensing, Photocatalytic, and Antimicrobial Applications**

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**Table 1. X-ray diffraction peak positions ( $2\theta$ ), corresponding Miller indices (hkl), and full width at half maximum (FWHM) values for pristine and Ce-doped ZnO samples.**

Samples	Ce0@Zn		Ce2@Zn		Ce4@Zn		Ce6@Zn	
	$2\theta$ ( $^{\circ}$ )	FWHM ( $^{\circ}$ )	$2\theta$ ( $^{\circ}$ )	FWHM ( $^{\circ}$ )	$2\theta$ ( $^{\circ}$ )	FWHM ( $^{\circ}$ )	$2\theta$ ( $^{\circ}$ )	FWHM ( $^{\circ}$ )
	-	-	25.49	0.18333	25.48	0.2745	25.52	0.2167
(100)	31.74	0.20885	31.8	0.26771	31.8	0.2635	31.8	0.2393
(002)	34.42	0.21808	34.48	0.26487	34.46	0.2428	34.48	0.2279
(101)	36.22	0.22336	36.28	0.28877	36.28	0.2666	36.34	0.2568
(102)	47.5	0.25888	47.6	0.33816	47.56	0.3203	47.66	0.2913
(110)	56.58	0.30199	56.66	0.17875	56.66	0.1183	56.7	0.3215
(103)	62.84	0.30011	62.88	0.4085	62.86	0.3826	62.9	0.3182
(200)	66.32	0.3856	66.34	0.47538	66.44	0.4495	66.46	0.3354
(112)	67.96	0.37327	67.95	0.4284	67.96	0.4498	68	0.3849
(201)	69.09	0.36831	69.14	0.47462	69.16	0.428	69.1	0.4318

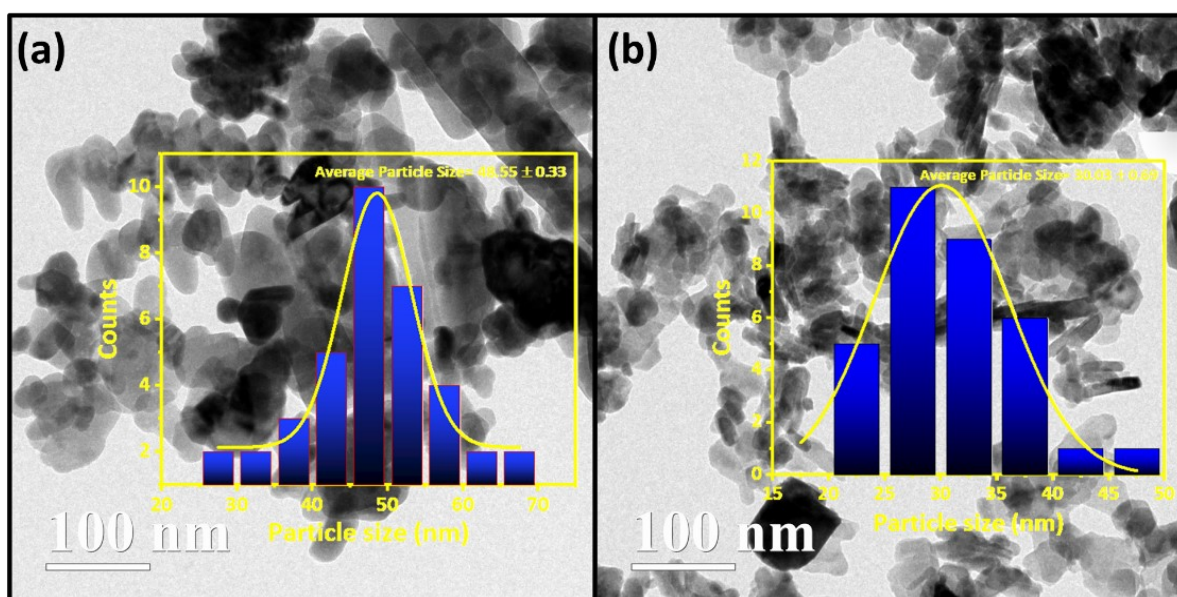


Figure S1. HRTEM images and corresponding particle size distribution histograms of (a) pristine ZnO and (b) Ce-doped ZnO (Ce-ZnO). The ZnO sample exhibits relatively larger and agglomerated nanoparticles with an average particle size of  $48.55 \pm 0.33$  nm, whereas Ce-ZnO shows reduced particle size ( $30.03 \pm 0.69$  nm) and improved dispersion, indicating that Ce incorporation effectively suppresses particle growth and promotes finer nanostructure formation.

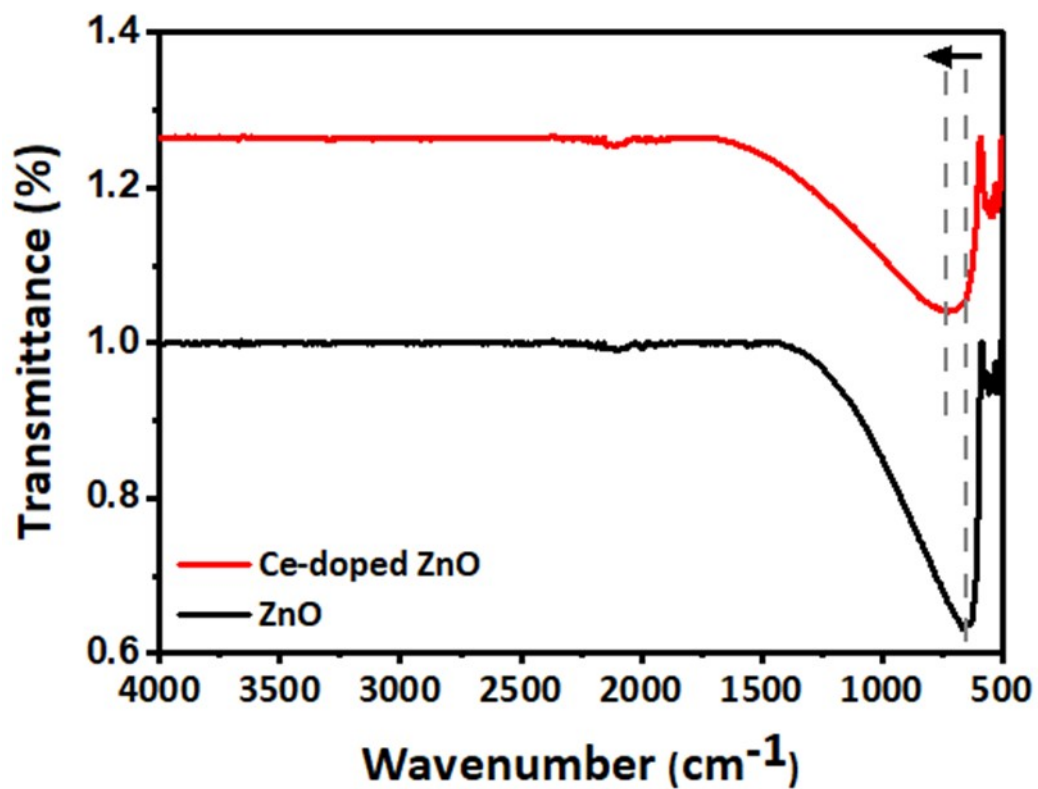


Figure S2. FTIR spectra of pristine ZnO and Ce-doped ZnO

**Table 2. Comparison of NO<sub>2</sub> gas sensing performance parameters of the present Ce-doped ZnO sensor with previously reported metal oxide-based NO<sub>2</sub> sensors.**

Materials	Preparation method	Gas response	Conc. (ppm)	Working temp. (°C)	Gases	Selectivity	Res./Reco. time (Sec.)	Lower detection limit (ppm)	Ref. No.
Ce doped ZnO	Hydrothermal		100	250	NO <sub>2</sub> , CO, H <sub>2</sub> , NH <sub>3</sub> , and acetone	NO <sub>2</sub>	11.8 /53.6	-	6
AlZnO	Reflux method	85 %	5	175	Acetone, CO <sub>2</sub> , NH <sub>3</sub> , NO <sub>2</sub> , LPG	NO <sub>2</sub>	-	5	7
Ni:ZnO	Co-precipitation	356%	100	200	NO <sub>2</sub> , H <sub>2</sub> S, Cl <sub>2</sub> , SO <sub>2</sub>	NO <sub>2</sub>	0.67/ 136.19	5	8
Ce:ZnO	Co-precipitation (Green approach)	7.5	20	190	NO <sub>2</sub> , H <sub>2</sub> S, Cl <sub>2</sub> , SO <sub>2</sub> , CO <sub>2</sub>	NO <sub>2</sub>		1	<b>This work</b>

**Table 3. Comparative summary of photocatalytic H<sub>2</sub> evolution performance of pristine ZnO and Ce-doped ZnO synthesized via different methods under various light sources and sacrificial agents.**

Sr. No.	Catalyst	Synthesis method	Light source	Sacrificial agents	H <sub>2</sub> evolution rates	Ref.
1	ZnO	One-pot Hydrothermal	300W	Methanol	36 μmol/g.h	34
	5% Ce/ZnO	One-pot hydrothermal	300W	Methanol	312 μmol/g.h	
2	ZnO	Mechanochemical method	300W	10% methanol	1.2 μmol/g.h	07
	2% Ce/ZnO	Mechanochemical method	300W	10% methanol	43 μmol/g.h	
3	ZnO	Combustion method	300W	Na <sub>2</sub> S/Na <sub>2</sub> SO <sub>3</sub>	0.36 mmol/g.h	35
	3%Ce/ZnO	Combustion method	300W	Na <sub>2</sub> S/Na <sub>2</sub> SO <sub>3</sub>	2.57 mmol/g.h	
4	ZnO	Biological method	450W	10% methanol	1.09 μmol/g.h	This work
	2% Ce/ZnO	Biological method	450W	10% methanol	5.94 μmol/g.h	

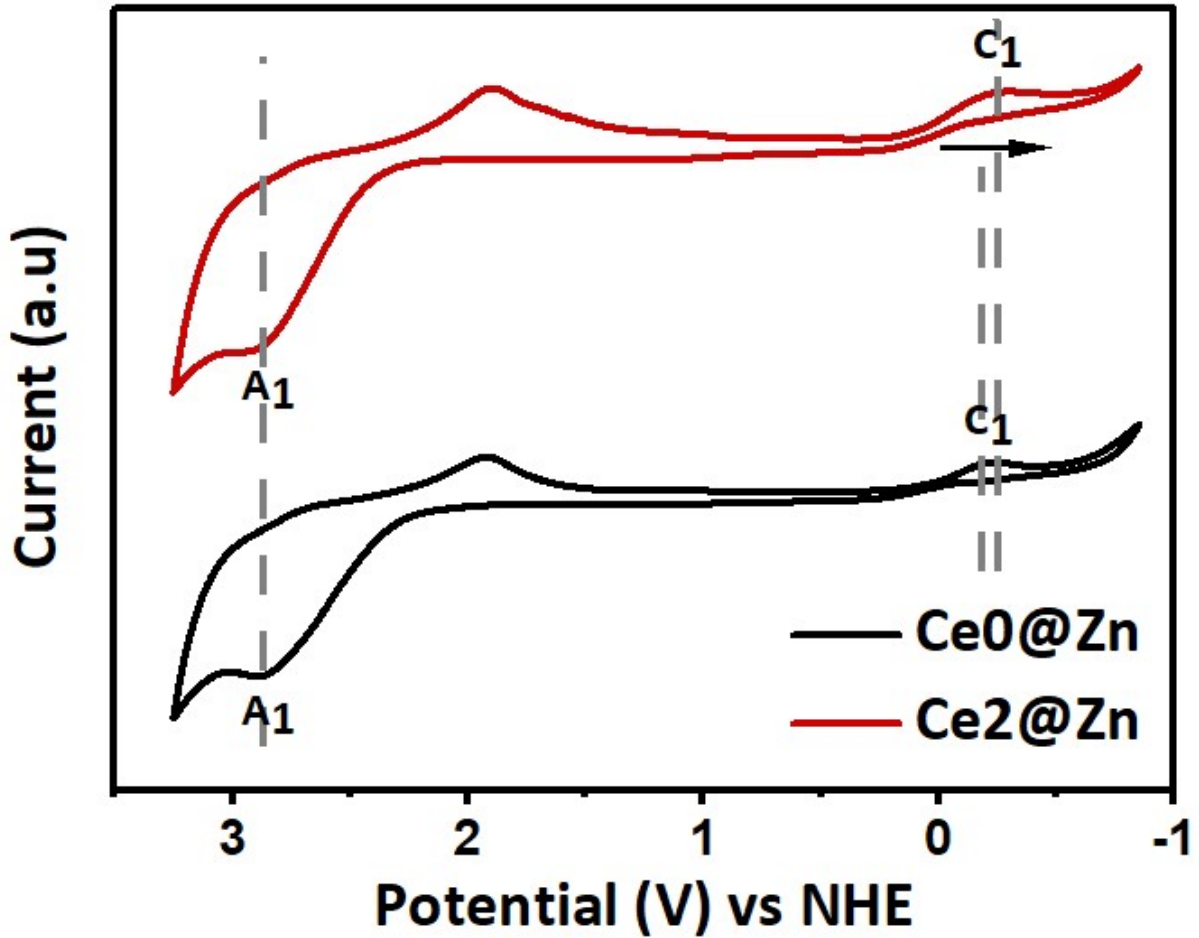


Figure S3. Cyclic voltammograms of Ce-doped ZnO samples ( $\text{Ce0@Zn}$  and  $\text{Ce2@Zn}$ ) recorded in a non-aqueous electrolyte versus NHE. The dashed lines indicate the onset potentials corresponding to the valence band maximum (VBM) and conduction band minimum (CBM). A noticeable shift in the band edge positions for  $\text{Ce2@Zn}$  compared to  $\text{Ce0@Zn}$  confirms the Burstein–Moss (BM) effect, arising from increased carrier concentration due to Ce doping, which leads to band filling and an apparent widening of the optical band gap.

**Table 3. Energy level positions and bandgap values of pristine ZnO and Ce-doped ZnO obtained from cyclic voltammetry (CV) and optical measurements.**

Sample	Cyclic Voltammetry		Electrochemical bandgap (eV)	Optical bandgap (eV)
	LUMO vs. Vacuum	HOMO vs. Vacuum		
pristine ZnO	-4.32	-7.39	3.07	3.20
Ce-doped ZnO	-4.24	-7.39	3.15	3.23

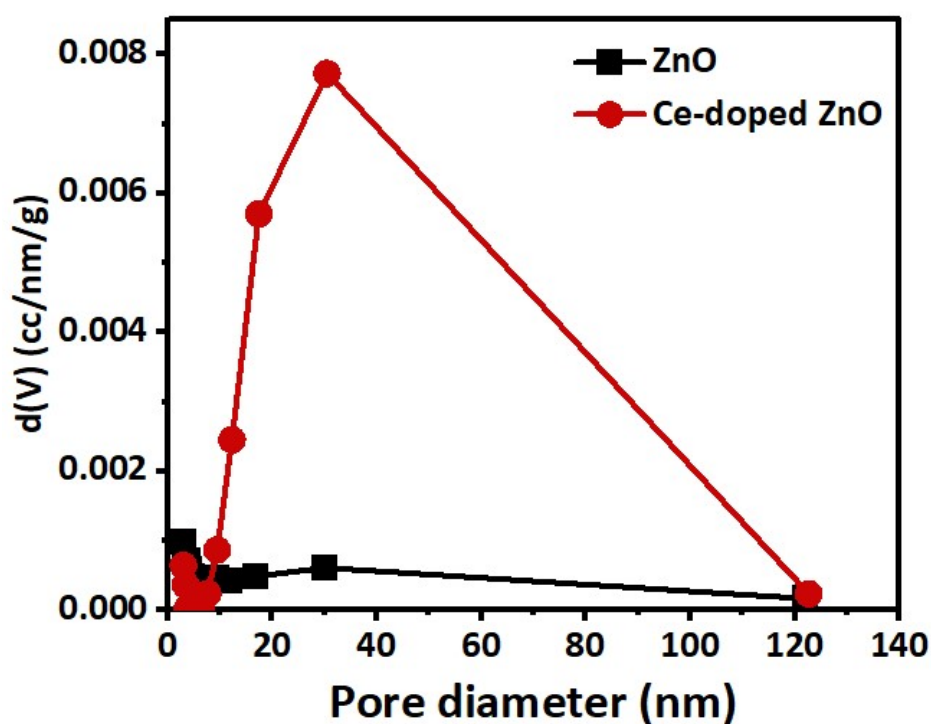


Figure S4. Pore size distribution curves of pristine ZnO and Ce-doped ZnO obtained from BET analysis of nitrogen adsorption–desorption isotherms.

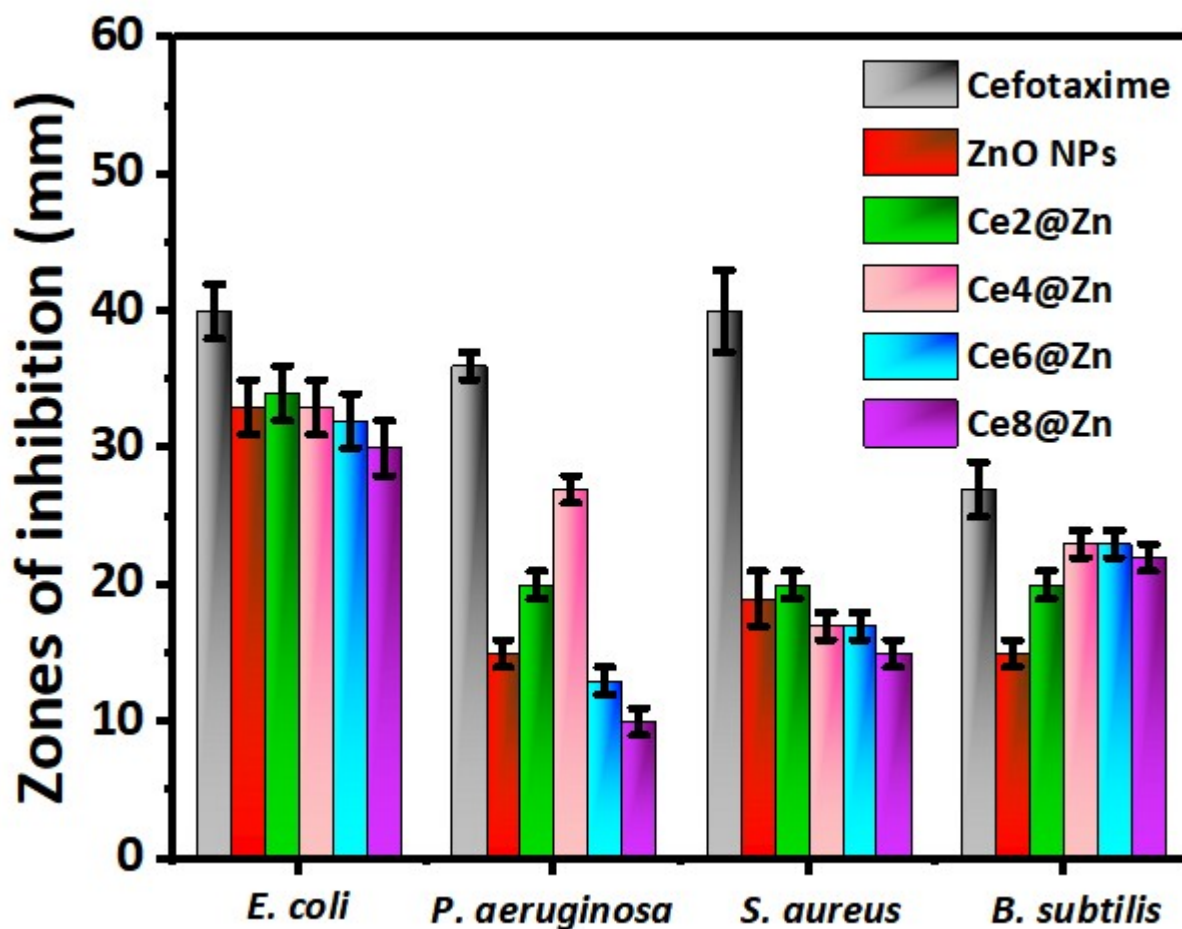


Figure S5. Comparative antibacterial activity of pristine ZnO and Ce-doped ZnO nanoparticles against different bacterial strains (*E. coli*, *P. aeruginosa*, *S. aureus*, and *B. subtilis*), expressed as zones of inhibition (mm). Cefotaxime is used as the positive control. The results show enhanced antibacterial performance for Ce-doped ZnO, with the 2% Ce-doped sample (Ce2@Zn) exhibiting superior activity compared to pristine ZnO and higher doping concentrations.