

† **Electronic Supplementary Information (ESI)**

**Insights into the Structural and Microscopic Origin of Magnetic and Optical Properties
of monodispersed γ -Fe₂O₃, ZnO, γ -Fe_{2-2x}Zn_{2x}O₃ and γ -Fe₂O₃@ZnO nanostructures**

Ruchi Agrawal^{a,b}, Manas Srivastava^a, Debashish Sarkar^{b,c} and Raghmani Singh
Ningthoujam^{a,b,*}

^aChemistry Division, Bhabha Atomic Research Centre, Mumbai 400085, India

^bHomi Bhabha National Institute, Anushaktinagar, Mumbai 400094, India

^cTechnical Physics Division, Bhabha Atomic Research Centre, Mumbai 400085, India

*Corresponding Author

Raghmani Singh Ningthoujam

Chemistry Division, Bhabha Atomic Research Centre, Mumbai 400085, India;

Homi Bhabha National Institute, Mumbai 400094, India;

orcid.org/0000-0002-4642-5990;

Email: rsn@barc.gov.in, nraghu_mani@yahoo.co.in

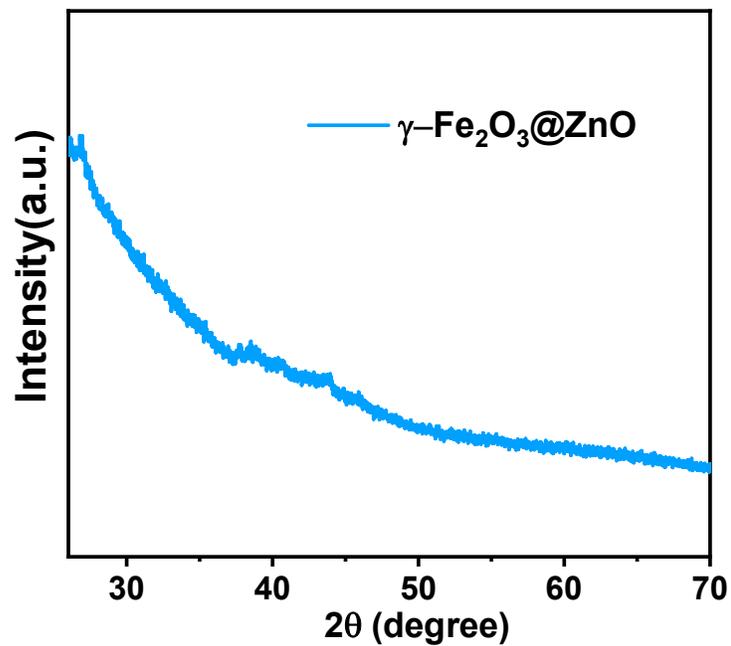


Fig. S1 Typical XRD pattern of $\gamma\text{-Fe}_2\text{O}_3@\text{ZnO}$ (CS).

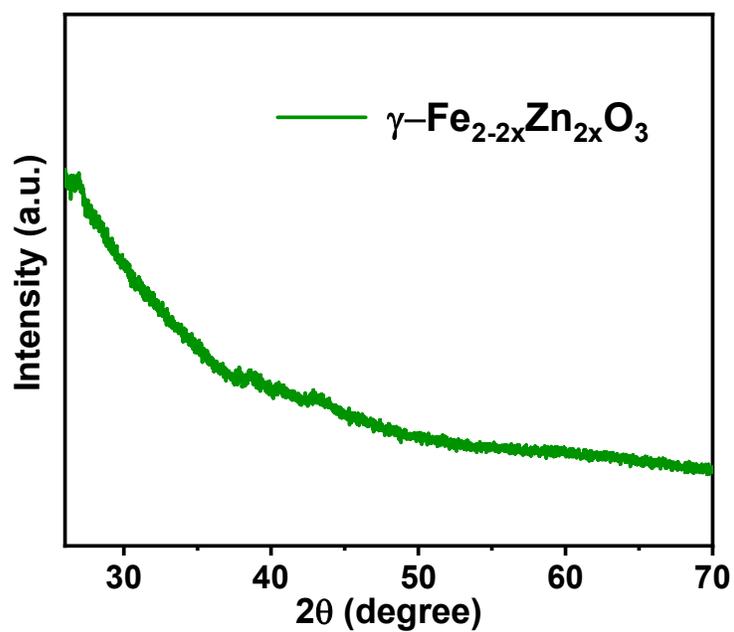


Fig. S2 Typical XRD pattern of $\gamma\text{-Fe}_{2-2x}\text{Zn}_{2x}\text{O}_3$ (SUB).

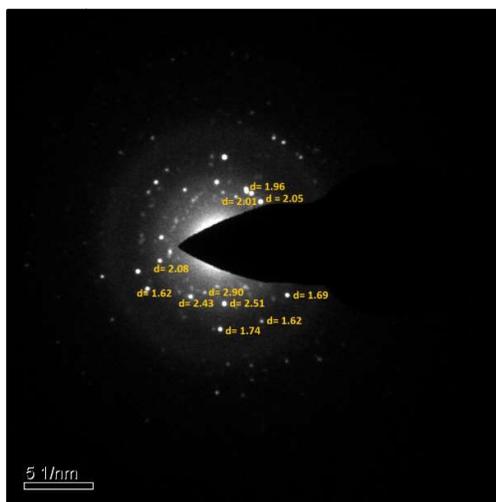


Fig. S3 Another SAED pattern of $\gamma\text{-Fe}_2\text{O}_3$.

Table S1 The d-values and corresponding planes of Fig. S3.

$\gamma\text{-Fe}_2\text{O}_3$	d-value (Å)	Plane
	2.90	220
	2.51	311
	2.05, 2.01, 2.08	400
	1.69, 1.74	422
	1.62, 1.62	511

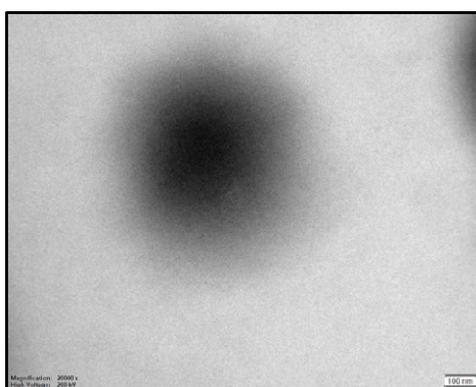


Fig. S4 TEM image of ZnO-300 (scale = 100 nm).

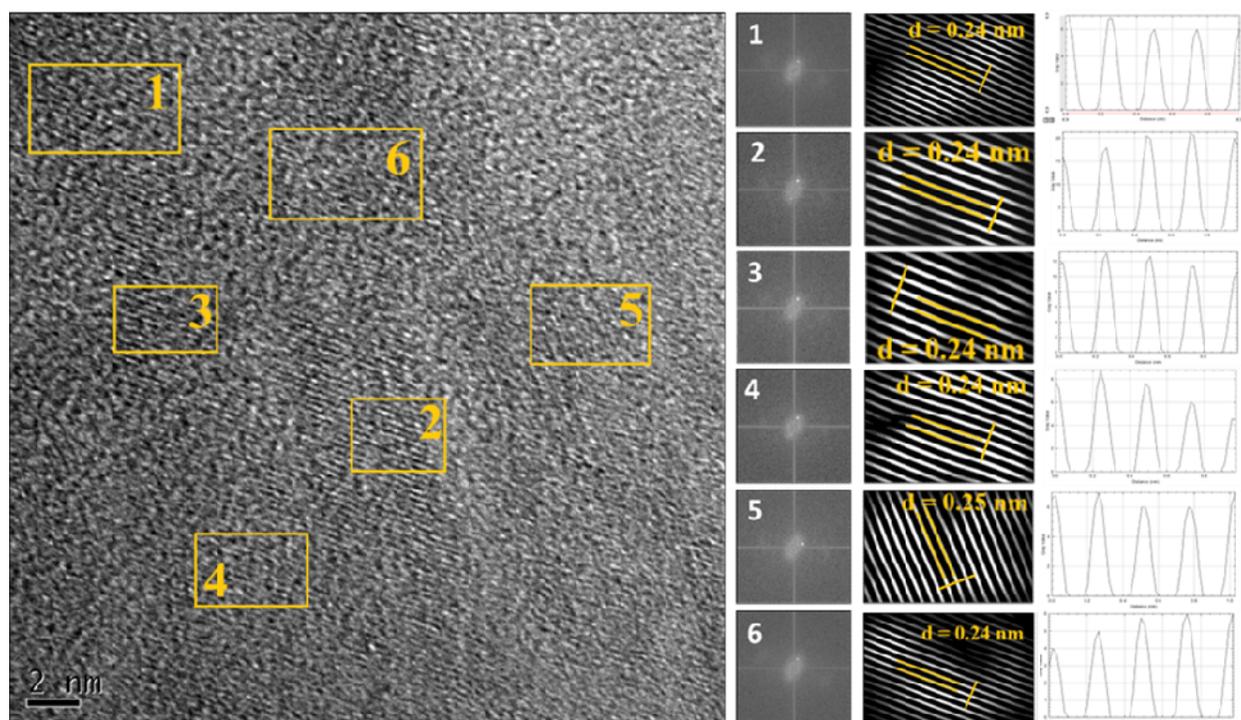


Fig. S5 Another HR-TEM image of CS: 6 different spots (1, 2, 3, 4, 5, 6) and their corresponding FFT images, inverse FFT and line profile images.

Table S2 The d-values and corresponding planes of **Fig. 5(c)**, **Fig. 5(d)** and **Fig. S5**.

SAED	d-value (Å)	Plane	
	3.37	211	γ-Fe₂O₃
	2.58	311	ZnFe₂O₄
	2.4	222	ZnFe₂O₄
	1.7	422	γ-Fe₂O₃/ ZnFe₂O₄
	1.5	440	ZnFe₂O₄
HR-TEM			
Spot	d-value (Å)	Plane	
Spot 1	2.5	311	γ-Fe₂O₃/ZnFe₂O₄
Spot 2	2.5	311	γ-Fe₂O₃/ZnFe₂O₄
Spot 3	3.0	220	γ-Fe₂O₃/ ZnFe₂O₄
HR-TEM			
Spot	d-value (Å)	Plane	
Spot 1	2.4	222	ZnFe₂O₄
Spot 2	2.4	222	ZnFe₂O₄
Spot 3	2.4	222	ZnFe₂O₄
Spot 4	2.4	222	ZnFe₂O₄
Spot 5	2.5	311	γ-Fe₂O₃/ZnFe₂O₄
Spot 6	2.4	222	ZnFe₂O₄

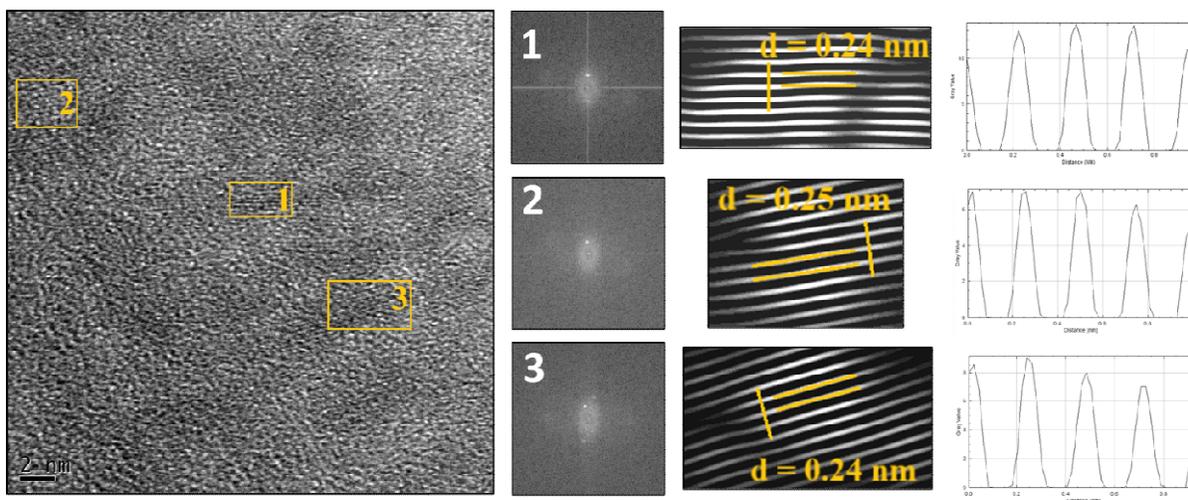


Fig. S6 Another HR-TEM image of SUB: 3 different spots (1, 2, 3) and their corresponding FFT images, inverse FFT and line profile images.

Table S3 The d-values and corresponding planes of **Fig. 6(c)**, **Fig. 6(d)** and **Fig. S6**.

$\gamma\text{-Fe}_{2-2x}\text{Zn}_{2x}\text{O}_4$ (SUB)			
SAED	d-value (Å)	Plane	
	3.0	220	$\gamma\text{-Fe}_2\text{O}_3/\text{ZnFe}_2\text{O}_4$
	2.58	311	ZnFe_2O_4
	2.2	400	ZnFe_2O_4
	1.6	511	ZnFe_2O_4
	1.5	440	ZnFe_2O_4
HR-TEM	d-value (Å)	Plane	
Spot 1	2.4	222	ZnFe_2O_4
Spot 2	3.0	220	$\gamma\text{-Fe}_2\text{O}_3/\text{ZnFe}_2\text{O}_4$
Spot 3	1.5	440	ZnFe_2O_4
HR-TEM	d-value (Å)	Plane	
Spot 1	2.4	222	ZnFe_2O_4
Spot 2	2.5	311	$\gamma\text{-Fe}_2\text{O}_3/\text{ZnFe}_2\text{O}_4$
Spot 3	2.4	222	ZnFe_2O_4

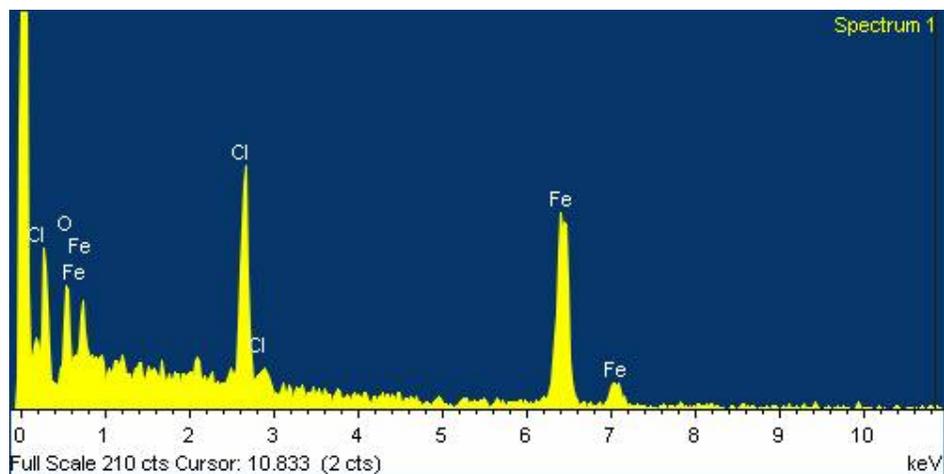


Fig. S7 EDX spectrum of $\gamma\text{-Fe}_2\text{O}_3$.

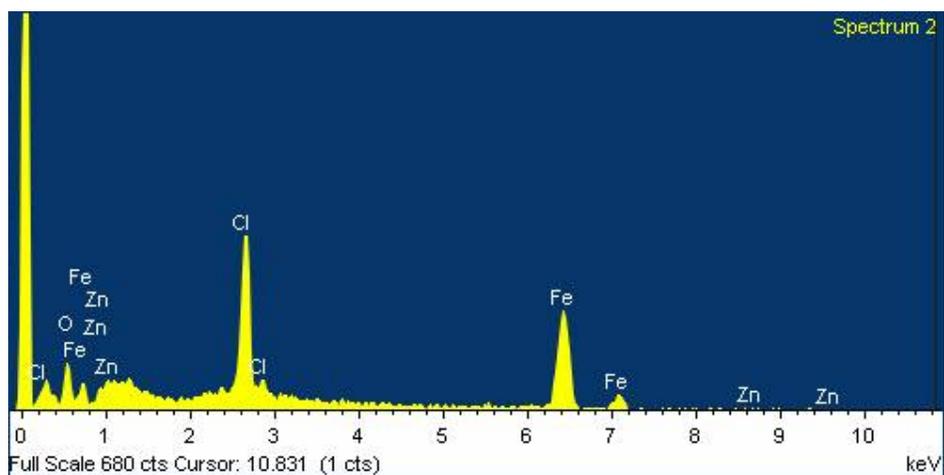


Fig. S8 EDX spectrum of $\gamma\text{-Fe}_2\text{O}_3@ZnO$ (CS).

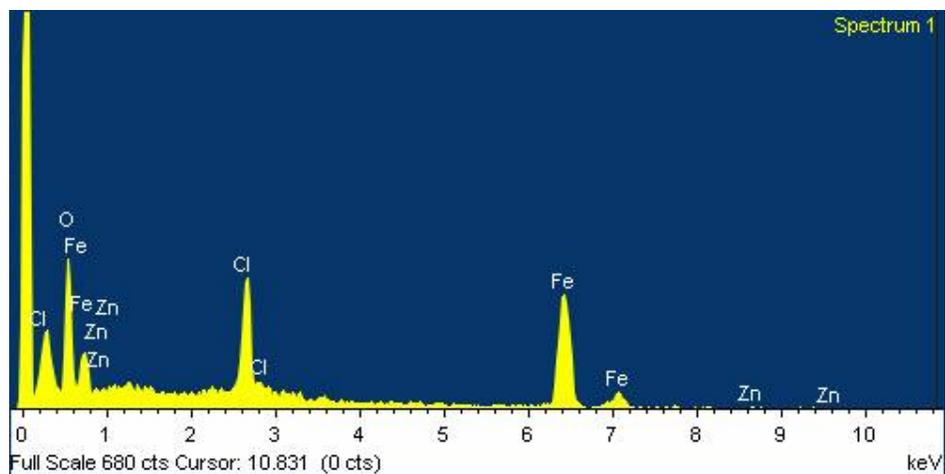


Fig. S9 EDX spectrum of $\gamma\text{-Fe}_{2-2x}\text{Zn}_{2x}\text{O}_3$ (SUB).

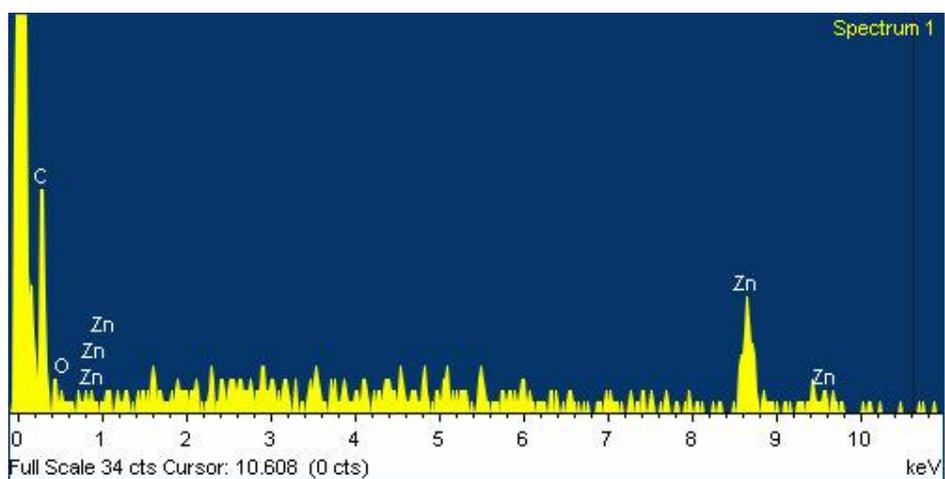


Fig. S10 EDX spectrum of ZnO.

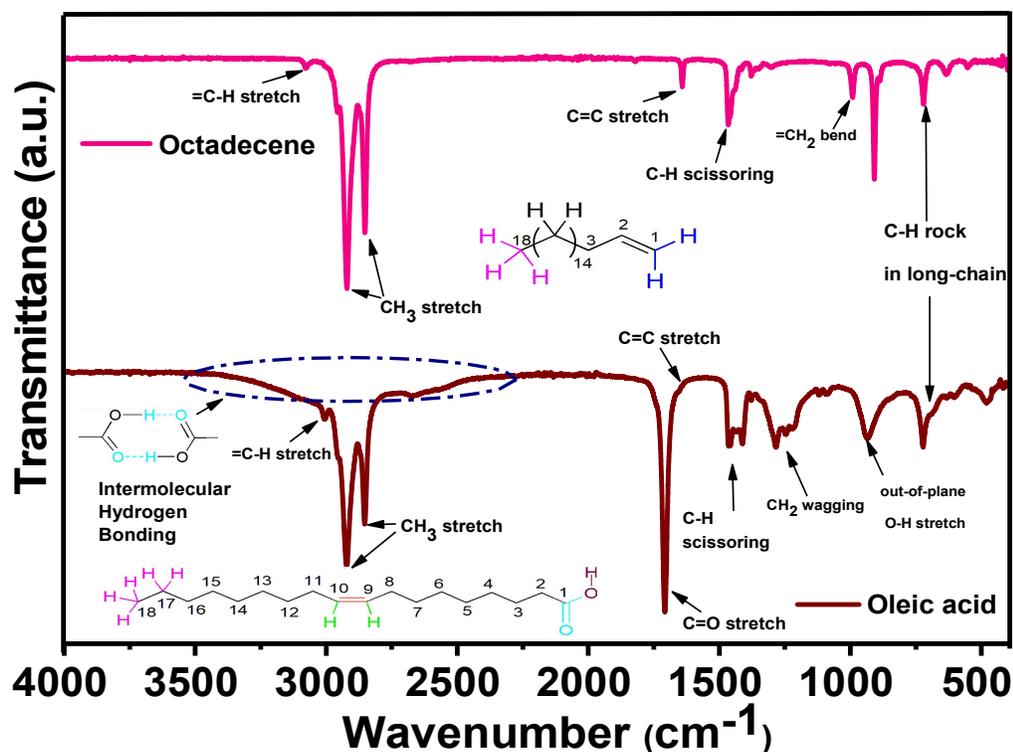


Fig. S11 FTIR spectra of pure oleic acid and 1-octadecene.

Table S4 FT-IR peak assignments of 1-octadecene and oleic acid.

1-Octadecene (cm ⁻¹)	Oleic acid (cm ⁻¹)	Peak assignments	References
3076	3005	=C-H stretch	2, 3
2919	2921	C-H stretch (asymmetric)	1, 2, 3
2851	2851	C-H stretch (symmetric)	1, 2, 3
-	2250-3500	O-H stretch Intermolecular hydrogen bonding	3
-	1709	C=O stretch	1, 3
1643	1643	C=C stretch	2

-	1462	In plane O-H stretch	1, 3
-	1284	C-O stretch	1, 3
-	931	Out-of-plane O-H stretch	2, 3
1380-1460	1380-1460	C-H scissoring	2, 3
-	1200-1300	C-H wagging	2
990	-	=CH ₂ bend	2
720	725	C-H rocking in long chain alkanes	2, 3

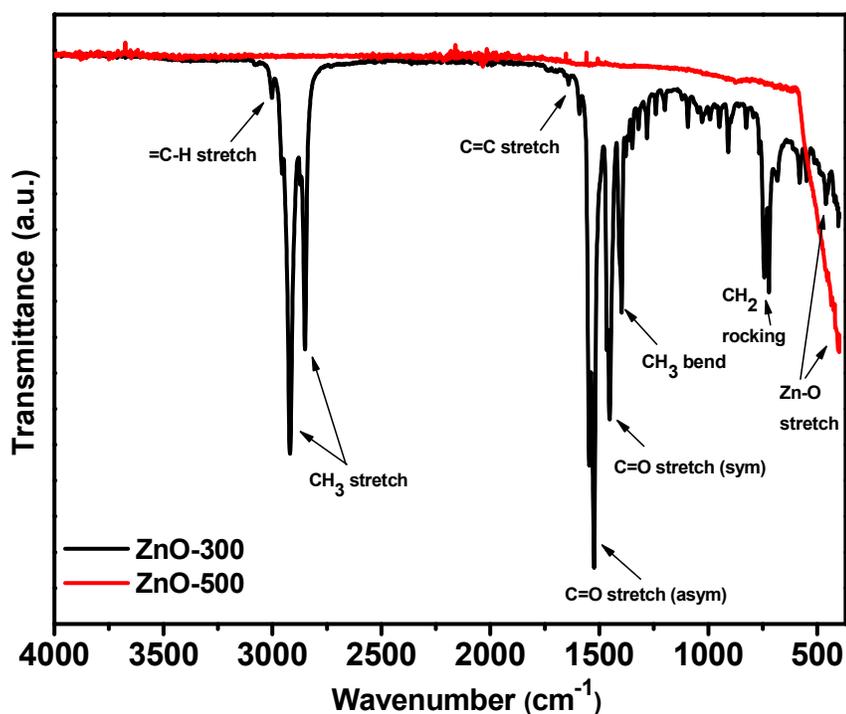


Fig. S12 FTIR spectra of ZnO-300 and ZnO-500 nanoparticles.

References:

- (1) J. Ibarra, J. Melendres, M. Almada, M. G. Burboa, P. Taboada, J. Juárez and M. A. Valdez, *Mater. Res. Express*, 2015, **2**, 095010.
- (2) R. Joshi, B. P. Singh, C. L. Prajapat, Y. Kashyap, C. Nayak, D. Bhattacharyya and R. S. Ningthoujam, *J. Phys. Chem. C*, 2021, **125**, 17971–17982.

- (3) N. Wu, L. Fu, M. Su, M. Aslam, K. C. Wong and V. P. Dravid, *Nano Lett.*, 2004, **4**, 383–386.

Table S5 Optical band gap energy of all the samples.

S.N.	Sample Name	Optical Band Gap Energy (eV)	
		Direct allowed transition	Indirect allowed transition
1	γ -Fe ₂ O ₃	2.78	2.40
2	γ -Fe ₂ O ₃ @ZnO (CS)	3.15	2.88
3	γ -Fe _{2-2x} Zn _{2x} O ₃ (SUB)	3.12	2.84
4	ZnO	3.58	3.02

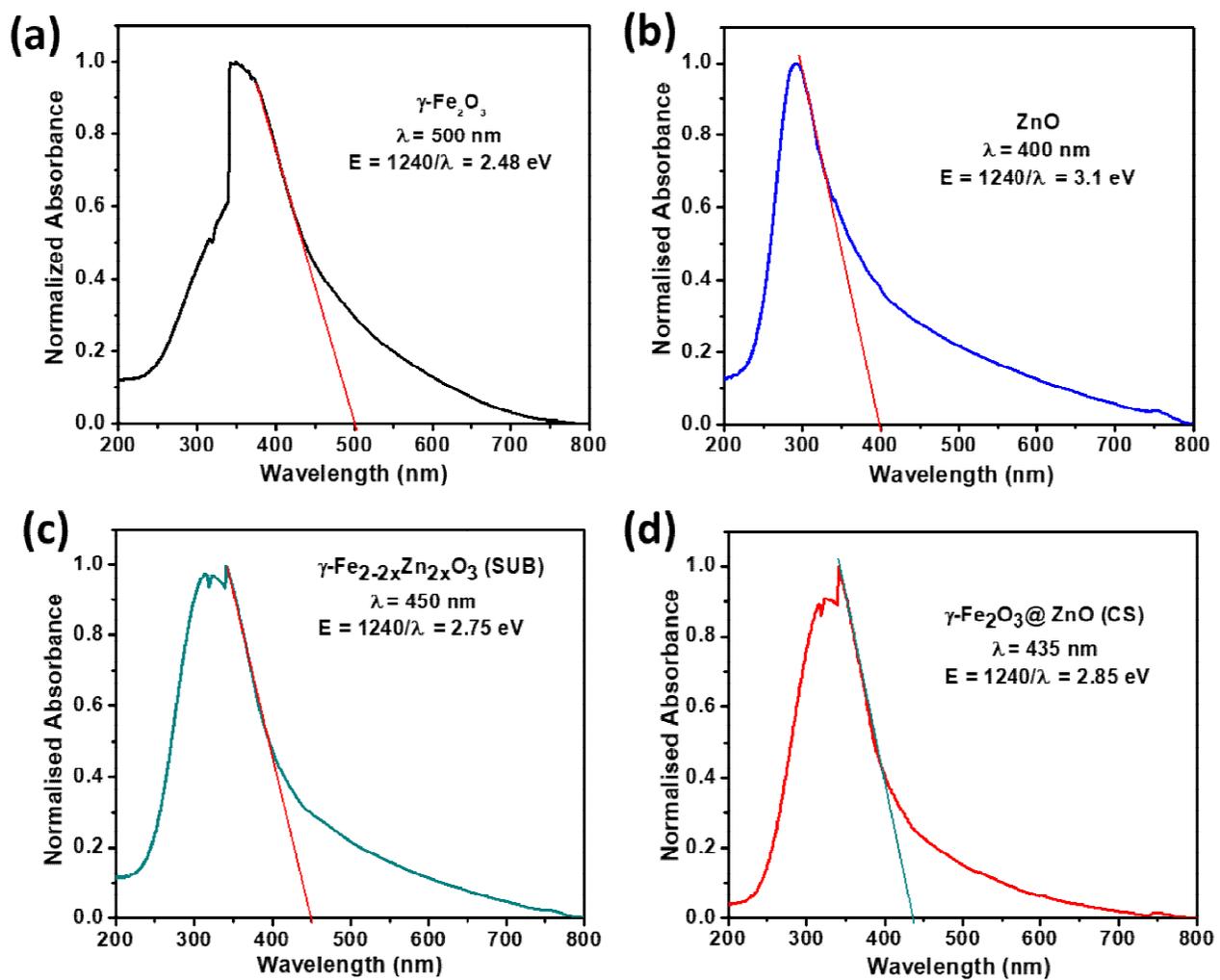


Fig. S13 Plotting of tangent/slope to UV-visible absorption curve of **(a)** $\gamma\text{-Fe}_2\text{O}_3$, **(b)** ZnO, **(c)** $\gamma\text{-Fe}_{2-2x}\text{Zn}_{2x}\text{O}_3$ (SUB) and **(d)** $\gamma\text{-Fe}_2\text{O}_3@ \text{ZnO}$ (CS).

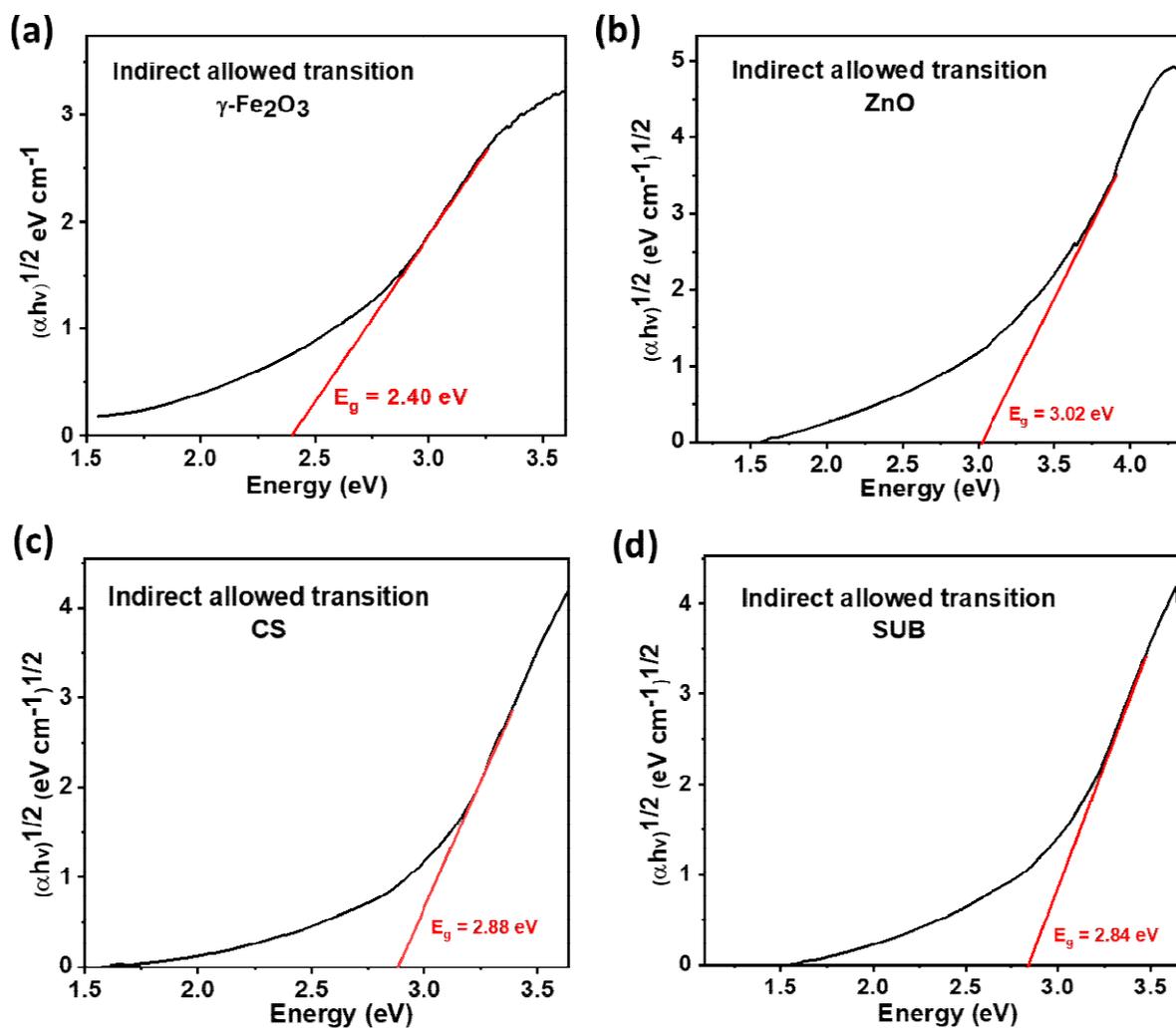


Fig. S14 The indirect optical band gap energies of (a) γ -Fe₂O₃, (b) ZnO, (c) γ -Fe₂O₃@ZnO (CS) and (d) γ -Fe_{2-2x}Zn_{2x}O₃ (SUB), respectively calculated using Tauc plot.