Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Supplementary Information

Significant reduction in the optical band-gap and defect assisted magnetic response in Fe-doped anatase TiO_2 nanocrystals as dilute magnetic semiconductors

V. R. Akshay[1, 2], B. Arun[1, 2], Guruprasad Mandal[3], Anupama Chanda[4] and M.Vasundhara[1, 2*]

[1]*Materials Science and Technology Division, CSIR-National Institute for Interdisciplinary Science and Technology, Trivandrum -695 019, India.*

[2] *Academy of Scientific and Innovative Research (AcSIR), CSIR-Human Resource Development Centre, Ghaziabad, Uttarpradesh, India.*

[3]*Centre for Rural and Cryogenic Technologies, Jadavpur University, Kolkata-700032*

[4]*Department of Physics, Dr Hari Singh Gour Central University, Sagar, India-470003*

[*]Corresponding authors: mvas@niist.res.in, vasu.mutta@gmail.com

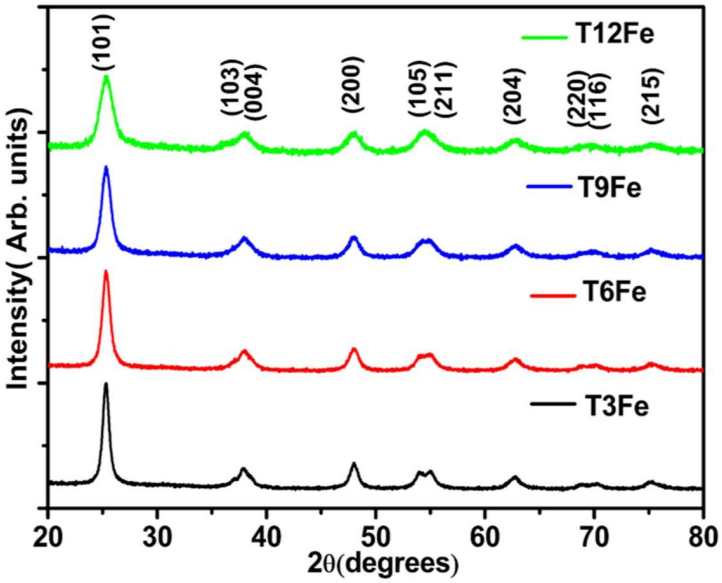

Fig.S1: XRD patterns of T3Fe, T6Fe, T9Fe and T12Fe

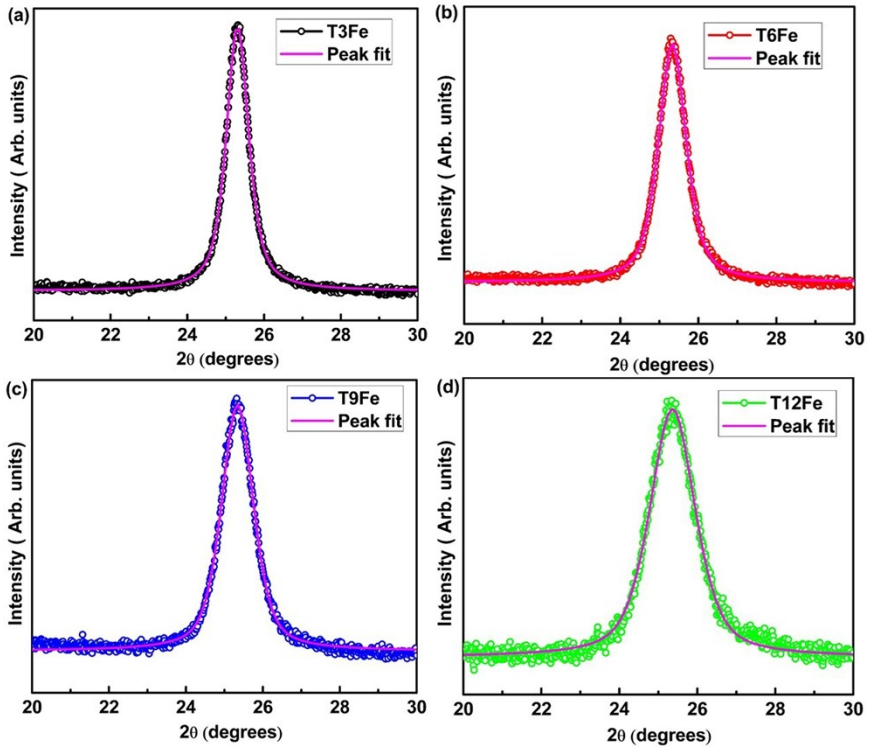

Fig.S2: Estimation of FWHM from the most intense (101) peak of (a) T3Fe (b) T6Fe (c) T9Fe and (d) T12Fe

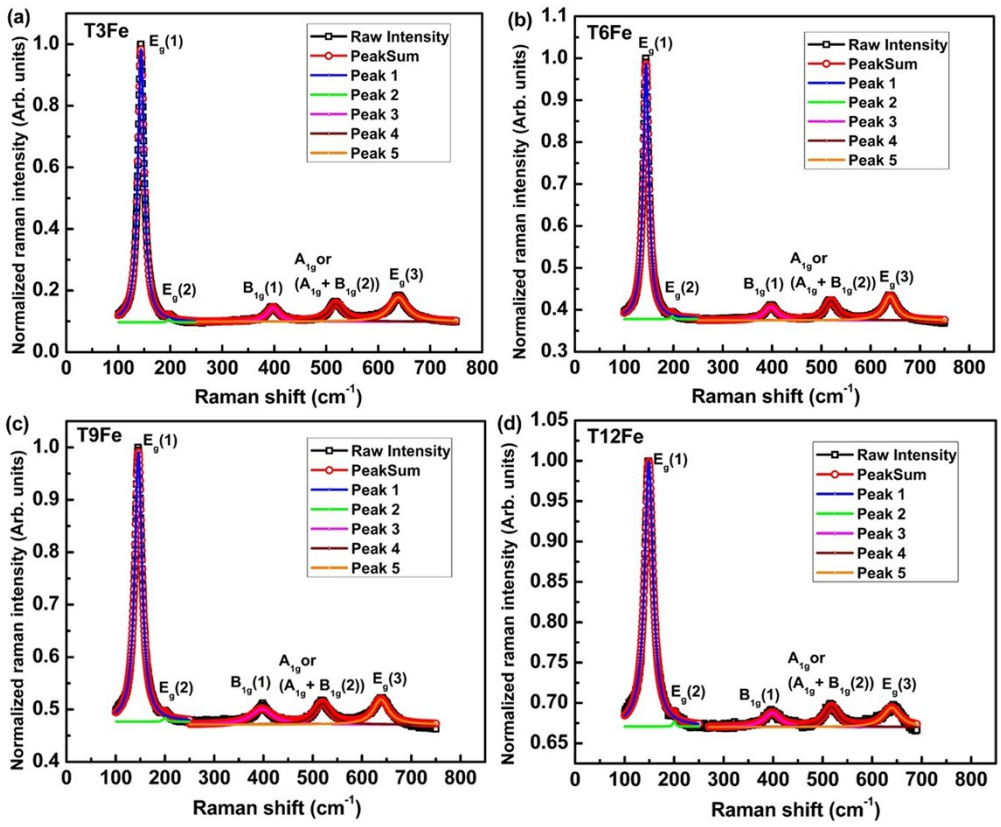

Fig.S3: Deconvoluted Raman spectra of (a) T3Fe (b) T6Fe (c) T9Fe (d) T12Fe

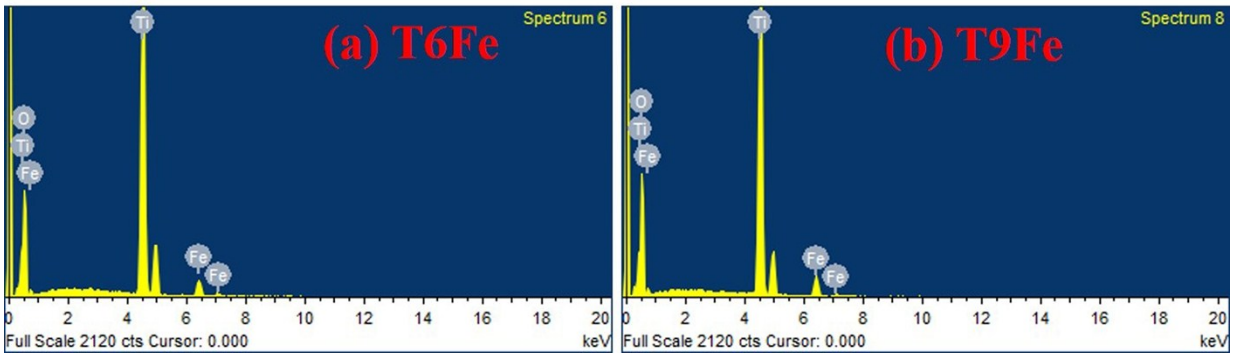

Fig.S4: SEM-EDS spectra of (a) T6Fe (b) T9Fe

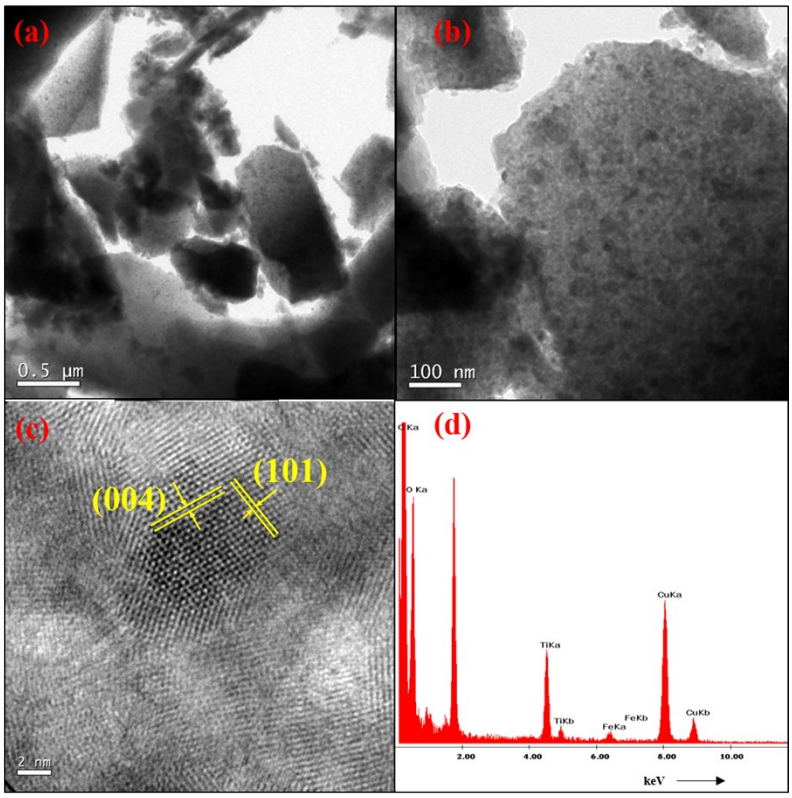

Fig.S5: (a), (b) Sheet formation in T3Fe samples (c) HR-TEM image showing the crystalline nature of stacked T3Fe sheets (d) EDS spectra of T3Fe from HR-TEM

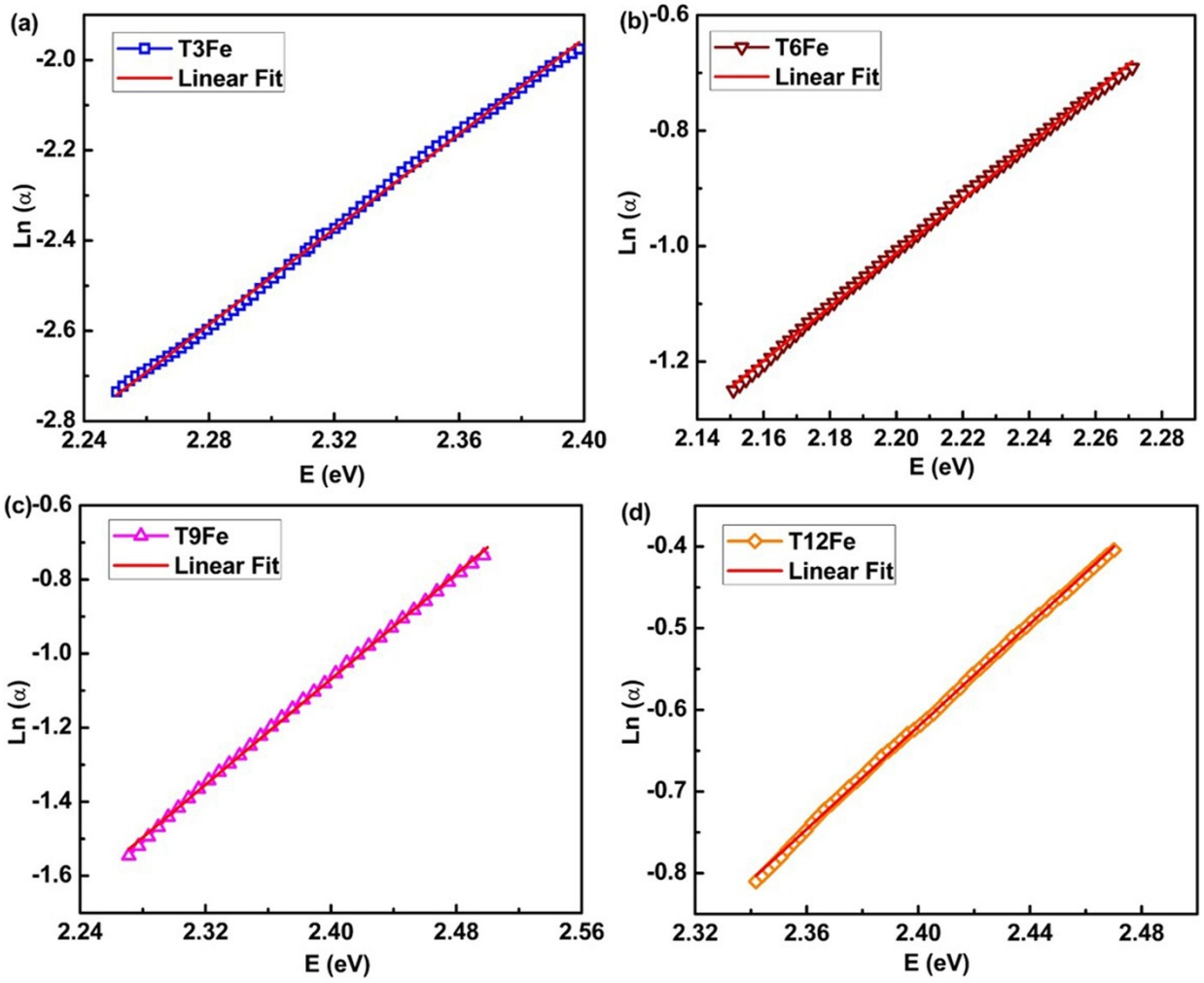

Fig.S6: Plot for Urbach energy estimation of (a) T3Fe, (b) T6Fe (c) T9Fe and (d) T12Fe

Table S1: Refinement parameters obtained for pristine and Fe-doped TiO_2 nanocrystals

Compound	**Pristine TiO_2**	**T3Fe**	**T6Fe**	**T9Fe**	**T12Fe**
Phase	Anatase				
Crystal Structure	Tetragonal				
Space Group	I 41/a m d				
Lattice Parameters					
a(Å)	3.7901 (1)	3.7834 (5)	3.7810 (2)	3.7793 (3)	3.7772 (5)
c(Å)	9.4923 (3)	9.4902 (1)	9.4881 (4)	9.4854 (1)	9.4843 (2)
Volume (Å)^3	136.35 (2)	135.81 (1)	135.64 (3)	135.45 (1)	135.29 (4)
Residual Parameters					
R_p	4.56	4.19	4.16	4.35	4.14
R_{wp}	5.77	5.23	5.44	5.33	5.39
χ^2	1.89	1.47	1.46	1.47	1.47

Table S2: ED-XRFS data obtained for T3Fe, T6Fe, T9Fe and T12Fe

Compound	**Percentage of elemental oxide**
T3Fe	96.9% TiO_2 + 3.1% Fe_2O_3
T6Fe	93.9% TiO_2 + 6.1% Fe_2O_3
T9Fe	90.9% TiO_2 + 9.1% Fe_2O_3
T12Fe	87.8% TiO_2 + 12.2% Fe_2O_3

Table S3 : Band Gaps and Urbach energy estimated for Fe-doped TiO_2 samples

Sample	Band gap (eV)	Urbach energy (meV)
T3Fe	2.30	190
T6Fe	1.89	214
T9Fe	1.80	281
T12Fe	1.76	318