Electronic supplementary information (ESI†)

Photocatalytic activity of SnO_2-α-Fe_2O_3 composite mixtures: exploration of number of active sites, Turnover number and Turnover Frequency.

L. Gomathi Devi*, R. Shyamala

Department of Post-Graduate Studies in Chemistry, Central College City Campus,

Dr Ambedkar Street, Bangalore University, Bangalore-560001

Email: ***gomatidevi_naik@yahoo.co.in***

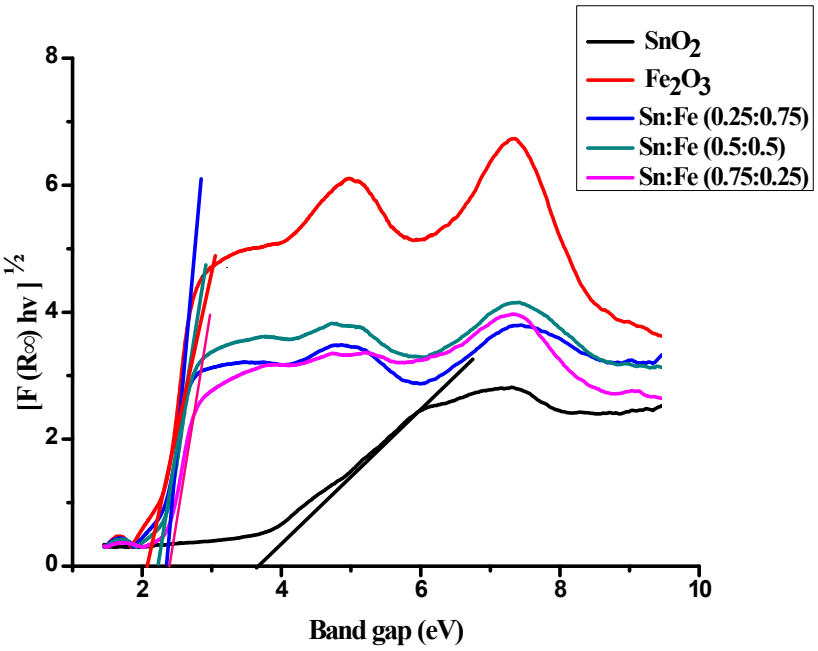
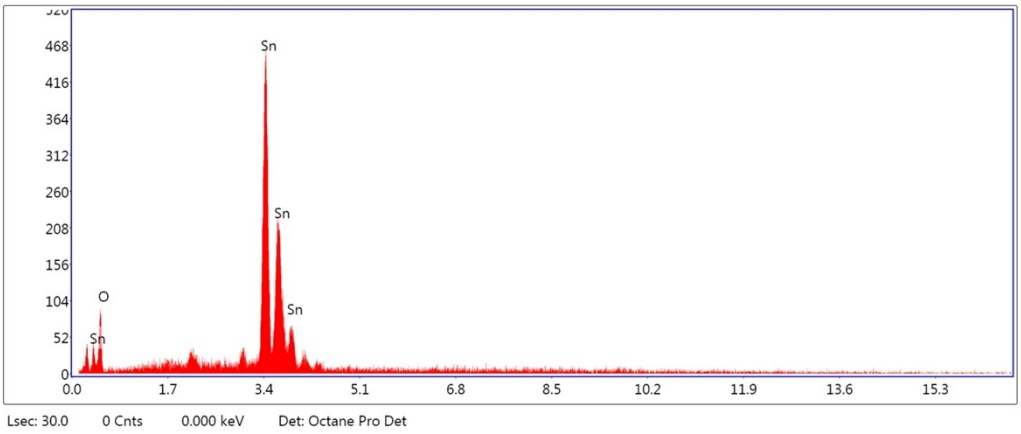


Fig.S1. The plots of [F (R_∞) hν] ^{½} v/s photon energy (hν) for α-Fe_2O_3, SnO_2 and SnO_2-α-Fe_2O_3 composites.

(a)



(b)

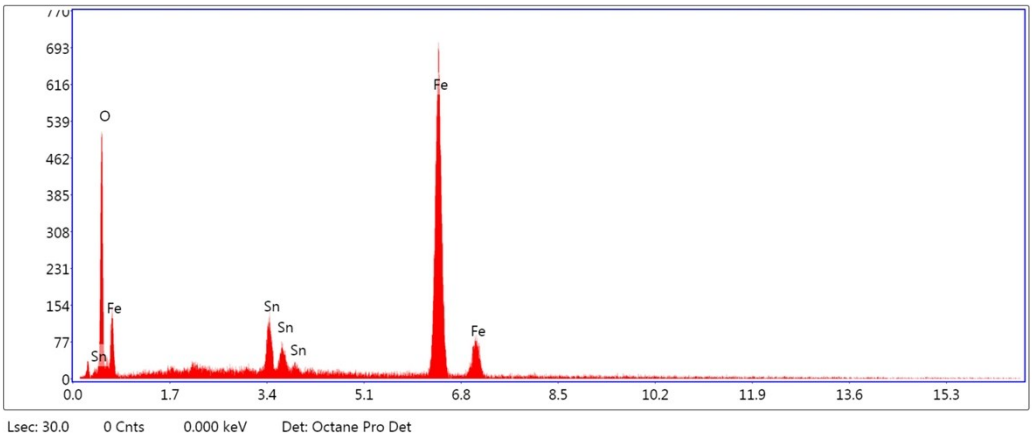


Fig.S2. EDAX of a) SnO_2 and b) Sn: Fe (0.75:0.25) composite.

S3: Detailed calculation of number of active sites, Turnover number (TON) and Turnover frequency (TOF) (for UV system in the absence of H_2O_2, refer to the Fig. 7(a))

1. **For SnO_2:**

Molecular weight of SnO_2 =150.7g/mol

Atomic weight of Sn =118.7g/mol

1.1. Calculation of number of active sites for SnO_2

150.7g/mol of SnO_2 contains 118.7g of Sn

Therefore 10mg of SnO_2 contains.....?

$$\frac{0.01\times118.7}{150.7}=0.0078\text{g of Sn}$$

1 mole of SnO_2 solution contains 150.7g SnO_2 of dissolved in 1L. Further this above solution contains 118.7g of Sn

Therefore 118.7g of Sn is present in 1 mole of SnO_2 solution

0.0078g of Sn is equivalent to.....moles

$$\frac{0.0078}{118.7}=6.571\times10^{-5}\text{moles of Sn ; number of active sites}$$

1.2. % conversion of substrate phenol under UV light illumination (as per data obtained from Fig.7.a)

94.1g of phenol in 1L gives 1M solution

0.02g (20ppm) of phenol in 250ml is equivalent to.....moles

$$\frac{0.02\times250\times1}{94.1\times1000}=5.313\times10^{-5}\text{moles}$$

250 ml of 20ppm phenol is 5.313×10^{-5} moles

35% of phenol is degraded under UV light with SnO_2 as catalyst (Fig.7.a)

35% of 5.313×10^{-5} moles is 2.0189×10^{-5} moles. More specifically 2.0189×10^{-5} moles were degraded in 120 min time period.

1.3. Calculation of Turnover number

$$\text{TON}=\frac{\text{Number of moles of phenol degraded}}{\text{Number of moles of SnO}_2\text{ taken}}$$
$$=\frac{2.0189\times10^{-5}\text{moles}}{6.571\times10^{-5}\text{moles}}$$
$$=0.3073$$

1.4. Calculation of Turnover frequency

$$\text{TOF}=\frac{\text{TON}}{\text{time}(\text{min})}=\frac{0.3073}{120}=2.5609\times10^{-3}\text{min}^{-1}$$

Similar procedure is used to calculate the number of active sites, TON and TOF of α-Fe_2O_3 sample.

2. Sn: Fe (0.25:0.75):

Molecular weight of Sn: Fe (0.25:0.75)=310.4g/mol

Molecular weight of Sn: Fe = Molecular weight of SnO_2 + Molecular weight of α- Fe_2O_3, Therefore in 310.4g/mol of Sn: Fe (0.25:0.75) composite contains SnO_2=28.51% and α-Fe_2O_3 =71.49% (as calculated from equation 3 and Table1)

100g of Sn: Fe (0.25:0.75) contains 28.51% of SnO_2

Therefore 310.4g of Sn: Fe (0.25:0.75) contains $\frac{310.4\times28.51}{100}=88.38\,\text{g of } SnO_2$

Calculation for α- Fe_2O_3: Similarly 310.4g of Sn: Fe (0.25:0.75) contains 221.9g of α-Fe_2O_3

2.1. Number of active sites for Sn: Fe (0.25:0.75) composite

310.4g of Sn: Fe (0.25:0.75) composite contains 88.38g of SnO_2

10mg of Sn: Fe (0.25:0.75) composite contains 2.851×10^{-3} g of SnO_2

150.7g/mol of SnO_2 contains 118.7g of Sn

Therefore 2.851×10^{-3} of SnO_2 contains $\frac{2.851\times10^{-3}\times118.7}{150.7}=2.2456\times10^{-3}\text{g of Sn}$

1 mole of SnO_2 solution contains 118.7g of Sn

2.2456x10^{-3} of Sn is equivalent to:

$\frac{2.2456\times10^{-3}}{118.7}=1.8918\times10^{-5}\text{moles of Sn}$; number of active sites

Similar calculation for α- Fe_2O_3,

310.4g of Sn: Fe (0.25:0.75) composite contains 221.9g of α- Fe_2O_3

10mg of Sn: Fe (0.25:0.75) composite contains 7.1580×10^{-3} g of α- Fe_2O_3

159.7g/mol of SnO_2 contains 111.7g of Fe

Therefore 7.1580×10^{-3} of α- Fe_2O_3 contains $\frac{7.1580\times10^{-3}\times111.7}{159.7} = 5.0065\times10^{-3}\text{g of Fe}$

1 mole of α- Fe_2O_3 solution contains 111.7g of Fe

5.0065x10^{-3}g of Fe contains:

$\frac{5.0065\times10^{-3}\text{g}}{111.7} = 4.4820\times10^{-5}\text{moles of Fe}$; number of active sites

Therefore total number of active sites in 10mg of Sn: Fe (0.25:0.75) composite containing 28.51% of SnO_2 +71.49% of α- Fe_2O_3 is 6.3738x10^{-5} moles ~ number of active sites

$(1.8918\times10^{-5}\text{moles} + 4.4820\times10^{-5}\text{moles})$

2.2. % conversion of substrate under UV light illumination

250ml of 20ppm of phenol contains 5.313×10^{-5} moles

60.14% of phenol is degraded under UV light (Fig.7.a) which is equivalent to 3.1953×10^{-5} moles.

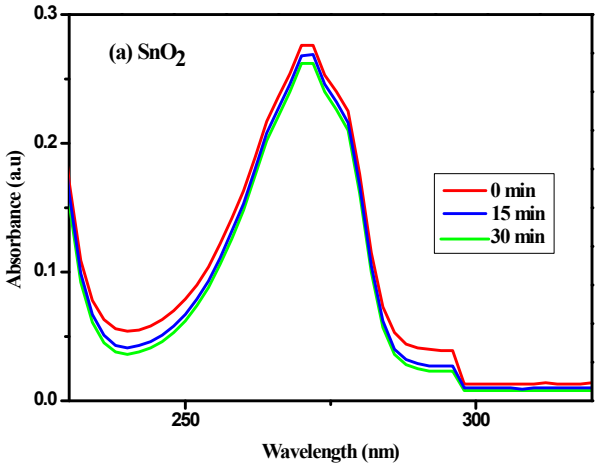
2.3. Calculation of TON

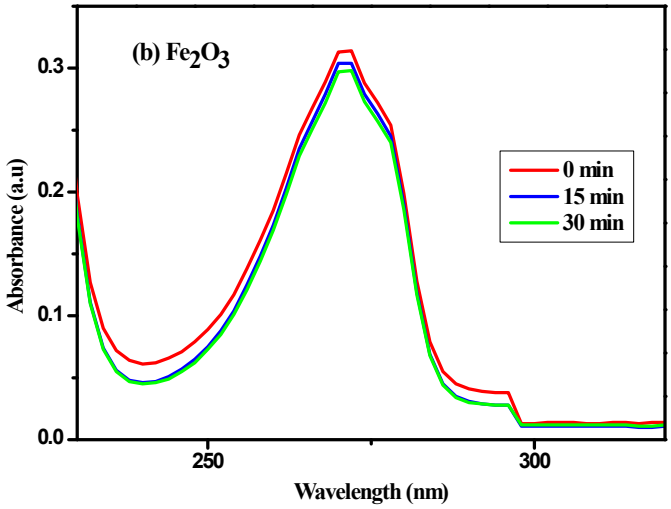
$$\text{TON} = \frac{\text{Number of moles phenol degraded}}{\text{Number of moles of composite catalyst taken}}$$
$$= \frac{3.1953\times10^{-5}\text{moles}}{6.3738\times10^{-5}\text{moles}}$$
$$= 0.5014$$

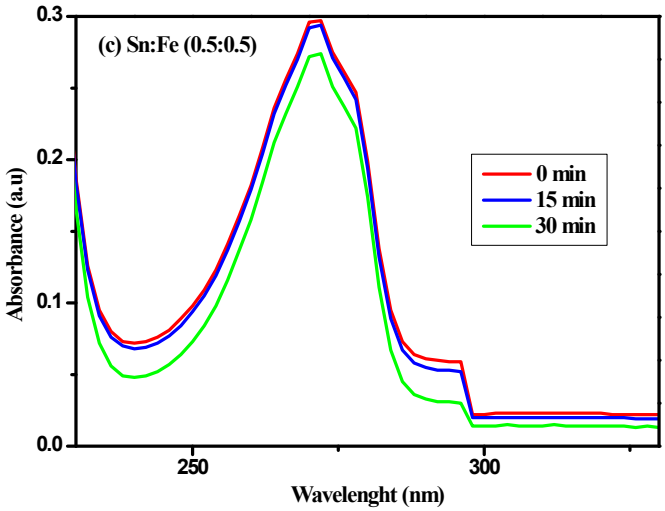
2.4. Calculation of TOF

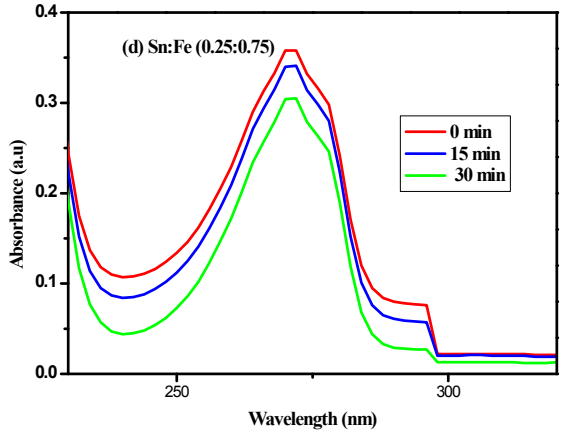
$$\text{TOF} = \frac{\text{TON}}{\text{time}(\text{min})} = \frac{0.5014}{120\text{min}} = 4.1784\times10^{-3}\text{min}^{-1}$$

Similar procedure is used to calculate the number of active sites, TON and TOF of the other two composites.


(a) SnO2
Absorbance (a.u)
Wavelength (nm)
0 min
15 min
30 min
0.0
0.1
0.2
0.3
250
300


(b) Fe2O3
Absorbance (a.u)
Wavelength (nm)
0 min
15 min
30 min
0.0
0.1
0.2
0.3
250
300


(c) Sn:Fe (0.5:0.5)
Absorbance (a.u)
Wavelenght (nm)
0 min
15 min
30 min
0.0
0.1
0.2
0.3
250
300



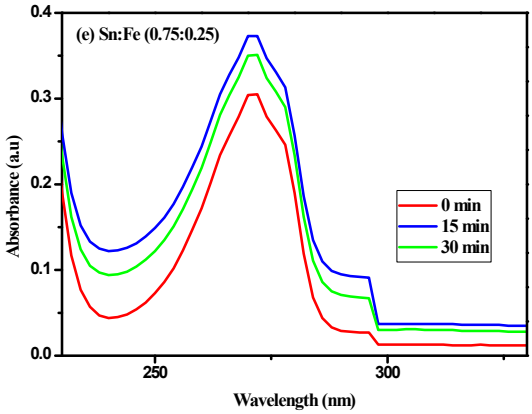
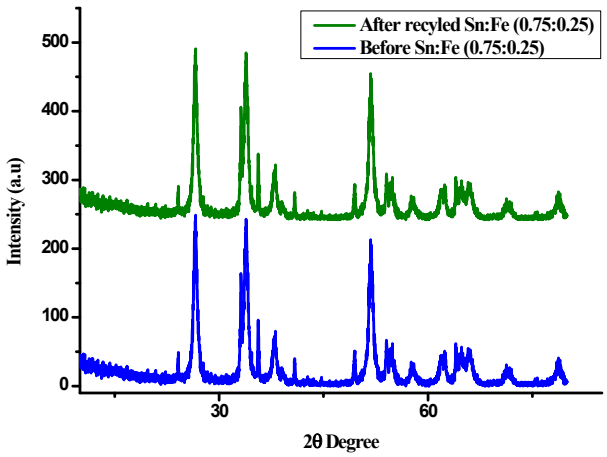


Fig.S4 The extent of adsorption of phenol on: (a) SnO_2 (b) α-Fe_2O_3 (c) Sn: Fe (0.5:0.5) (d) Sn: Fe (0.25:0.75) and (e) Sn: Fe (0.75:0.25) catalysts.

Catalysts	C_o (ppm)	C (ppm)	(C_o-C) (ppm)	q_e (mg g^{-1})
SnO_2	20	18.98	1.01	25.42
α-Fe_2O_3	20	19.01	0.98	24.53
Sn:Fe (0.25:0.75)	20	17.52	2.47	61.95
Sn:Fe (0.5:0.5)	20	18.45	1.55	38.72
Sn:Fe (0.75:0.25)	20	17.07	2.92	73.20

Table.S5. Extent of adsorption q_e, for SnO_2, α-Fe_2O_3 and various SnO_2- α-Fe_2O_3 composite photocatalysts, in the time period of 30 min.

(a)



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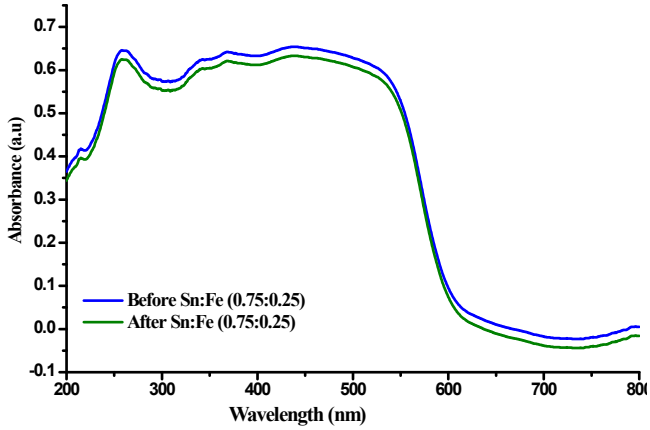

Fig.S6. (a) PXRD and (b) UV-visible spectra of Sn: Fe (0.75:0.25) before and after the three repetitive cycles.