Electronic supplementary information (ESI†)

Photocatalytic activity of SnO$_2$-α-Fe$_2$O$_3$ composite mixtures: exploration of number of active sites, Turnover number and Turnover Frequency.

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Fig.S1. The plots of $[F (R_\infty) h\nu]^{1/2}$ v/s photon energy ($h\nu$) for α-Fe$_2$O$_3$, SnO$_2$ and SnO$_2$-α-Fe$_2$O$_3$ composites.

(a)
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$_2$O$_2$, 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..........?
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

\[
\frac{0.0078}{118.7} = 6.571 \times 10^{-5} \text{ moles of Sn; number of active sites}
\]

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

\[
\frac{0.02 \times 250 \times 1}{94.1 \times 1000} = 5.313 \times 10^{-5} \text{ moles}
\]

250 ml of 20ppm phenol is $5.313 \times 10^{-5}$ moles

35% of phenol is degraded under UV light with SnO$_2$ as catalyst (Fig.7.a)

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

1.3. Calculation of Turnover number

\[
\text{TON} = \frac{\text{Number of moles of phenol degraded}}{\text{Number of moles of SnO}_2 \text{ taken}} = \frac{2.0189 \times 10^{-5} \text{ moles}}{6.571 \times 10^{-5} \text{ moles}} = 0.3073
\]

1.4. Calculation of Turnover frequency

\[
\text{TOF} = \frac{\text{TON}}{\text{time(min)}} = \frac{0.3073}{120} = 2.5609 \times 10^{-3} \text{ min}^{-1}
\]
Similar procedure is used to calculate the number of active sites, TON and TOF of $\alpha$-$Fe_2O_3$ 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 $\alpha$-Fe$_2$O$_3$,

Therefore in 310.4g/mol of Sn: Fe (0.25:0.75) composite contains SnO$_2$=28.51% and $\alpha$-Fe$_2$O$_3$=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 $\frac{310.4 \times 28.51}{100} = 88.38$g of SnO$_2$

**Calculation for $\alpha$-Fe$_2$O$_3$**: Similarly 310.4g of Sn: Fe (0.25:0.75) contains 221.9g of $\alpha$-Fe$_2$O$_3$

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 $2.851 \times 10^{-3}$g of SnO$_2$

150.7g/mol of SnO$_2$ contains 118.7g of Sn

Therefore $2.851 \times 10^{-3}$ of SnO$_2$ contains $\frac{2.851 \times 10^{-3} \times 118.7}{150.7} = 2.2456 \times 10^{-3}$g of Sn

1 mole of SnO$_2$ solution contains 118.7g of Sn

$2.2456 \times 10^{-3}$ of Sn is equivalent to:

$\frac{2.2456 \times 10^{-3}}{118.7} = 1.8918 \times 10^{-5}$ moles of Sn ; number of active sites

**Similar calculation for $\alpha$-Fe$_2$O$_3$**,

310.4g of Sn: Fe (0.25:0.75) composite contains 221.9g of $\alpha$-Fe$_2$O$_3$

10mg of Sn: Fe (0.25:0.75) composite contains $7.1580 \times 10^{-3}$g of $\alpha$-Fe$_2$O$_3$

159.7g/mol of SnO$_2$ contains 111.7g of Fe
Therefore \( 7.1580 \times 10^{-3} \) of \( \alpha\)-Fe\(_2\)O\(_3\) contains \( \frac{7.1580 \times 10^{-3} \times 111.7}{159.7} \) = \( 5.0065 \times 10^{-3} \) g of Fe

1 mole of \( \alpha\)-Fe\(_2\)O\(_3\) solution contains 111.7 g of Fe

5.0065 x 10\(^{-3}\) g of Fe contains:

\[
\frac{5.0065 \times 10^{-3} \text{ g}}{111.7} = 4.4820 \times 10^{-5} \text{ moles of Fe} \quad \text{; number of active sites}
\]

Therefore total number of active sites in 10 mg of Sn: Fe (0.25:0.75) composite containing 28.51% of Sn\(_2\)O\(_2\) + 71.49% of \( \alpha\)-Fe\(_2\)O\(_3\) is \( 6.3738 \times 10^{-5} \) moles ~ number of active sites

\[
(1.8918 \times 10^{-5} \text{ moles} + 4.4820 \times 10^{-5} \text{ moles})
\]

2.2. % conversion of substrate under UV light illumination

250 ml of 20 ppm of phenol contains \( 5.313 \times 10^{-5} \) moles

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

2.3. Calculation of TON

\[
\text{TON} = \frac{\text{Number of moles phenol degraded}}{\text{Number of moles of composite catalyst taken}} = \frac{3.1953 \times 10^{-5} \text{ moles}}{6.3738 \times 10^{-5} \text{ moles}} = 0.5014
\]

2.4. Calculation of TOF

\[
\text{TOF} = \frac{\text{TON}}{\text{time (min)}} = \frac{0.5014}{120 \text{ min}} = 4.1784 \times 10^{-3} \text{ min}^{-1}
\]

Similar procedure is used to calculate the number of active sites, TON and TOF of the other two composites.
(a) SnO$_2$

(b) Fe$_2$O$_3$

(c) Sn:Fe (0.5:0.5)
Fig S4 The extent of adsorption of phenol on: (a) SnO$_2$ (b) α-Fe$_2$O$_3$ (c) Sn: Fe (0.5:0.5) (d) Sn: Fe (0.25:0.75) and (e) Sn: Fe (0.75:0.25) catalysts.

<table>
<thead>
<tr>
<th>Catalysts</th>
<th>$C_0$ (ppm)</th>
<th>$C$ (ppm)</th>
<th>$(C_0-C)$ (ppm)</th>
<th>$q_e$ (mg g$^{-1}$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>SnO$_2$</td>
<td>20</td>
<td>18.98</td>
<td>1.01</td>
<td>25.42</td>
</tr>
<tr>
<td>α-Fe$_2$O$_3$</td>
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<td>19.01</td>
<td>0.98</td>
<td>24.53</td>
</tr>
<tr>
<td>Sn:Fe (0.25:0.75)</td>
<td>20</td>
<td>17.52</td>
<td>2.47</td>
<td>61.95</td>
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<tr>
<td>Sn:Fe (0.5:0.5)</td>
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<td>18.45</td>
<td>1.55</td>
<td>38.72</td>
</tr>
<tr>
<td>Sn:Fe (0.75:0.25)</td>
<td>20</td>
<td>17.07</td>
<td>2.92</td>
<td>73.20</td>
</tr>
</tbody>
</table>

Table S5. Extent of adsorption $q_e$, for SnO$_2$, α-Fe$_2$O$_3$ and various SnO$_2$- α-Fe$_2$O$_3$ composite photocatalysts, in the time period of 30 min.
Fig. S6. (a) PXRD and (b) UV-visible spectra of Sn: Fe (0.75:0.25) before and after the three repetitive cycles.