Electronic Supplementary Material (ESI) for RSC Advances.


# *Supplementary information*

## Structural, Optical and Magnetic Properties of Pure and 3d Metal Dopant Incorporated $SnO_2$ Nanoparticles

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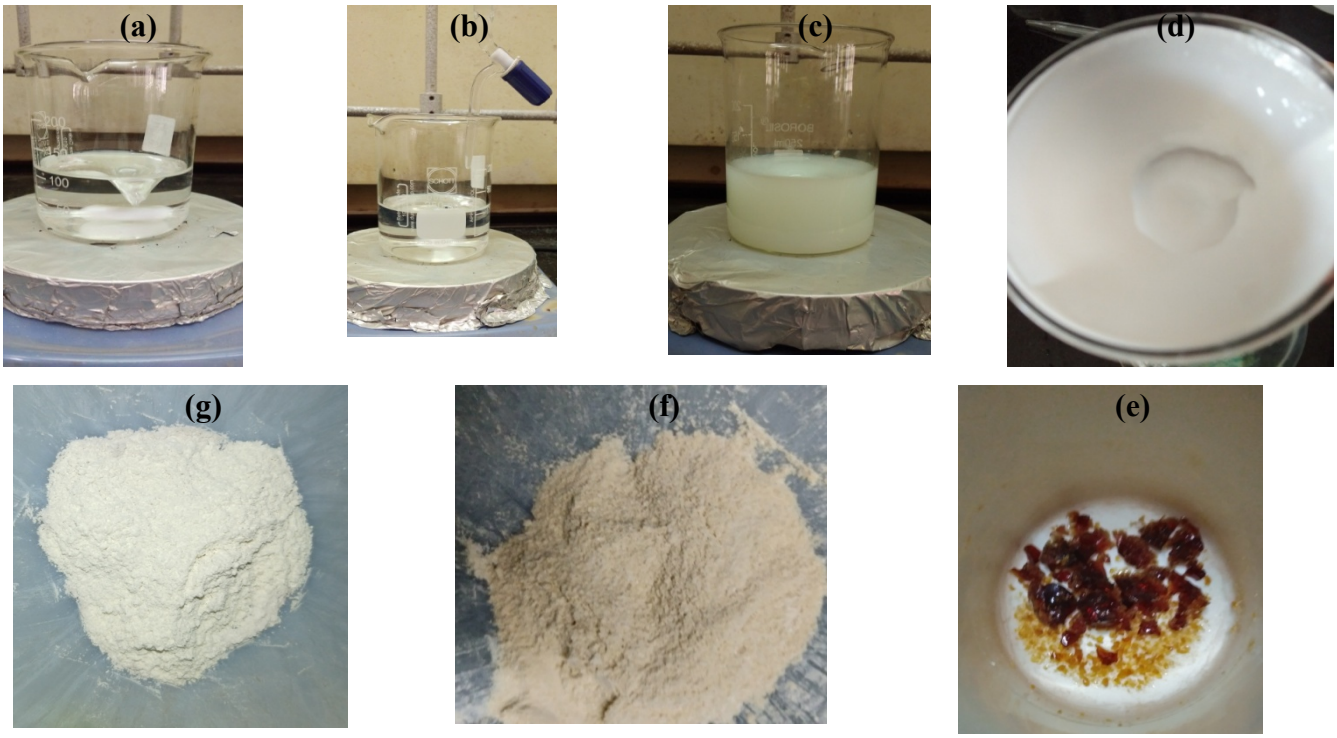
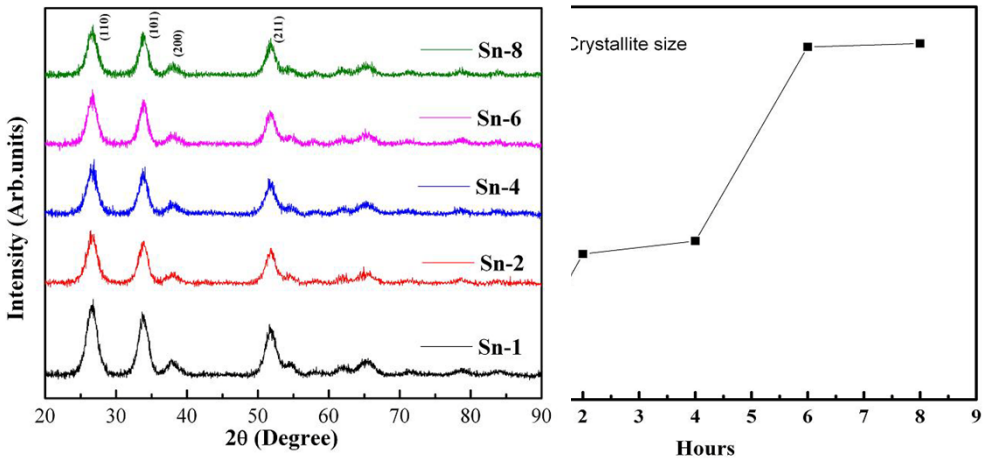



**S Fig. 1:** Stepwise photographic representation of synthesis process of $SnO_2$ nanoparticles (a) mixed solution of $SnCl_4.5H_2O$ and ethylene glycol, (b) & (c) Drop-wise addition of aqueous ammonia under constant magnetic stirring forming the gel (d) gel of $SnO_2$ nano crystallites after filtration and washing, (e) dried $SnO_2$ nanoparticles at $150^0$C for 2 h (f) powdered samples of dried $SnO_2$ and (g) powdered samples calcinated at $400^0$C

(a) (b)




**S Fig. 2(a):** XRD patterns of Sn-1, Sn-2, Sn-4, Sn-6 and Sn-8 samples. **2(b):** Variation of crystallite size with calcinations hours Variation of crystallite size with calcinations hours

**S Table1:** Refinement parameters obtained for pure and doped $SnO_2$ nanocrystals.

| Samples / Refined parameters | Sn-2 | SnFe-3 | SnCo-3 | SnNi-3 |
|---|---|---|---|---|
| **Crystal Structure** | Tetragonal | Tetragonal | Tetragonal | Tetragonal |
| **Space group:** | P42/mnm | P42/mnm | P42/mnm | P42/mnm |
| **Cell Parameters:** | | | | |
| ***a=b (A⁰)*** | 4.7386 | 4.7469 | 4.7408 | 4.7410 |
| ***c(A⁰)*** | 3.1909 | 3.1949 | 3.1893 | 3.1907 |
| **Volume (Å³)** | 71.6472 | 71.9913 | 71.6801 | 71.7195 |
| **α= β= ϒ** | 90 | 90 | 90 | 90 |
| **Positions:** | | | | |
| **Sn(x)** | 0.00000 | 0.00000 | 0.00000 | 0.00000 |
| **Sn (y)** | 0.00000 | 0.00000 | 0.00000 | 0.00000 |
| **Sn (z)** | 0.00000 | 0.00000 | 0.00000 | 0.00000 |
| **Fe/Co/Ni(x)** | - | 0.00000 | 0.00000 | 0.00000 |
| **Fe/Co/Ni(y)** | - | 0.00000 | 0.00000 | 0.00000 |
| **Fe/Co/Ni (z)** | - | 0.00000 | 0.00000 | 0.00000 |
| **O (x)** | 0.29797 | 0.28498 | 0.29126 | 0.28384 |
| **O (y)** | 0.29797 | 0.28498 | 0.29126 | 0.28384 |
| **O (z)** | 0.00000 | 0.00000 | 0.00000 | 0.00000 |
| **Density (g/cm³)** | 6.608 | 6.435 | 6.416 | 6.598 |
| **$B_{iso}$:** | | | | |
| **Sn** | 7.04728 | 7.92788 | 7.91514 | 7.91239 |
| **Fe/Co/Ni** | - | 7.92788 | 7.91514 | 7.91239 |
| **O** | 6.93872 | 6.34257 | 7.57134 | 7.52507 |
| **Site Occupation:** | | | | |
| **Sn** | 1.0003 | 0.9699 | 0.9705 | 0.9702 |
| **Fe/Co/Ni** | - | 0.3063 | 0.0300 | 0.0301 |
| **O** | 1.0478 | 1.0736 | 1.09862 | 1.07522 |
| **Agreement factors:** | | | | |
| **$R_p$** | 14.7 | 18.2 | 26.7 | 20.2 |
| **$R_{wp}$** | 17.1 | 20.4 | 26.7 | 21.9 |
| $\chi^2$ | 1.01 | 1.14 | 1.34 | 1.18 |

**S Table 2.** Brief analysis of high-resolution XPS of O 1s.

| **Sample** | **O 1s spectrum** | | | |
|---|---|---|---|---|
| | Oxygen type | B.E (eV) | FWHM | Area |
| **Sn-2** | $O_L$ | 530.95 | 1.41 | 38113 |
| | OH | 531.85 | 1.85 | 12989 |
| **SnFe-3** | OL | 531.17 | 1.57 | 2669 |
| | OH | 532.67 | 1.47 | 393 |
| **SnCo-3** | $O_L$ | 531.03 | 1.65 | 2926 |
| | OH | 532.67 | 1.37 | 365 |
| **SnNi-3** | OL | 530.45 | 1.42 | 3249 |
| | OH | 531.85 | 1.51 | 587 |

**S Table 3**. Evaluation of $O_V$ with respect to parent $SnO_2$ O 1s spectra.

| **Sample** | **O 1s spectrum** | |
|---|---|---|
| | Oxygen type | % Area |
| **Sn-2** | $O_L$ | 74.58 |
| | OH | 25.42 |
| **SnFe-3** | $O_L$ | 7.00 |
| | OH | 3.03 |
| | $O_V$ | 89.97 |
| **SnCo-3** | $O_L$ | 7.68 |
| | OH | 2.81 |
| | $O_V$ | 89.52 |
| **SnNi-3** | $O_L$ | 8.53 |
| | OH | 4.52 |
| | $O_V$ | 86.95 |