

Supporting information

Surface functionalization induced magnetism in SnO₂ nanoparticles and its correlation to Photoluminescence properties

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Octadecyltrichlorosilane (OTS) molecules are linked to SnO₂ nanoparticles (NPs) through a self-assembly process by forming covalent bonds. Figure S1 shows the Raman spectra of OTS treated SnO₂ NPs, which show the allowed modes for rutile SnO₂ phase along with molecular vibrations from OTS molecules. Peak around 570 cm⁻¹(*D*) is due to in-plane 'O' vacancy.¹ Raman spectroscopy has been widely used to understand ordered and disordered phases of the covalently bonded OTS to silica surfaces.^{2,3} Molecular vibrations originating from the breadth and asymmetry of CH₂ twist (τ -CH₂) and bending of CH₂ (δ -CH₂) modes were observed at 1293, and 1441 cm⁻¹, respectively (Fig. S1). Similarly symmetric (ν_s) and asymmetric (ν_a) stretching modes of CH₂ and CH₃ modes were also shown in Figure S1. Vibrational modes of ν_s (CH₂) and ν_a (CH₂) were observed at 2846 and 2881 cm⁻¹, respectively whereas the same for ν_s (CH₃) and ν_a (CH₃) appeared at 2935 and 2962 cm⁻¹, respectively. In the ordered phase of OTS, τ -CH₂ mode was reported to shift to lower frequency in comparison to the disordered phase of OTS at 1304 cm⁻¹. The τ -CH₂ mode at 1294 cm⁻¹ supports the formation of an ordered OTS on the SnO₂ surfaces. Moreover, the intensity ratio of ν_a (CH₂) to ν_s (CH₂) is described to be higher than 0.9 for the ordered phase. In the present study, intensity ratio of the above modes exhibits around 1.3 extending support to the formation of ordered OTS on SnO₂ surfaces. The intensity ratio, however is found to be lower than the reported value of 1.6 - 2 for the crystalline phase of OTS on micron sized silica surfaces.^{2,3} In the present context, spherical NPs of SnO₂ allows only limited surface area for the ordering to be observed.

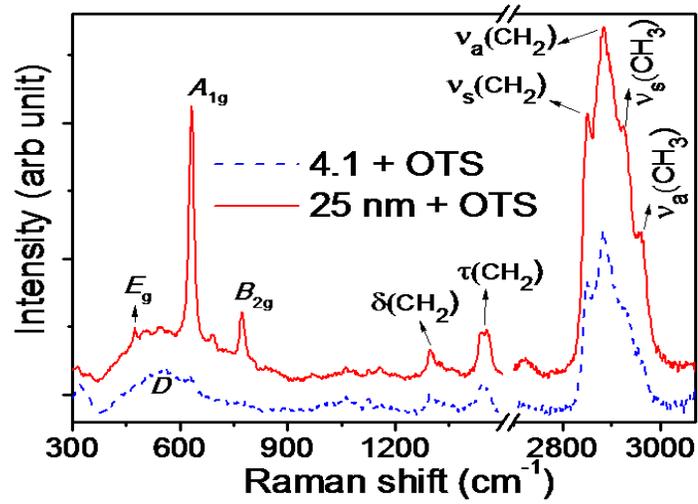


Fig. S1 Raman spectra of OTS treated SnO₂ nanoparticles of 4 nm, and 25 nm

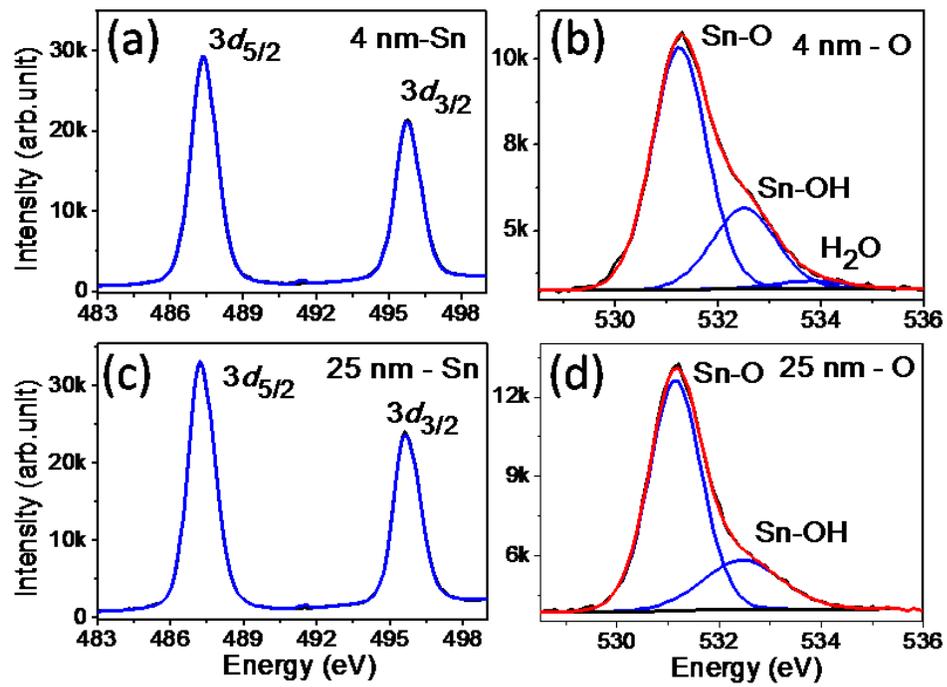


Fig. S2 XPS spectra of (a) Sn 3d (b) O 1s of SnO₂ (4 nm) and (c) Sn 3d (b2) O 1s of SnO₂ (25 nm).

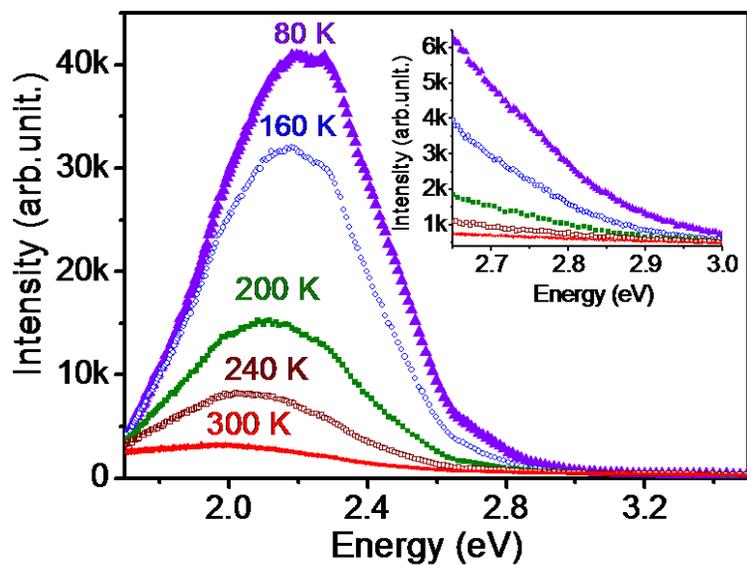


Fig. S3 Temperature dependent photoluminescence of pristine 25 nm SnO₂ nanoparticles. Inset showing the zoomed region between 2.65 to 3 eV.

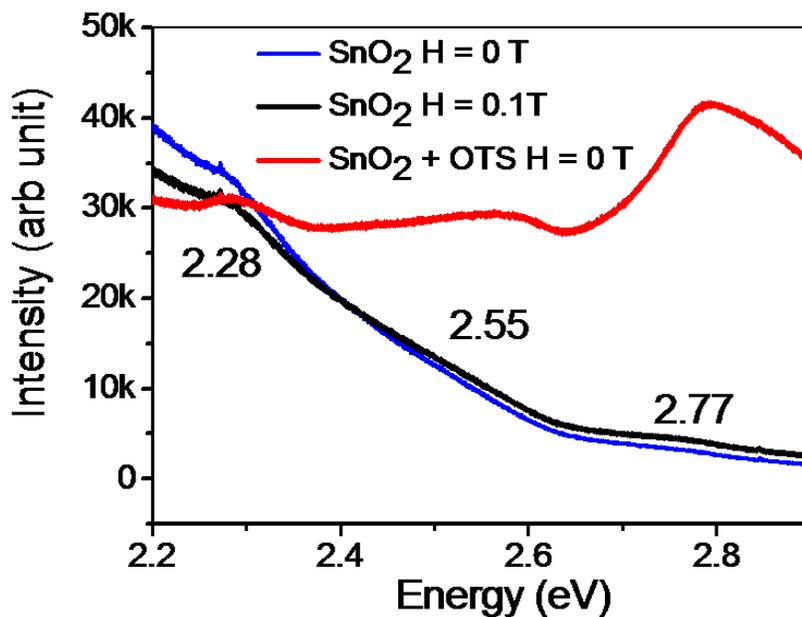


Fig. S4 Zoomed region of Fig. 4 showing no new peak after functionalization.

REFERENCES

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