Electronic Supporting Information

Efficiency Enhancement of Cubic Perovskite $BaSnO_3$ Nanostructures Based Dye Sensitized Solar Cells

N. Rajamanickam[a,b], P. Soundarrajan[b], Venkat K. Vendra[a], Jacek B. Jasinski[a], Mahendra K. Sunkara[a], and K. Ramachandran[b]

[a] Conn Center for Renewable Research and Department of Chemical Engineering, University of Louisville, Louisville, KY – 40292, USA.

[b] School of Physics, Madurai Kamaraj University, Madurai – 625021, TN, India.

* Corresponding author E-mail: nrajamku@gmail.com

*Tel. No: +91-0452-2458471 (352)

*Fax: +91-0452-2458471

XRD analysis

The crystallite size is estimated from the peak width of the XRD pattern using Scherrer's formula, $D = K\lambda/\beta\cos\theta$. where, D is the grain size in m, λ is the wavelength of X-ray in m ; λ = 1.54 Å, β is the full width at half maximum of the diffraction peak in radians, θ is the angle of diffraction in degrees, K is Scherrer's constant (0.9).

Dislocation density in the prepared sample is calculated using, $\rho = \frac{1}{D^2} lines/m^2$

Because of the quantum confinement in nanomaterials, the bulk system gets strained and this is estimated approximately using the formula, $\eta = \left[\frac{\lambda}{D\cos\theta} - \beta\frac{\pi}{180}\right]\frac{1}{\tan\theta}$

The Rietveld refinement parameters are calculated from Fullprof suit software (version 2.05) package.

Raman analysis

Figure S1 shows the room temperature Raman spectra of BSO NS. BSO NS have $Pm\bar{3}m$ (221) structure and it shows first order Raman spectrum because of the centro-symmetric crystal structure. Raman shift observed in the sample may be attributed to defects induced in the samples at high temperatures. The formation of oxygen vacancies also contributed to the structural changes. BSO nanomaterials exhibited the Raman modes at 413, 548, 645, 670, 831, 988, 1058, 1066 and 1149 cm^{-1} and these Raman peaks are assigned on the basis of the six fundamental vibrations of SnO_6 octahedron which has O_h symmetry in the distorted perovskite structure. The Raman active mode $\nu_2 E_g$ is observed at 548 cm^{-1}.

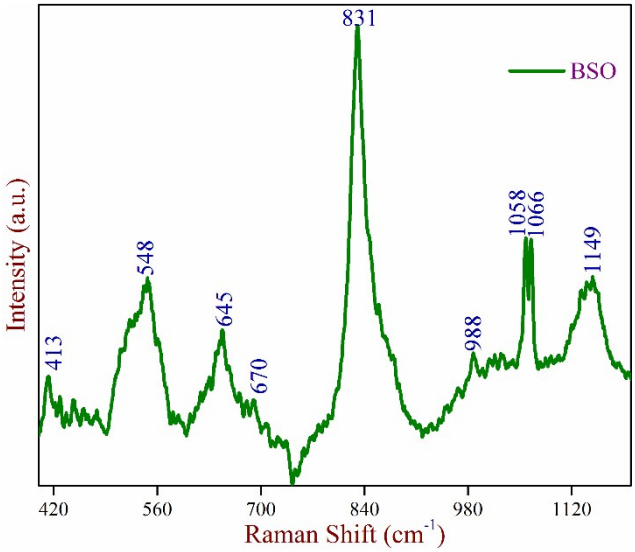

Figure S1. Raman spectrum of BSO nanostructures.

HRTEM with EDS Analysis

HRTEM image of the TiO_2 and ZnO are shown in Fig. 1. The measured inter-planar spacing value of TiO_2 and ZnO are 1.92 Å and 2.88 Å respectively which is corresponding to the (200) and (100) plane respectively. From the HRTEM images, tetragonal anatase and hexagonal wurtzite phase confirmed for TiO_2 and ZnO, respectively.

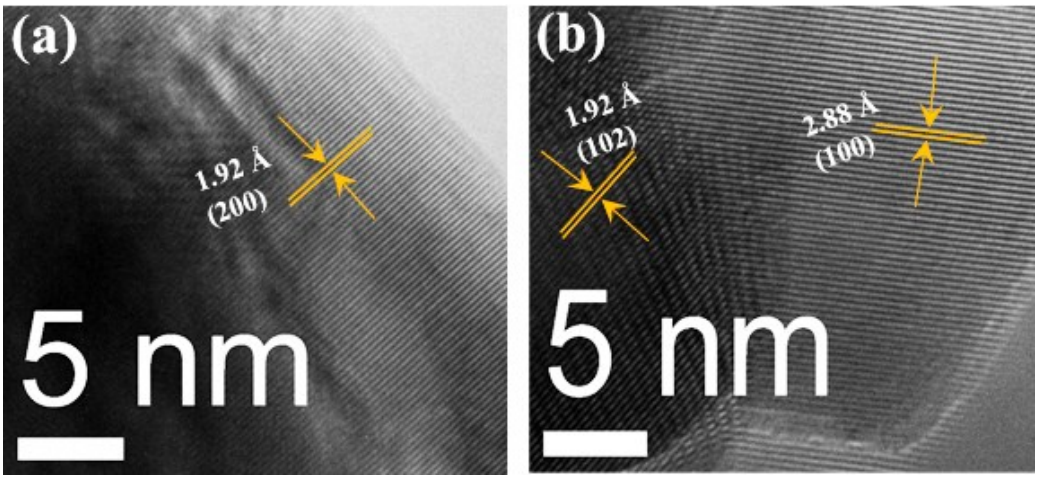

Figure S2. HRTEM Image of (a) TiO_2 and (b) ZnO nanostructures

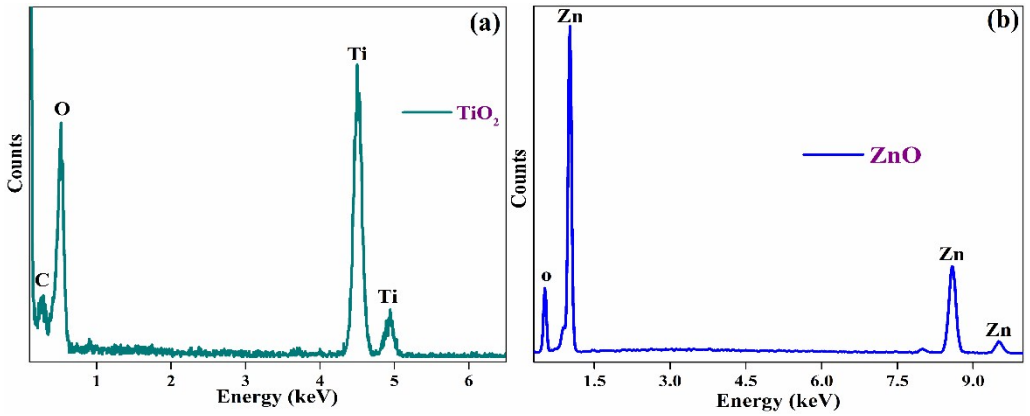

Figure S3. EDS spectrum of synthesized (a) TiO_2 and (b) ZnO nanoparticles.

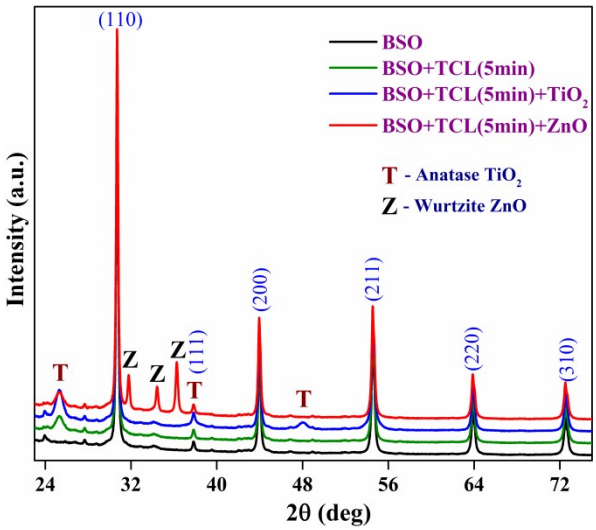

Figure S4. XRD patterns of BSO, BSO/5 min TCL, BSO/5 min TCL/TiO_2 scattering layer and BSO/5 min TCL/ZnO scattering layer photoelectrodes. (TCL – $TiCl_4$ treatment)