Electronic Supplementary Material (ESI) for Journal of Materials Chemistry C.

Tuning the properties of F:SnO_2 (FTO) nanocomposites with S:TiO_2 nanoparticles as promising hazy transparent electrodes for photovoltaics applications

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Supplementary Information:

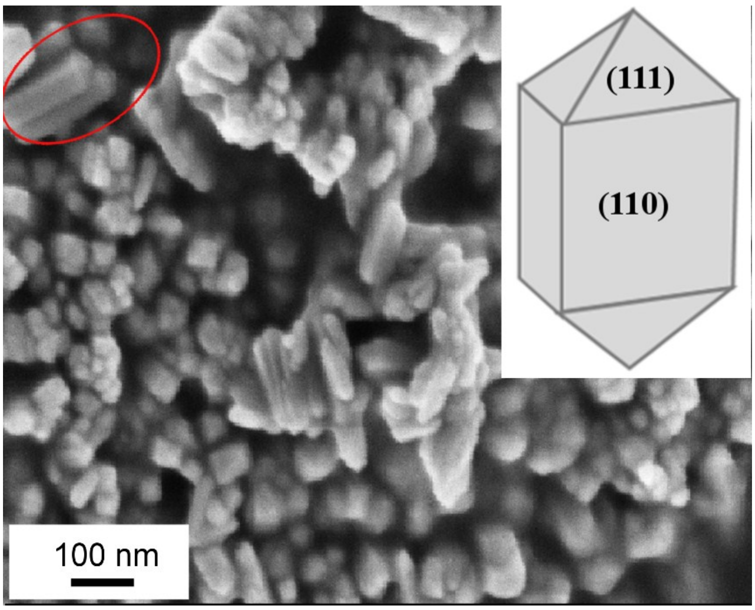

Fig. S1 SEM image of the as-synthesized rutile S:TiO_2 nanoparticles. The two nanoparticles marked with the red circle clearly demonstrate that the 3D shape of a single S:TiO_2 nanoparticle has the form as schematically drawn in the inset.

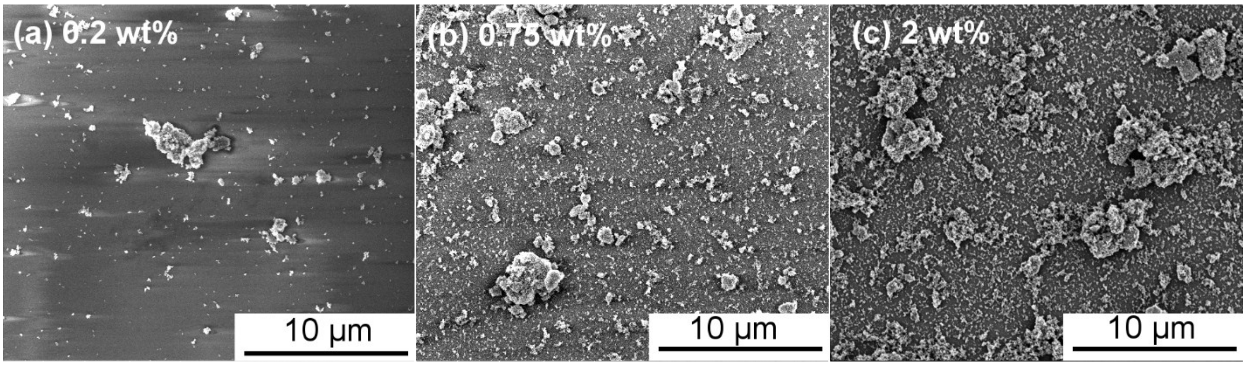

Fig. S2 The SEM image showing the surface morphology of (a) 0.2 wt%, (b) 0.75 wt%, and (c) 2 wt% S:TiO_2 nanoparticle substrates. The stripes in (a) are due to serious charging during acquisition.

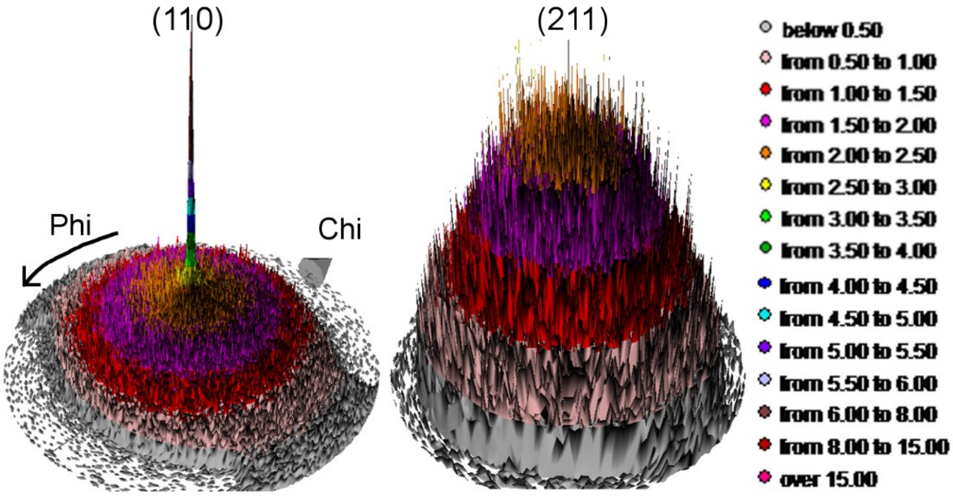

Fig. S3 The 3D x-ray pole figures of the 2 wt% S:TiO_2 nanoparticle substrate collected on the rutile TiO_2 (110) and (211) diffraction peaks. The radial angle (Chi) increases from 0° in the centre towards 90° at the circumference while the azimuthal (Phi) angle changes from 0° to 360° by rotating along the circle. The intensities are scaled in colours as shown.

The intense central peak in the (110) pole figure suggests that the majority of S:TiO_2 nanoparticles orient their {110} planes parallel to the glass surface, i.e. the S:TiO_2 nanoparticles preferentially orient along <110> directions. In contrast, for the (211) pole figure, only weak intensities are seen at all Chi and Phi angles suggesting that the distribution of S:TiO_2 nanoparticles orientating their (211) planes parallel to the glass surface is random (as powder samples). In fact the small amount of randomly oriented S:TiO_2 nanoparticles contributes also in the (110) pole figure by constituting a weak bottom background whose intensity is similar to that of (211) pole figure.

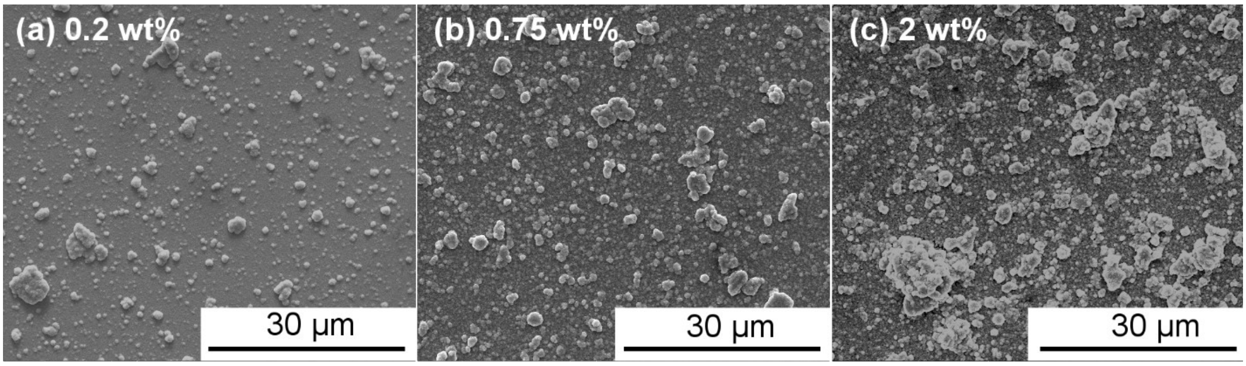

Fig. S4 The SEM image showing the surface morphology of (a) 0.2 wt%, (b) 0.75 wt%, and (c) 2 wt% S:TiO_2-FTO nanocomposites.

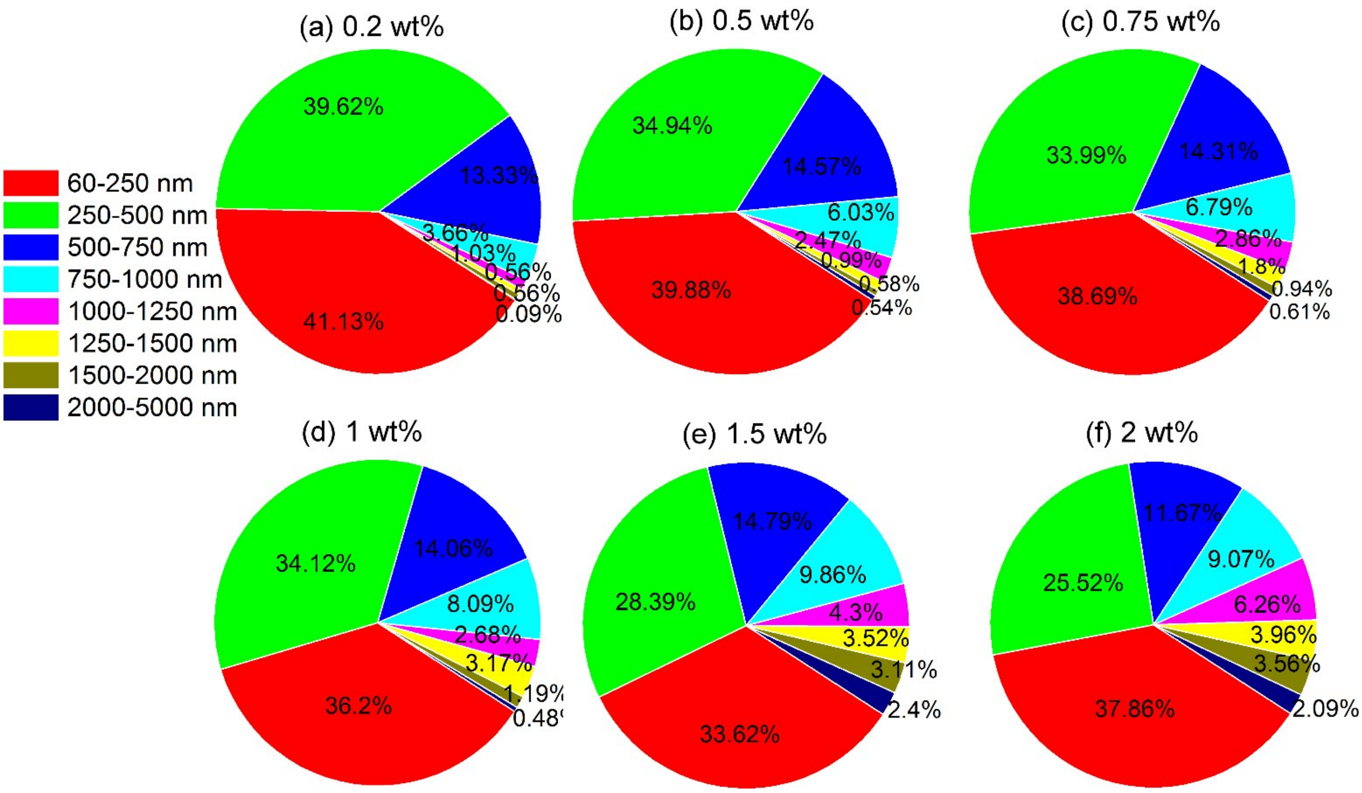

Fig. S5 The relative fractions for the 8 nanoparticle agglomerate groups (categorized based on R_{eq}) summarized for (a) 0.2 wt%, (b) 0.5 wt%, (c) 0.75 wt%, (d) 1 wt%, (e) 1.5 wt%, and (f) 2 wt% S:TiO_2-FTO nanocomposite.

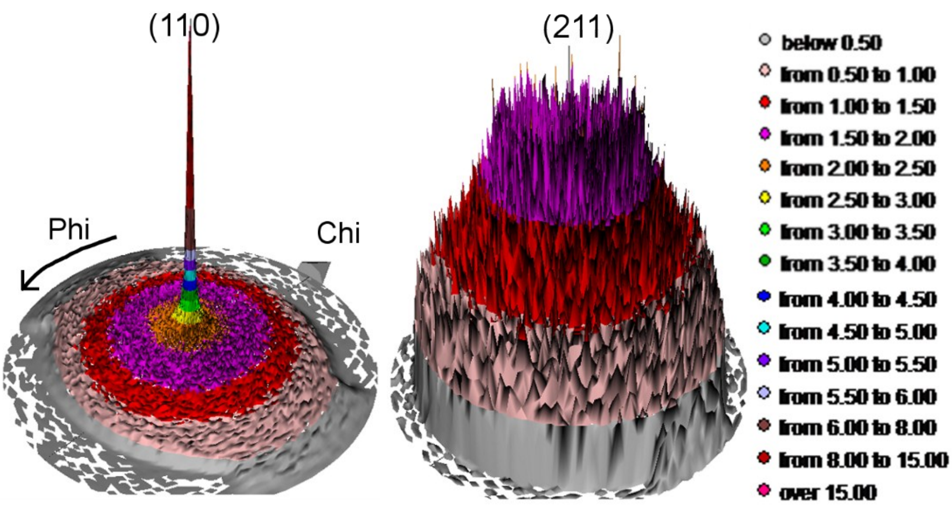

Fig. S6 The 3D x-ray pole figures of the S:TiO_2-FTO nanocomposite collected on the SnO_2 (110) and (211) diffraction peaks. The radial angle (Chi) increases from 0° in the centre towards 90° at the circumference while the azimuthal (Phi) angle changes from 0° to 360° by rotating along the circle. The intensities are scaled in colours as shown.

The intense central peak in the (110) pole figure suggests that the majority of FTO grains orient their {110} planes parallel to the glass surface, i.e. the FTO film preferentially orient along <110> directions. In contrast, for the (211) pole figure, only weak intensities are seen at all Chi and Phi angles suggesting that the distribution of FTO grains orientating their (211) planes parallel to the glass surface is random (as powder samples). In fact the small amount of randomly oriented FTO grains contributes also in the (110) pole figure by constituting a weak bottom background whose intensity is similar to that of (211) pole figure.

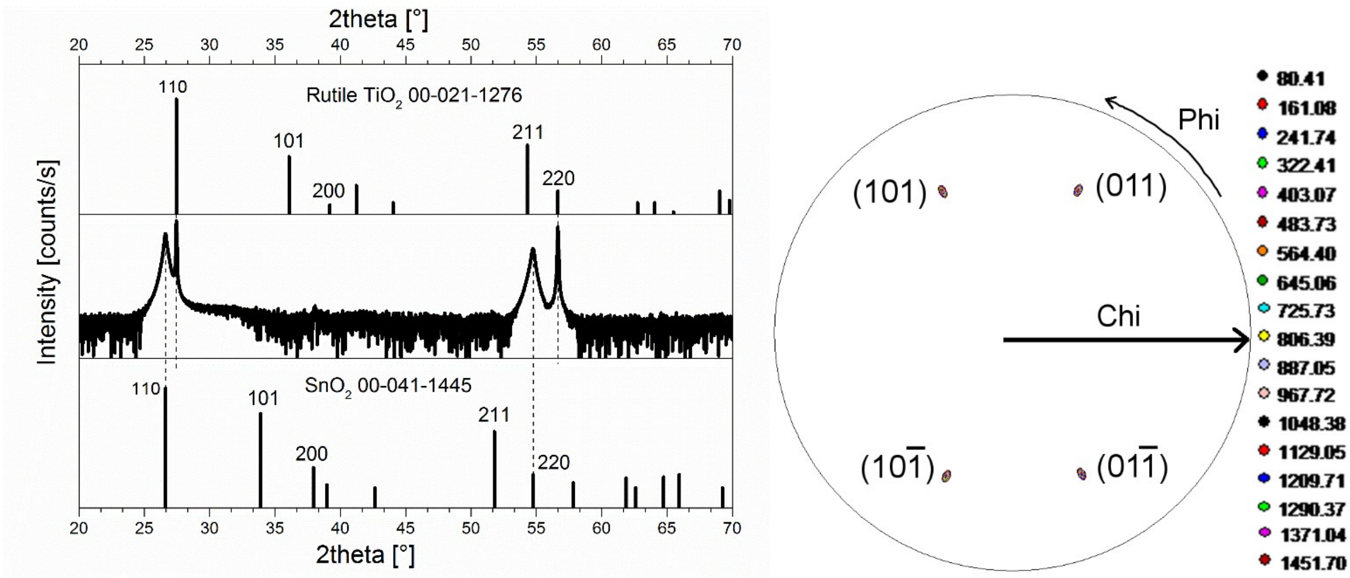

Fig. S7 (a) Bragg-Brentano XRD pattern of a FTO film (300 nm) deposited by ultrasonic spray pyrolysis on a commercial (110) rutile TiO_2 single crystal. The PDF patterns of both rutile TiO_2 (00-021-1276) and SnO_2 (00-041-1445) are shown for reference. (b) 2D x-ray pole figure of the FTO film collected on the SnO_2 (101) diffraction peak. It shows 4 distinct peaks indexed as indicated. The radial angle (Chi) increases from 0° in the centre towards 90° at the circumference while the azimuthal (Phi) angle changes from 0° to 360° by rotating along the circle.

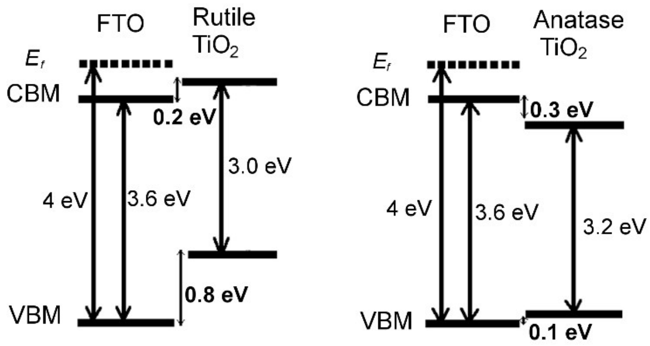

Fig. S8 The proposed intrinsic band alignment between FTO with rutile/anatase TiO_2 based on Ref. 1. CBM and VBM represent the conduction band minimum and valence band maximum respectively. E_f represents the Fermi level of FTO.

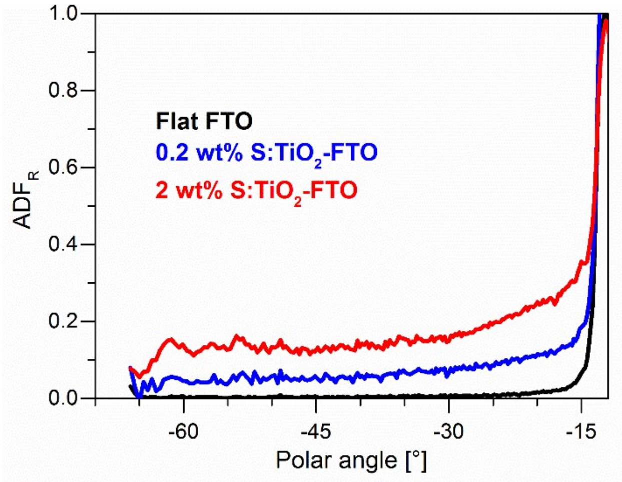

Fig. S9 ADF_R normalized on the horizontal cross sections of angular space images (Fig. 9c and d) for flat FTO, 0.2 wt% and 2 wt% S:TiO_2-FTO nanocomposites.

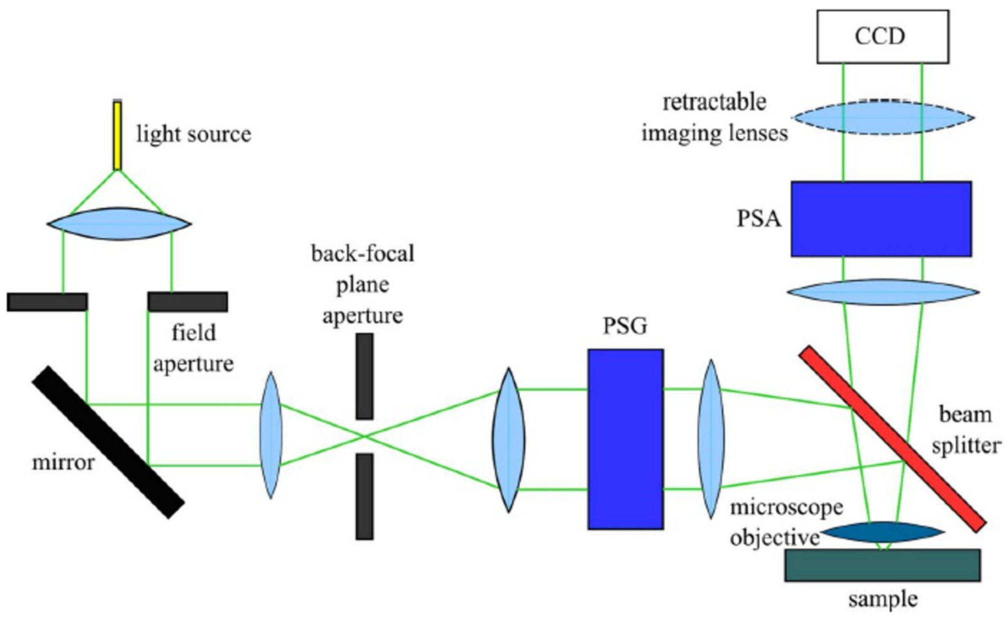

Fig. S10 Schematic drawing of the angle-resolved Mueller matrix polarimeter.[2] PSG refers to polarization state generator while PSA refers to polarization state analyser.

References

1 S. Li, F. Chen, R. Schafranek, T. J. M. Bayer, K. Rachut, A. Fuchs, S. Siol, M. Weidner, M. Hohmann, V. Pfeifer, J. Morasch, C. Ghinea, E. Arveux, R. Günzler, J. Gassmann, C. Körber, Y. Gassenbauer, F. Säuberlich, G. V. Rao, S. Payan, M. Maglione, C. Chirila, L. Pintilie, L. Jia, K. Ellmer, M. Naderer, K. Reichmann, U. Böttger, S. Schmelzer, R. C. Frunza, H. Uršič, B. Malič, W.-B. Wu, P. Erhart and A. Klein, *Phys. Status Solidi RRL – Rapid Res. Lett.*, 2014, **8**, 571–576.

2 M. Foldyna, M. Moreno, P. R. i Cabarrocas and A. De Martino, *Appl. Opt.*, 2010, **49**, 505.