



# Synthesis of a high efficiency novel working electrode scandium/HOMBIKAT in dye-sensitized solar cells



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## ABSTRACT

In this work, scandium supported TiO<sub>2</sub> HOMBIKAT UV 100 (Sc/TiO<sub>2</sub>) in different wt.% were prepared by simple wet impregnation method. Inductively coupled plasma (ICP) confirmed that Sc/TiO<sub>2</sub> contains scandium in 2 and 4 wt.%. Different characterization tools were used to investigate the prepared samples. X-ray diffraction (XRD) and Raman analysis showed that no peaks characteristic for scandium was detected. Surface properties showed that the prepared samples display isotherms of Type II according to the IUPAC classification, with the presence of mesoporous pores. Surface morphology shows that the aggregation increases as the scandium content increase. High-resolution transmission electron microscopy (HRTEM) showed the increase in size upon increase in scandium content. The electrical properties for Sc/TiO<sub>2</sub> and TiO<sub>2</sub> were investigated by measuring the current density–voltage (*J*–*V*) under illumination condition. 4 wt.% Sc/TiO<sub>2</sub> showed the highest electrical properties. The open circuit voltage (*V*<sub>OC</sub>), short circuit current density (*J*<sub>SC</sub>) and energy conversion efficiency (*η*) were found to be 0.835 V, 20.46 mA/cm<sup>2</sup> and 10.34%, respectively. The shunt resistance calculation indicates that 4 wt.% Sc/TiO<sub>2</sub> showed a high efficiency solar cell. Fourier transform infrared spectroscopy (FTIR) was carried out to investigate the anchored groups on the catalyst surface which differ according to the concentration of Rose Bengal dye (RB) used. Also, the orientation of benzene ring depends on the concentration of RB and has an impact on the activity. Different factors affecting the performance of the cell such as photosensitizer concentration and pH, active area of photoanode, thickness of counter electrode, and effect of electrolyte concentration were studied.

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## 1. Introduction

Utilizing solar energy is certainly one of the most viable ways to solve the world's energy crisis. Dye sensitized solar cells (DSSCs) have emerged as promising candidates for harnessing solar power because of their low cost, flexibility, ease of production, relatively high energy conversion efficiency, and low toxicity to the environment (O'Regan et al., 1991). Since this type of solar cells being introduced by Grätzel and co-workers in 1991, many strategies have been employed to achieve high-performance DSSCs, including novel counter electrodes (Jeon et al., 2015), electrolytes (Hashmi et al., 2015), dyes (Yum et al., 2012), and semiconductor photoanode materials (Fei et al., 2014). Among these, the photoanode plays a crucial role in determining the cell performance. So far, titanium dioxide (TiO<sub>2</sub>)-based material is one of the most promising materials for a DSSCs due to its low cost, abundance, nontoxicity, safety,

large surface area for maximum dye uptake and matched energy and band structure (Tao et al., 2013; Chen et al., 2012). However, the major drawback associated with the use of TiO<sub>2</sub> is its random electron transport, which will cause the electron–hole recombination process and hence affect the overall performance (van de Lagemaat et al., 2000; Kopidakis et al., 2005). There is an active search to overcome the deficiency of TiO<sub>2</sub>-based DSSCs through surface modification with metal nanoparticles, doping of metals and non-metals, semiconductor coupling, and hybridizing with carbon materials (Lai et al., 2010; Macak et al., 2007; Yang et al., 2007; Zhao et al., 2007).

In the present decade, surface of TiO<sub>2</sub> has been modified with different metal nanoparticles (Rao et al., 2014; Zhu et al., 2015) co-sensitized vertically aligned anatase TiO<sub>2</sub> nanowire arrays but scandium was seldom used as dopant. That's why it was interesting to study its effect upon impregnating on TiO<sub>2</sub>.

Sensitizer dyes in DSSCs play a key role in harvesting sunlight and transforming solar energy into electric energy and so it is important for the efficiency of photovoltaic cell and its performance

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(Chang et al., 2010). It attaches to the surface of a wide band-gap mesoporous semiconductor serving as electron transporter (Sarica and Erten-Ela, 2012). Ruthenium-based dye sensitizers are used but they are very expensive and hard to prepare, which restricts their large-scale applications in solar cells. Another alternative was to use the Rose Bengal (RB) dye. It has been used as dye sensitizer in DSSCs and photogalvanic cells (Mahmoud and Fouad, 2015; Mahmoud et al., 2014; Mahmoud and Mohamed, 2015) and has shown high energy conversion efficiency. Rose Bengal dye is relatively cheap, non-toxic, and environmentally friendly.

In the present study, we successfully developed a facile synthesis method to prepare uniformly distributed scandium nanoparticles deposited on TiO<sub>2</sub> using a simple method for DSSCs application. The prepared materials were characterized using various suitable analytical techniques and used as photoanodes in the DSSCs.

## 2. Experimental

### 2.1. Materials and characterization techniques

#### 2.1.1. Materials

Titanium dioxide (HOMBIKAT UV 100) of anatase modification, the HOMBIKAT refers to the trading name of the product of Huntsman Pigments and Additives Company, Germany. Scandium nitrate Sc(NO<sub>3</sub>)<sub>3</sub>·3H<sub>2</sub>O was purchased from Merck. Indium tin oxide (ITO) conducting glass slides (8–12 Ω sq<sup>-1</sup>) and the Rose Bengal (RB) dye were purchased from Sigma–Aldrich. Fig. 1 shows the structure of Rose Bengal.

#### 2.1.2. Characterization techniques

Nitrogen adsorption–desorption isotherms of the synthesized samples were measured on ASAP2010, at –196 °C after degassing at 200 °C for 4 h.

X-ray diffraction patterns were recorded with a Pan Analytical Model X' Pert Pro, which was equipped with Cu Kα radiation (λ = 0.1542 nm).

Scanning Electron Microscopy (SEM) investigation was performed on JEOL JEM 3500 electron microscope. High-Resolution Transmission electron microscopy (HRTEM) studies were carried out using a JEOL JEM-1230 electron microscope operating at 120 kV.

Ultraviolet–Visible absorption spectroscopic analysis was measured using Jasco, V-570, NIR spectrophotometer.

Raman spectra were collected using a Renishaw Via 2000 system with an argon ion laser emitting at 100 and 800 nm.

FT-IR spectra of the samples were carried out using ATI unicam (Mattson 936) Bench Top spectrometer

### 2.2. Synthesis of Sc/TiO<sub>2</sub> nanomaterials

Two samples of Sc/TiO<sub>2</sub> were prepared by wet impregnation method. Briefly, 500 mg of TiO<sub>2</sub> HOMBIKAT UV 100 was added

to aqueous solutions that contain different amounts of Sc(NO<sub>3</sub>)<sub>3</sub>·3H<sub>2</sub>O corresponds to (2 and 4 wt.% of scandium). Each mixture was vigorously stirred for 12 h at room temperature. The prepared samples were dried in an oven at 120 °C then calcined at 400 °C for 4 h.

### 2.3. Fabrication of Sc/TiO<sub>2</sub> photoanode

Sc/TiO<sub>2</sub> photoanodes were synthesized using the following procedure: initially, 0.2 g of the materials (TiO<sub>2</sub>, 2 wt.% Sc/TiO<sub>2</sub> and 4 wt.% Sc/TiO<sub>2</sub>) was mixed separately with Triton X-100 and acetic acid at room temperature. Finally, the materials were coated on a conducting ITO slide. In order to obtain a stable photoanode, the film was dried at room temperature, sintered at 450 °C for 30 min in a muffle furnace, and then cooling down to room temperature.

### 2.4. Fabrication of DSSCs and evaluation of their performances

After cooling, the coated substrates (photoanodes) were immersed in a dye bath containing RB at different concentrations range from 10.16 × 10<sup>-8</sup> to 10.16 × 10<sup>-3</sup> M in ethanol for 12 h. The dye-adsorbed photoanode was withdrawn from the solution and gently cleaned with ethanol. The counter electrode made of carbon (candle flame) coated ITO glass. The photoanode and counter electrode were clamped firmly together. A redox electrolyte solution (iodine in ethanol) was introduced into the cell assembly by capillary action. Different concentrations of electrolyte; 100% iodine (iodine free ethanol), 80, 50 and 20 in ethanol were used. Different active areas of 1.5, 2.3, 3.0, 3.4, 4.4 and 5.0 cm<sup>2</sup> were fabricated to measure the cell performance. The counter electrode was coated with different thickness of carbon. The photocurrent density–voltage (*J*–*V*) measurements were performed using light intensity lamp of 10 mW cm<sup>-1</sup> calibrated using Radiometer (International Light Technologies).

From the analysis of the *J*–*V* curves, parameters of the cell's operation are obtained. Open-circuit photovoltage (*V*<sub>OC</sub>), short-circuit photocurrent density (*J*<sub>SC</sub>), fill factor (FF), calculated using Eq. (1), and the overall energy conversion efficiency (*η*) is calculated using Eq. (2)

$$FF = V_{\max} J_{\max} / V_{OC} J_{SC} \quad (1)$$

$$\eta = V_{OC} J_{SC} FF / I_s \quad (2)$$

where *V*<sub>max</sub> and *J*<sub>max</sub> are voltage and current density for maximum power output, respectively. *I*<sub>s</sub> is the intensity of the incident light (mW/cm<sup>2</sup>).

## 3. Results and discussion

### 3.1. Surface analysis

The BET surface area and pore size distribution were calculated and the results are represent in Table 1. The BJH method based on desorption branches of nitrogen isotherms was used to calculate the pore size distribution. The prepared samples display isotherms of Type II according to the IUPAC classification, with the presence of mesoporous (IUPAC, 1985) (Fig. 2a–c). Table 1 shows that as the scandium content increases the surface area decreases from 316.0 to 144.5 m<sup>2</sup>/g. The pore volume decreases from 0.35 to 0.34 cm<sup>3</sup>/g and the average pore diameter increases from 39.1 to 69.9 Å. This is because scandium oxide helps the TiO<sub>2</sub> particles to agglomerate forming bigger pores with a loss of accessible surface. The inset view at the top of Fig. 2 shows the pore size distribution. The peak of the pore size distribution increases with increase in

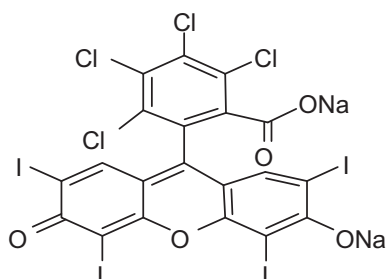


Fig. 1. Structure of Rose Bengal (IUPAC name: 4, 5, 6, 7-Tetrachloro-2', 4', 5', 7'-tetraiodofluorescein sodium salt).

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