Optimization of organic meso-superstructured solar cells for underwater IoT^2 self-powered sensors.

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***Abstract*—The effectiveness of the mesoporous TiO_2 layer, which acts as an active n-type semiconductor layer in dye sensitized solar cells (DSSCs) was investigated by varying the $AgVO_3$-doping. To optimize the meso-superstructure, the doping concentration was varied from 0% to 25% using experimentally validated simulations. Moreover, performance comparisons between experimentally fabricated DSSCs based on natural beetroot and the commonly used N719 dye were made. A 15%-doping concentration was found optimum for our DSSC, which delivered an output power of 19.24 mW, 6.1% power conversion efficiency, as well as an open circuit voltage, V_{oc}, of 0.5 V and a short circuit current, I_{sc}, of 21 mA/cm^2 in diffused light conditions. Based on these performance results, we integrated our optimized DSSC in an underwater sensing unit as a light harvester.**

***Index Terms*— $AgVO_3$ doping, Dye Sensitized Solar Cells, mesoporous TiO_2, Natural dye, Numerical optoelectronic modeling.**

I. Introduction

Titanium dioxide (TiO_2) is considered an n-type indirect band gap semiconductor. Among the many TiO_2 structures, the meso-superstructured porous (mp) form has become increasingly useful in dye sensitized solar cells (DSSCs) [1] and perovskite solar cells (PSCs) [2].

In hybrid DSSCs with mesoporous TiO_2, the photovoltaic performance is based on the effective absorption of the dye. TiO_2 is a relatively high energy band-gap semiconductor (3.15 eV) and photon absorption is constrained to the UV spectrum [2]. Therefore, dye based DSSCs demonstrate relatively low efficiencies. To boost DSSC efficiency, the optoelectronic properties of TiO_2 can be tuned via doping [3], which leads to improved carrier transport in solar cells. In fact, the doping concentration influences the energy bandgap of the mp-TiO_2 structure and enables the optical absorption spectrum to be extended to the visible region [4].

In this paper, we demonstrate the optimized photovoltaic performance of meso-superstructured DSSCs, which were previously published in the literature [5]. Our approach relied on replacing the inorganic N719 dye with a low-cost organic dye based on beetroot. Additionally, we numerically optimized and fabricated $AgVO_3$-doped TiO_2 cells. DSSCs with double absorption effect were demonstrated, where the dye and narrow-band TiO_2 influence the cell's spectral absorption in the visible region.

Moreover, an optoelectronic carrier transport model was developed, where the doping concentration was varied between 0% and 25%. Our simulation results were experimentally validated using cells that were fabricated for an IoT^2 underwater self-powered sensor. Due to this underwater environment, our cells were characterized using diffused light conditions.

II. Optoelectronic Model

A numerical simulation platform known as Solar Cell Capacitance Simulator (SCAPS-1D) was used to predict the I-V characteristics of our DSSCs and to optimize the $AgVO_3$-doping concentration with respect to the output conversion efficiency. The input simulation parameters were extracted from the literature[1, 6-8]. During doping, Silver Vanadate ($AgVO_3$) was introduced as extrinsic doping in the mesoporous layer, while the organic dye was treated as an absorbing layer with extinction properties from experimentally measured data. The optical reflectance was considered due to the variation in the optical refractive index in the air-glass interface. Moreover, diffused AM1.5 global irradiation conditions were used to match the experimental conditions.

III. Experimental Work and Characterization

TiO_2 nanoparticles were prepared using the sol-gel method described in the literature [5]. Moreover, $AgVO_3$ was prepared from the reaction between sodium vanadate ($NaVO_3$) and silver nitrate ($AgNO_3$). TiO_2 was doped with different $AgVO_3$ concentrations, varying from 0% to 25%.

In comparison to our previously published work in [5], we replaced the commonly used N719 dye with an organic natural dye. Moreover, mp-TiO_2 was replaced with an $AgVO_3$-doped mp-TiO_2 layer, as discussed in the previous section. Herein, beetroot was used as a natural organic dye, which has a dark reddish purple color and has good sunlight absorption

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capabilities [9]. For the sake of comparison, yellowish green N719 dye was prepared. All DSSCs were sealed using a hot press at a temperature of 120 °C.

In order to study and characterize the fabricated DSSCs, an LED-based solar simulator with an integrated NIR-UV-Vis spectrometer and Keithley 2401 current-voltage source meter were used [10]. For optical characterisation, a V-770 UV-Visible/NIR Spectrophotometer was used, which has a wavelength range from 190 nm to 2700 nm.

IV. Results and Discussions

One of the main advantages of doping with $AgVO_3$ is to reduce the energy bandgap of the mesoporous TiO_2 layer. Typically, TiO_2 is a UV absorber with an energy bandgap of 3.15 eV [1, 11], where the dye is the main absorber in standard DSSCs [5]. However, mp-TiO_2 can be tuned by doping with $AgVO_3$ (2.01 eV band-gap energy [12]) to shift the absorption spectrum of the formed composite to the visible range. Figure 1 shows the tauc plots of the mesoporous TiO_2 layer before and after doping with $AgVO_3$. This reduction in the bandgap is directly attributed to the absorption capabilities of the newly proposed doped TiO_2 active layer in DSSCs.

First, numerical optoelectronic simulations (described in section 2) were used for optimizing the doping concentration of $AgVO_3$. Figure 2 shows the variation in total conversion efficiency of our DSSCs with doping concentration, along with experimentally measured data. The optimization process showed maximum efficiency for a 15% doping concentration.

According to the simulation data shown in figure 2, the left portion of the curve shows improved cell efficiency with increasing doping concentration. We attribute this behaviour to bandgap narrowing and increased carrier mobility. However, the conversion efficiency starts to decrease for higher doping concentrations, which reduce electron mobility and increase the recombination rate. These phenomena agree with reported investigations in the literature in [13].

Experimental results were used for validating our simulation data. Figure 3 shows a comparison between the experimental and simulated J-V curves for different doping concentrations. Herein, the term Stand-DSSC refers to a DSSC with undoped mesoporous TiO_2 as an active layer. The simulation results agree with the experimental data and a root mean square error below 5% was observed near the open-circuit voltage point. We attribute this error to the fluctuated series parasitic resistance associated with the measurements. Another observation related to the non-linear proportionality between short-circuit current and doping concentration can be also detected. This is simply due to the variation of the fill-factor with doping concentration.

Finally, the impact of using a natural beetroot dye is shown in figure 4. Here, photon absorption in the UV region (hot photons) and below 500 nm is attributed to the enhanced narrow-band mp-TiO_2 layer, while the mid-visible photons (around 550 nm) are absorbed by the natural dye. This justifies the enhanced performance of the beetroot-based DSSC in comparison to N719 DSSC whenever $AgVO_3$ doping was used. On the other hand, N719 dyes demonstrate better performance with bare mp-TiO_2 cells (cf. figure 4).

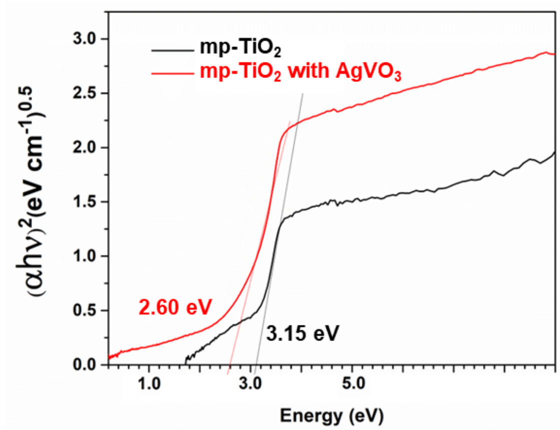

Figure 1: Tauc plots of bare mp-TiO_2 and the $AgVO_3$ doped sample. The band gap of the mp-TiO_2 layer can be shifted from 3.15 eV to 2.6 eV by adding a $AgVO_3$ layer.

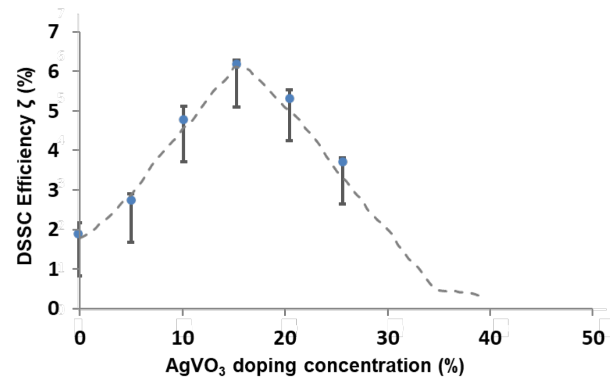

Figure 2: Optimizing the $AgVO_3$ doping concentration in DSSC TiO_2 active layer using the SCAPS-1D numerical model. Data from experimentally fabricated DSSCs are shown as blue dots with corresponding error bars to account for variations in successive measurements.

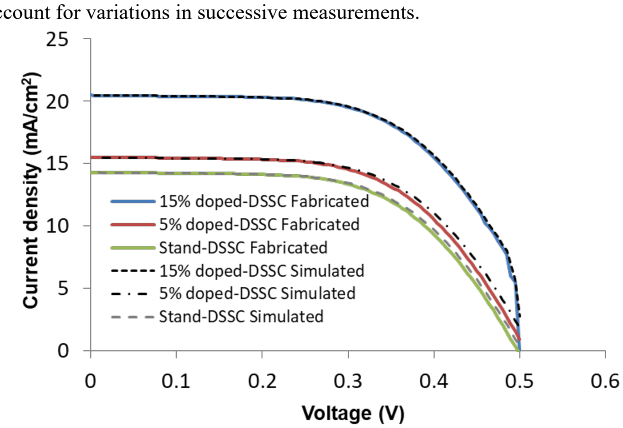

Figure 3: J-V characteristics of Stand-DSSC and DSSC with mp-TiO_2, which were doped with 5% and 15% $AgVO_3$. Our results show good agreement between experimental and simulation results.

V. Optimized DSSC for IoT[2] underwater sensing

In this section, the optimized DSSC cell was used for powering an underwater sensor that was previously described in the literature [14]. The sensor has an on-power of 500 mW with a 10 ms operating time, while the off-power is 0.5 mW (see the appendix of [14]).

We designed a complete experiment that involved submerging the sensor with our DSSC in a 1 m deep water tank, under a standard solar simulator. The power degradation profile against versus underwater depth was experimentally measured and plotted in figure 5. Since the sensor was submerged underwater, diffused light ($\theta_{incident} > 45^o$) was the dominant light component reaching the sensor. Considering a diffused-light efficiency of $D_{45} = 59\%$, only 4.2 cm^2 area was needed from the 15% doped-DSSC with beetroot dye to supply the sensor unit, assuming a 10 cm underwater depth. This records a significant reduction in area with respect to monocrystalline silicon-based harvesters. Knowing that the harvested power density of the silicon cell reached 51.3 mW/cm^2 at optical injection of one Sun. However, a significant reduction was observed under diffused light conditions (nearly 66.6%). Accordingly, our improved meso-superstructured DSSC demonstrated enhanced energy harvesting capabilities and improved power densities for such underwater applications. However, the stability and long term performance of these cells needs to be investigated in the future..

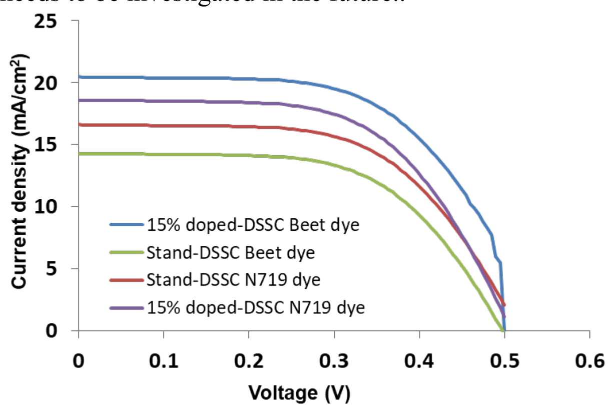

Figure 4: Measured J-V characteristics for Stand-DSSC as well as DSSC with mp-TiO_2 doped with 15% $AgVO_3$. Both N719 and natural beetroot dyes were used. Beetroot dyes showed better J-V performance and higher output power.

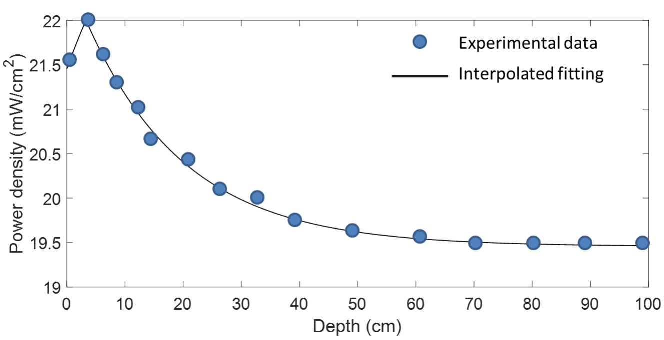

Figure 5: Measured power density degradation versus underwater depth for DSSCs with 15% doped $AgVO_3$.

VI. Conclusion

In this manuscript, we described the optimization process of a Dye Sensitized Solar Cell (DSSC), which demonstrated a power conversion efficiency of 6.1%, from diffused light conditions. We achieved this by narrowing the energy bandgap of the active mesoporous TiO_2 layer from 3.15 eV to 2.6 eV and by integrating a natural beetroot dye. Experimentally validated simulations tools were used to optimize the doping concentration with respect to the total conversion efficiency. The optimized cell, which yields an energy harvesting density of 19.24 mW in diffused light conditions, was integrated in a self-powered millimeter scale underwater sensing unit. Our optimized cell showed better performance in comparison to Si-based harvesters under the same conditions.

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