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DFT Analysis on the Photovoltaic Performance of ZnO Based Dye Sensitized Solar Cell.

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ABSTRACT

A dye sensitized solar cell based on ZnO photoanode sensitized with Sudan IV dye was fabricated. Morphological study on ZnO photoanode reveals spherical shaped nanoparticle with evenly distributed grains for large area sensitization. Power conversion efficiency of the fabricated device was obtained as 0.33 %. Electronic properties of the chosen dye were analyzed through density functional theory to investigate the photovoltaic performance.

Keywords: ZnO; Sudan IV; Dye sensitized solar cell; Density functional theory;

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INTRODUCTION

Energy crisis has become an economical case in today's scenario. Renewable resources are the excellent substitute for fossil fuels, with solar energy being the most favorable. A solar cell (Photovoltaic cells) that utilizes solar energy has now been employed generally for electricity generation. Dye sensitized solar cell (DSSC), which is similar to a photoelectrochemical cell have attracted much attention, owing to flexibility in designing and being economical [1]. A DSSC with TiO_2 as photoanode and ruthenium sensitizer as dye has attained 11 % of power conversion efficiency [2]. ZnO, a wide band-gap (3.37 eV) material is also of much interest as photoanode in DSSC due to its excellent opto-electronic properties [3]. Metal free dyes are also a noticeable candidate in regard with low cost and high molar absorbance [4]. Density functional theory (DFT) [5] has been adopted to investigate the optical and electronic properties of materials to analysis the device performance. The dye in a DSSC acts as solar energy harvesting material and contributes majorly in the device performance. In this work, ZnO based DSSC with a metal free dye as photosensitizer was fabricated and the photovoltaic performance of the fabricated device was analyzed with the DFT investigation on the electronic properties of the chosen dye.

MATERIALS AND METHODS

Materials

Precursor salt, Zinc acetate dihydrate $(Zn(CH_3COO)_2 \cdot 2H_2O)$ of 99.99 % pure obtained from Merck and Indium Tin Oxide (ITO) coated glass substrate of sheet resistance 70 – 100 Ω/sq obtained from Sigma Aldrich were used to prepare the photoanode. Sudan IV $(C_{24}H_{20}N_4O)$ obtained from Loba chemie was used as the sensitizer. Anhydrous Lithium Iodide of 99.90 % pure and 0.1 N of Iodine solution obtained from Sigma Aldrich were used to prepare the electrolyte solution. A 0.5 mm thick Platinum foil obtained from Sigma Aldrich along with ITO coated glass substrate was employed as the counter electrode.

ZnO thin film preparation

Precursor salt solution containing 0.05M of zinc acetate dihydrate dissolved in 50 mL of deionized water was deposited onto the ITO glass substrate through spray pyrolysis technique [6] at a deposition temperature of 250 °C to prepare the ZnO photoanode and the reaction is described as,

$$(Zn(CH_3COO)_2 \cdot 2H_2O)_{(aq)} \xrightarrow[\Delta 250^\circ C]{} ZnO_{(s)} + CH_3COCH_{3(g)} + CO_{2(g)} + 2H_2O_{(g)} ----(1)$$

DSSC fabrication

The ZnO photoanode was sensitized with 0.05 mM of Sudan IV dissolved in methanol for a period of 12 hrs. The electrolyte solution was prepared with 0.5 M Lithium iodide and 0.05 M iodine. Platinum foil was sealed over ITO glass substrate to prepare the counter electrode. The electrolyte solution was introduced in between the photoanode and counter electrode to obtain the DSSC assembly.

Characterization studies

Structural analysis of the prepared ZnO thin film was characterized using XPERT-PRO diffractometer system with Cu-Kα_1 (λ=1.54060 Å) radiation. Surface morphology of ZnO thin film was characterized with field-emission scanning electron microscope (FE-SEM, JEOL-6701F). Optical property of Sudan IV was analyzed with UV–Vis spectrophotometer (Perkin Elmer, Lambda 25). Nicolet Magna 560 FTIR spectrometer was used to analyze the FT-IR spectrum of Sudan IV. The photovoltaic performance of the device was analyzed by illuminating 500 W xenon lamp of 100 mW/cm^2 over 1 cm^2 of the device.

Computational method

DFT study on electronic properties and optimized structure of Sudan IV were carried out with Becke-3-parameter-Lee-Yang-Parr (B3LYP) exchange correlation and Los Alamos National Laboratory 2-double-z (LANL2DZ) basis set. Gaussian 09 [7] software was used to perform the simulations.

RESULTS AND DISCUSSION

Morphological and Optical analysis

Fig. 1 shows the FE-SEM image of the deposited ZnO thin film. It represents spherical nanoparticle morphology with evenly distributed grains. This uniformly distributed particle has the capability to provide more surface area for the dye molecules to get adsorbed and thereby enhancing the light harvesting capacity. The UV-Vis absorbance spectrum of Sudan IV dye dissolved in methanol is shown in Fig. 2. From the spectrum it is inferred that, Sudan IV shows maximum absorbance around 510 nm in the visible region. This strong absorbance characteristic of Sudan IV in the visible region is of interest to employ it as photosensitizer in DSSC.

Photovoltaic studies

The I-V characteristic of the DSSC fabricated with Sudan IV dye is shown in Fig. 3. Power conversion efficiency (η) of the device is obtained as (0.33 %). The photovoltaic parameters were obtained using the following relation.

Fill Factor (FF) = $$\frac{I_{\max} \times V_{\max}}{I_{sc} \times V_{oc}} \quad (1)$$

Efficiency: η (%) = $$\frac{I_{sc} \times V_{oc} \times FF}{P_{in}} \times 100 \quad (2)$$

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Table 1: Obtained photovoltaic parameters of the fabricated DSSC

Photoanode	Dye	Counter electrode	Isc (mA)	Voc (V)	FF	η (%)
ZnO	Sudan IV	Platinum foil	1.78	0.490	0.3875	0.3

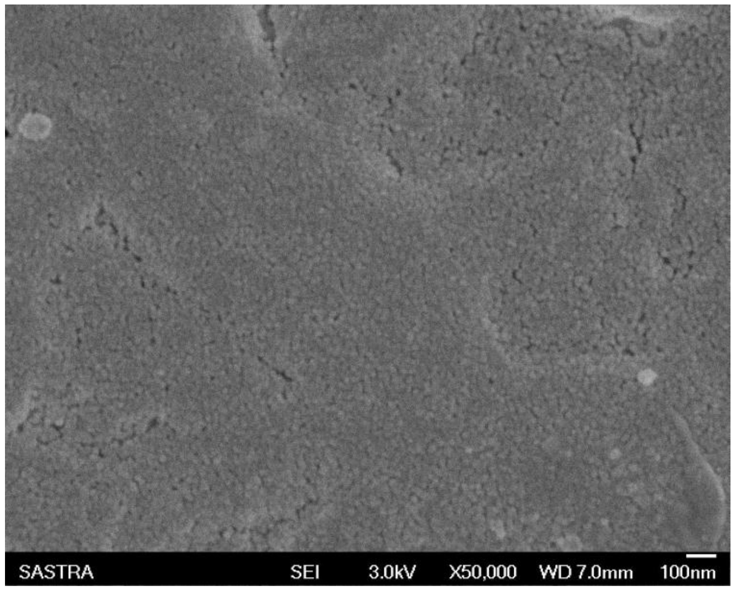

Figure 1: FE-SEM image of ZnO photoanode

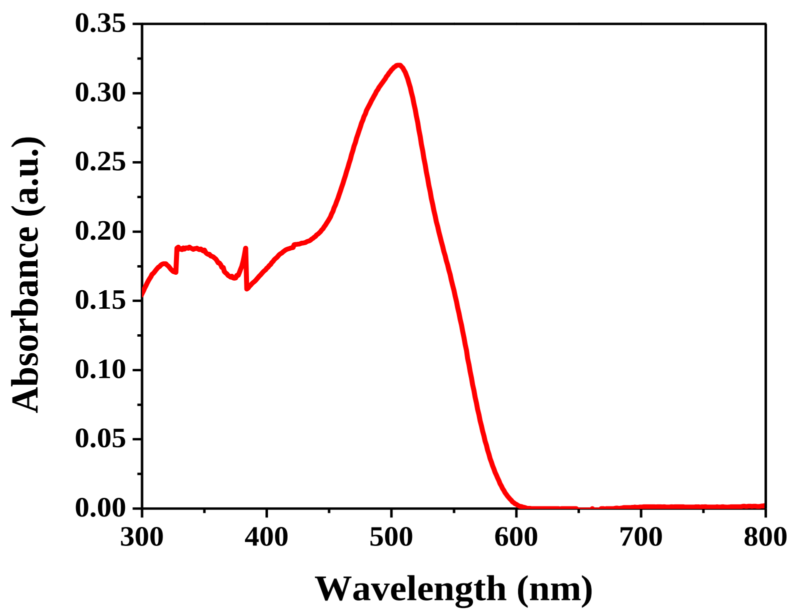

Figure 2: UV-Vis absorbance characteristic of Sudan IV dye

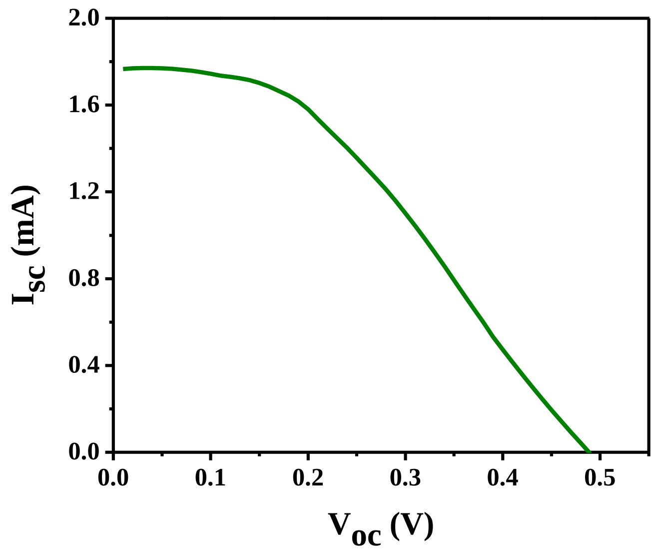

Figure 3: I - V characteristic of the fabricated DSSC

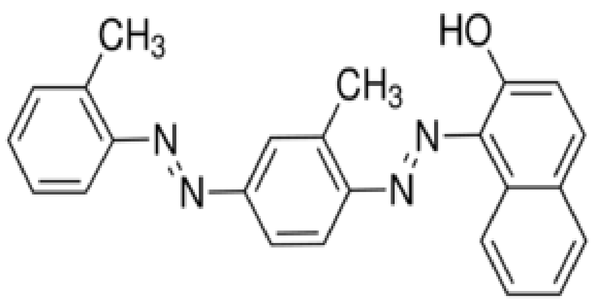

Figure 4: Molecular structure of Sudan IV dye

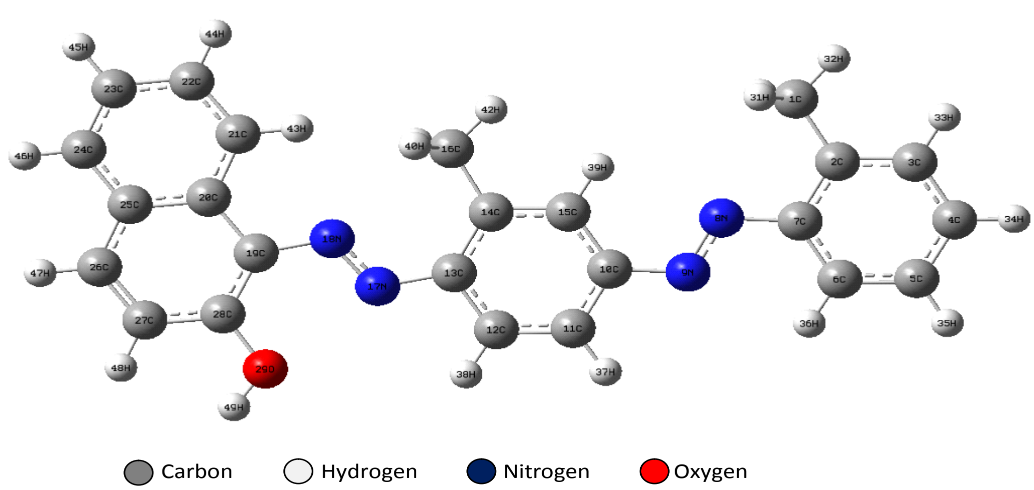

Figure 5: Optimized structure of Sudan IV molecule

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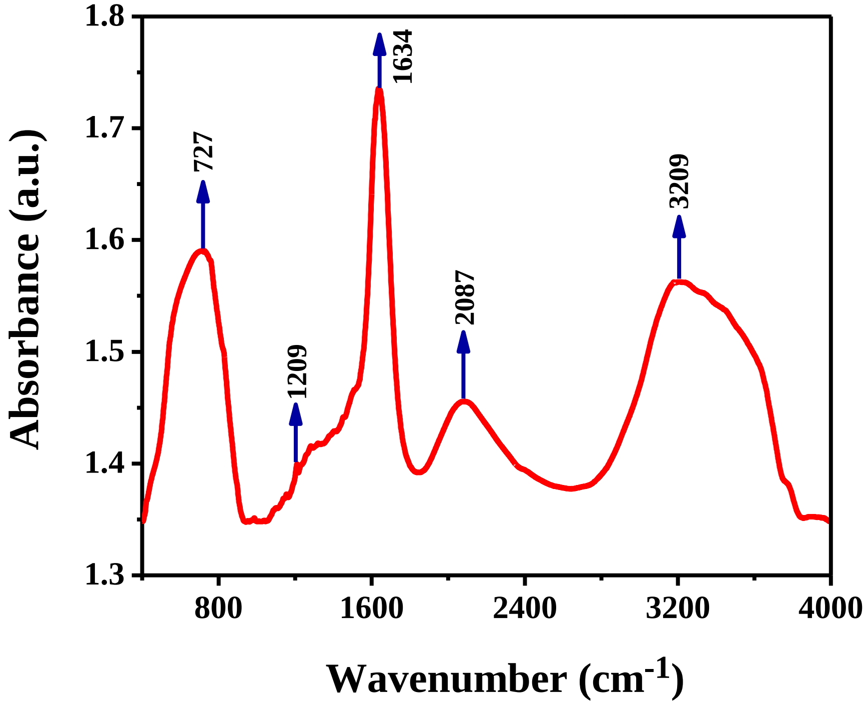


Figure 6: FTIR spectrum of Sudan IV dye

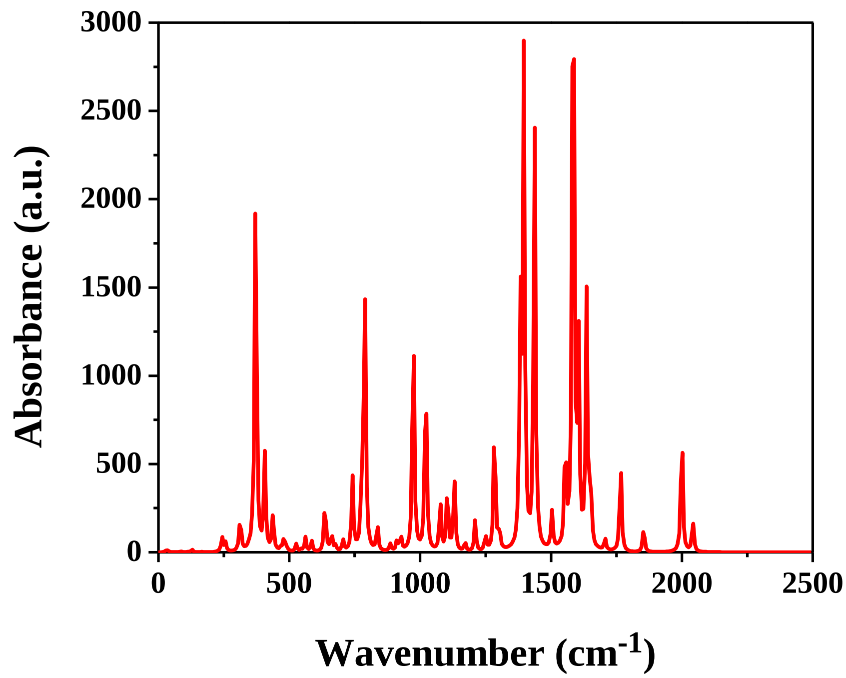


Figure 7: Simulated FTIR spectrum of Sudan IV molecule

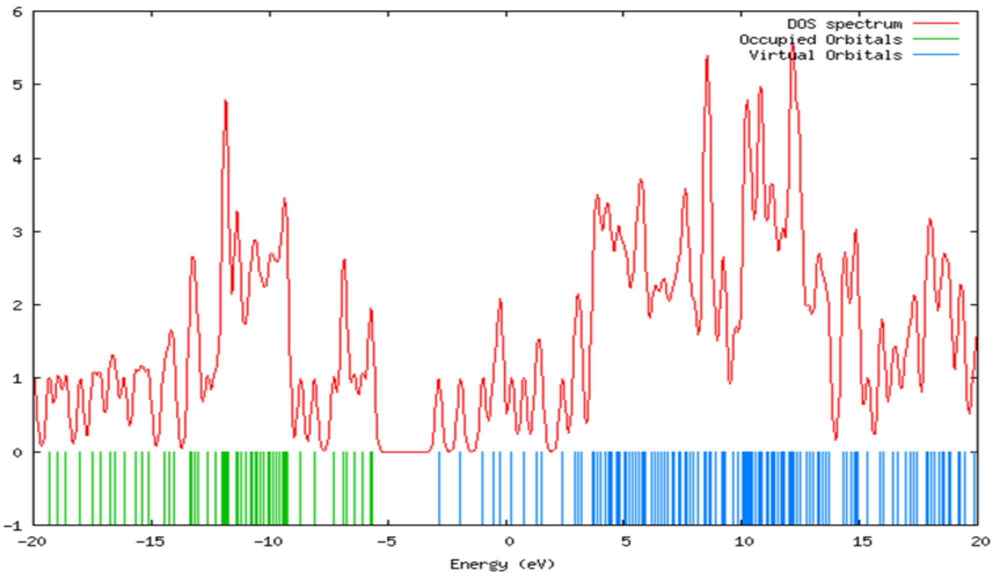
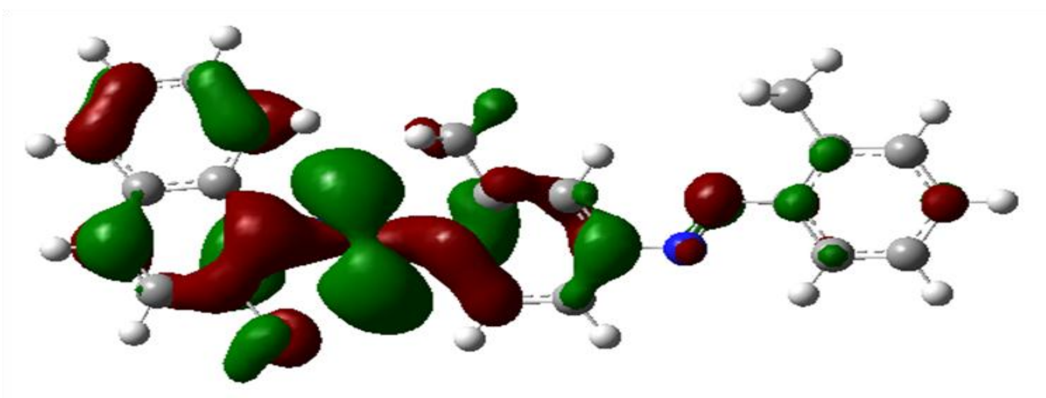


Figure 8: DOS spectrum of Sudan IV molecule



(a)

(b)

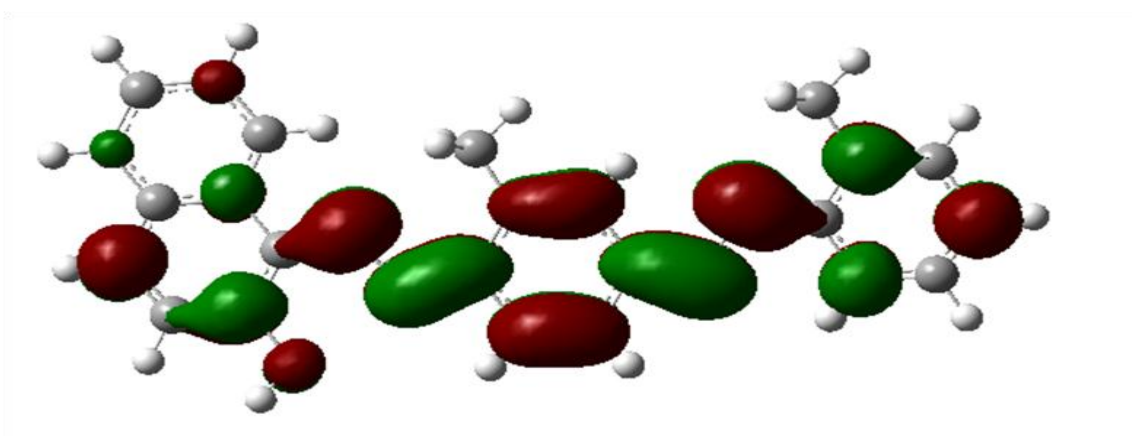


Figure 9: (a) HOMO and (b) LUMO of Sudan IV molecule

The obtained photovoltaic parameters are shown in Table 1. The low performance of the device is ascribed to the low I_{sc} (1.78 mA) and V_{oc} (0.49 V) values. It indicates that the recombination of charge carriers at the interfaces has major reflection in the device performance.

DFT analysis on the electronic properties of Sudan IV

The molecular structure of Sudan IV is shown in Fig. 4. The N=N group provides the bridge for the electron transportation within the molecule. The anchoring part of Sudan IV is carboxylic group. The optimized structure of Sudan IV having energy of -521.97938 hartree, obtained through DFT study is depicted in Fig. 5. The simulated and characterized FTIR spectrum of Sudan IV molecule is shown in Fig. 6 and Fig. 7. It indicates that the experimental result is in agreement with the simulated result, and hence this confirms that the optimized structure of Sudan IV molecule is valid. Density of states (DOS) spectrum of Sudan IV obtained through DFT is shown in Fig. 8. The LUMO and HOMO energy levels were found to be – 2.83 eV and – 5.67 eV respectively. The electron densities in the highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO) of Sudan IV were determined through DFT analysis. Fig. 9 (a) indicates that the distribution of electron density in the HOMO (ground state) is considerable in the alkyl, amine and aromatic group and weak in the hydroxyl group. Furthermore, the electron density due to photo excitation is shown in Fig. 9 (b). It is observed that in the excited state, the electron density is shifted towards the hydroxyl part, favoring for electron injection onto the oxide material. It is also observed that the electron distribution in the anchoring part is weak and hence there is less favorable charge injection from the dye, which is confirmed from the low I_{sc} and saturation current in the IV curve shown in Fig. 3.

CONCLUSION

Photovoltaic performance of the fabricated DSSC was analyzed and the parameters were obtained as I_{sc} = 1.78 mA, V_{oc} = 0.49 V, FF = 0.3875 and η = 0.33 %. To analyze the device performance, the electronic properties of Sudan IV dye were studied. Electron density distribution in HOMO and LUMO indicates that the dye has major contribution in the device performance. Even though the performance of the fabricated DSSC is poor, synthesizing Sudan IV dye for tuning the electronic properties and ZnO photoanode with specific morphology could improve the efficiency of the device.

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