STUDY OF DSSC DYE USING DENSITY FUNCTIONAL THEORY

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Abstract

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1. INTRODUCTION

Dye Sensitized Solar Cell (DSSC) is a photovoltaic device that converts light into electricity in presence of metal oxide semiconductors which have a wide bandgap photosen-sitization property. Another main reason of interest is the low cost solar energy conversion technique [1]. Thus, with the help of new combination of metal complexes and dyes, we can improve photo-conversion efficiency [1,2].

The working of DSSC is based on the separation of charge carriers controlled by reactions involved [3]. Most of efficient DSSC have power convrsion efficiency of 11% hav-ing ruthenium based complexes as dye materials. But high cost of ruthenium-based com-plexes [4] made to search for alternate photosensitizers with proper combination of photo-

electrodes. Synthetic dye production is not only very expensive but also environmentally

unfriendly [5]. Again, the use of natural dye as sensitizer over synthetic dyes have several advantages [6] and they can be easily extracted with minimal chemical procedures, thereby attracting interest in producing cost efficient sensitizer [7].

In the present paper, we consider a DSSC, having Rose Bengal dye as a photosensitizer, absorbed in metal oxide semiconductor. The experimental studies are limited to TiO_2 and ZnO as photo-electrode. Computational modeling was carried out to provide the further understanding of different energy levels, UV-Vis spectra and the electron clouds of different photo-electrode used in DSSC.

2. EXPERIMENTS

2.1 Optical Properties:

UV-Vis spectra of Rose Bengal dye is shown in the Fig. (1). Analysis shows an absorption peak at 378 nm having oscillatory strength 0.0029. The absorption peak is around the visible spectrum of sunlight, hence the dye can be used as light absorbing material.

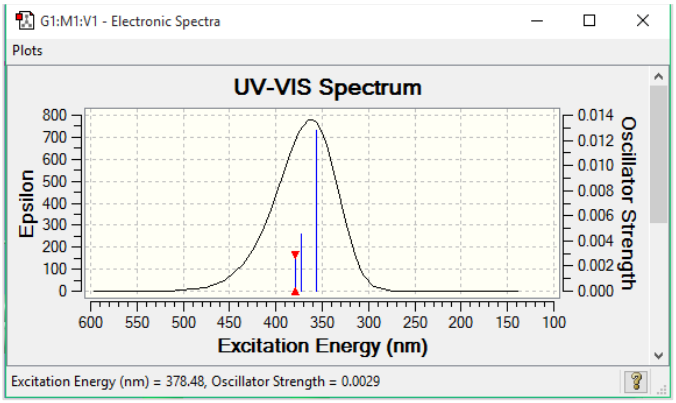


Fig 1 Computed UV-Viz spectra from DFT Studies.

2.2 Electro-chemical Properties:

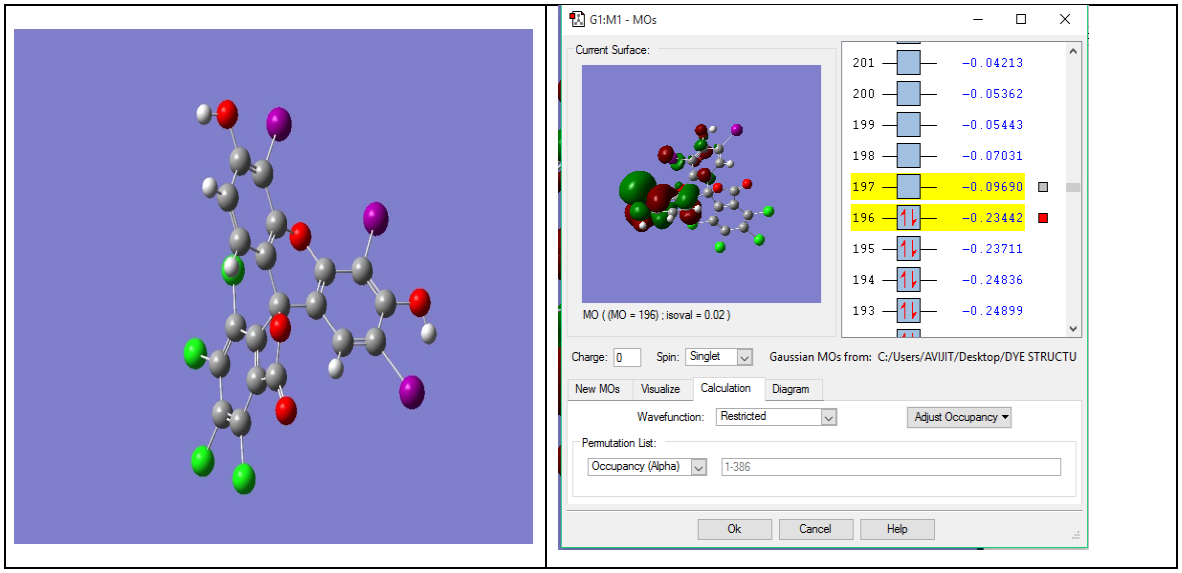
The electro chemical property of the Rose Bengal dye was investigated and the study showed the possibility of electron injection from the excited state of dye to the conduction band of semiconductor. The HOMO level is the major factor of electron donar mechanism. Higher positive energy value of HOMO level means lower electron donating ability. Here we find both HOMO and LUMO levels of Rose Bengal, TiO_2 and ZnO thereby comparing the donating ability to both the metal oxide semiconductor from the photosensitizer.

3. RESULT AND DISCUSSION:

3.1 Computational Study:

The molecular structures of TiO2, ZnO and Rose Bengal dye (fig. 1) were computed using ChemDraw Ultra 8.0 software. Both Density Functional Theory (DFT) and Time Dependent Density Functional Theory (TD-DFT) were performed using Gaussian 09W software. Here we used B3LYP hybrid functional and 3-21G basis set as calculation methods. The various energy levels including Highest Occupied Molecular Orbitals (HOMO), Lowest Unoccupied Molecular Orbitals (LUMO) and the electron densities were visualized using Gauss-View version 5.0.

The computational generated energy levels of HOMO and LUMO of Rose Bengal dye is shown in the Fig. (2). In order to transfer electrons, the LUMO level of the photosensitizer must be higher than the conduction band edge of photo electrode i.e. either TiO_2 or ZnO. Optimizing the dye structure and then calculating it is seen that the HOMO level is 196 having energy -0.23442 A.U. while the Lowest Unoccupied Molecular Orbital (LUMO) is 197 and its energy is -0.09690 A.U. Converting in electron volts, the HOMO, LUMO energies were found to be -6.38 ev and -2.64 ev respectively. Hence bandgap is 3.74 ev.



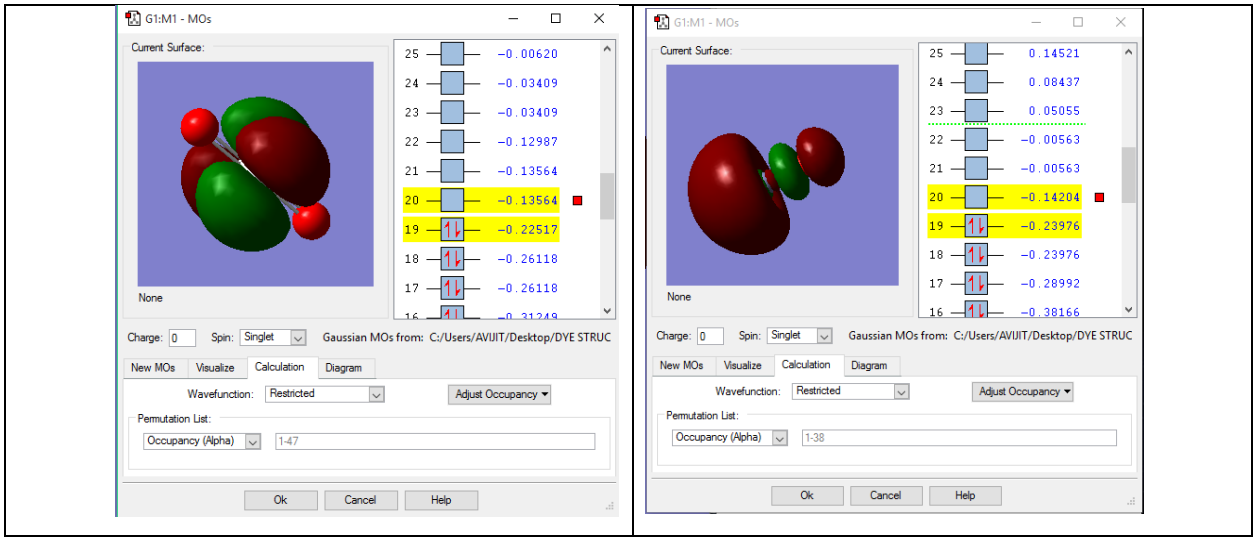
(a) (b)

Fig 2(a) Structure of Rosebengal dye and (b) gave HOMO LUMO levels of dye material

Table I – HOMO LUMO levels and Bandgap of Rose bengal dye.

Photosensitizer / Photo anode	**HOMO LEVEL**	**LUMO LEVEL**	**E_{HOMO}(EV)**	**E_{LUMO}(EV)**	**Bandgap(ev)**
Rose Bengal dye	196	197	-6.38	-2.64	3.74
TiO_2	19	20	-6.13	-3.69	2.44
ZnO	19	20	-6.52	-3.86	2.66

Again by using the same procedure for TiO_2, we found the HOMO, LUMO levels energies to be -0.22517 A.U. and -0.13564 A.U (fig. 3). In terms of electron-volt, these energies become -6.13 ev and -3.69 ev having a band gap of 2.44 ev. For ZnO, the HOMO, LUMO levels were at -0.23976 A.U. and -0.14204 A.U. which means at -6.52ev and -3.86ev respectively, which produces a bandgap of 2.66 ev. (fig. 4)



(a) (b)

Fig 3(a) The HOMO LUMO levels of TiO_2 and Fig 3(b) give HOMO LUMO levels of ZnO

Here it is clearly seen that the LUMO of Rose Bengal dye is higher than the conduction band edge of TiO_2 and ZnO while HOMO were more negative. It indicate that, both

TiO_2 and ZnO can be used as a suitable photo electrode in presence of Rose Bengal dye as photosensitizer.

4. CONCLUSION:

Dye sensitized solar cells were designed with TiO2 and ZnO photo anodes with Rose Bengal dye as a photosensitizer. We mainly focused on the properties of the dye used in dye sensitized solar cell (DSSC), calculated the HOMO-LUMO energy levels of the dye as well as the photo anode TiO_2/ZnO using Gaussian software. Here we discuss the energy band structures of these two photo anodes. The results show that efficiency of DSSCs using ZnO photo anode is greater than the TiO_2 photo anodes.

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