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Study of new Azo Dyes for DSSCs using DFT

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Abstract: The world panorama consumption increasingly migrates to the clean and easy energy production. Some alternatives to the usual sources are proved by the historically environmental degradation combined to the impact on the life quality of people. In this context, solar energy has emerged as a potential alternative with an open field for research and development.

This project aims precisely at deepening about the technology and operation of the components of the Dye Sensitized Solar Cells (DSSC) [1] with focus to the production of organic azo dyes in order to generate clean energy applying the green chemistry principles. The azo dyes are given special attention, since they are widely used in the paint industry [2], but little reported in the literature of DSSCs. A schematic diagram of DSSC work system is shown in Figure. 1.

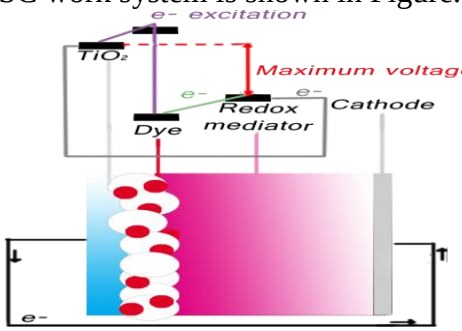


Figure 1. Schematic of a DSSC operation

The two azo compounds chosen for this work have been proposed to be synthetized based originally on the methodology described on [3] with some modifications and additional steps. They are illustrated in Figure. 2:

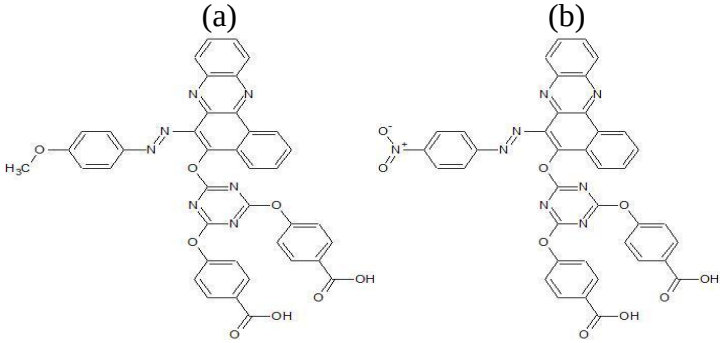
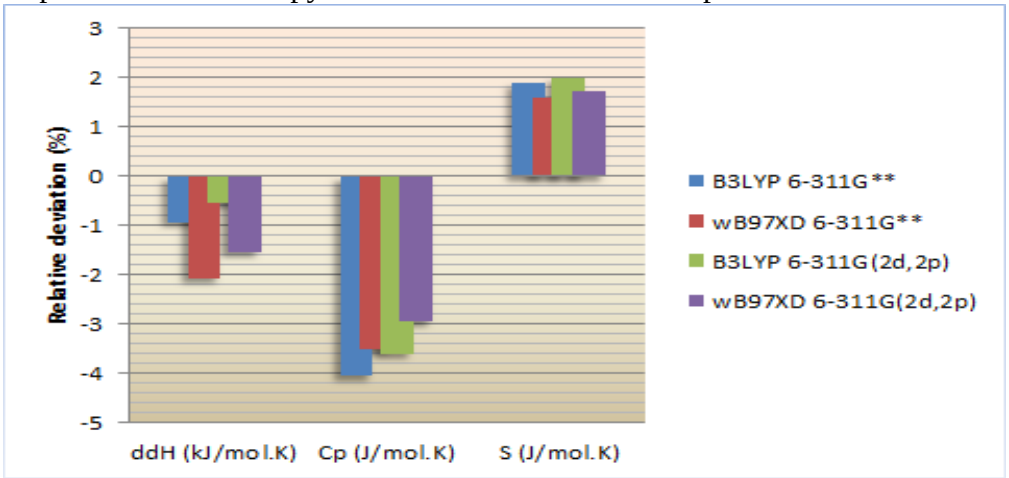


Figure 2. Azo Dyes. (a) Azo 1 (b) Azo 2

DSSC's dyes have been already investigated with DFT method to understand orbitals energy levels [4]. In order to validate the computational methodology, some calculations were performed with the pyrrole due to the similar structure and constituent atoms. From the pyrrole calculations was observed that the functionals B3LYP and wB97XD using 6-311G** or 6-311G(2d,2p) basis set have good agreement with the experimental data shown on [5] (about less than 2% of deviation for enthalpy content and entropy and about less than 4% of deviation for heat capacity – all data collected for 298,15K) and was chosen to be used for the azo dyes calculations. The percentual deviations of thermodynamic properties from the experimental data for pyrrole are shown below on Graphic 1.



Graphic 1: Percentual deviation of thermodynamic values

DFT calculations are being performed for the Azo 1 and Azo 2 and in sequence the electronic and structural properties will be analyzed. The energy levels, thermodynamic parameters and electron population will be used to predict some properties of a dye sensitized solar cell prepared with those organic dyes. Based on that, we expected with the results of this work to validate a solid methodology for predictions of new organic dyes to ensure a lower financial and environmental costs.

Key-words: Azo compounds, Organic Dyes, Solar Cells, Dye Sensitized Solar Cells, DSSCs, DFT

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References:

[1] C. Lee et al RSC Adv. 5 (2015) 23810-23825
[2] Labd-Alredha, R. Mhessn et al E-Journal of Chemistry 9 (2012) 465-470
[3] A. I. Francisco, M. D. Vargas, V. F. Ferreira et al J. Braz. Chem. Soc. 21 (2010)
[4] A. Hagfeldt et al Chem. Rev. 110 (2010) 6595-6663
[5] http://cccbdb.nist.gov/exp2.asp - NIST, Pyrrole - access in 08/2017