

# Computational studies of optical properties of (E)-2-(5-methacrylamido-2, 3-bis (methylthio) phenyl) diazenesulfonate dye for solar cell using DFT and TD-DFT Methods

M. Kiasadegh<sup>a</sup>, B. Sohrabi<sup>a\*</sup>, J. Beheshtian<sup>b</sup>

a Department of Chemistry, Surface Chemistry Research Laboratory, Iran University of Science and Technology, P.O. Box 16846-13114, Tehran, Iran.

b Department of Chemistry, Shahid Rajaee Teacher Training University, P.O. Box 16785-163, Tehran, Iran.

Email: [Sohrabi\\_b@iust.ac.ir](mailto:Sohrabi_b@iust.ac.ir), [sohrabi\\_b@yahoo.com](mailto:sohrabi_b@yahoo.com)

**Key words:** Solar cell, DFT, TD-DFT, dye, CPCM.

## Abstract:

In this work, the (E)-2-(5-methacrylamido-2, 3-bis (methylthio) phenyl) diazenesulfonate dye molecules was optimized by DFT/6-31G (d, p) method in gas phase and Ethanol solvent by using CPCM model. The UV-Vis spectra of dyes have been studied in gas phase and Ethanol solvent.

## Introduction:

Organic solar cells have been attracted much attention because of the good efficient, low-cost and easy fabrication in recent years. The performance of an organic dye in real devices depends sensitively on its structure and electronic/optical properties, such as the binding stability, the band alignment, and the absorption maximum and intensity [1]. These types of solar cell form a donor- acceptor system, which dyes are donor and semiconductors are acceptor [2]. Design a suitable linker, which contain a bridge between dye and anchoring group, is an important factor to improve efficient of solar cells.

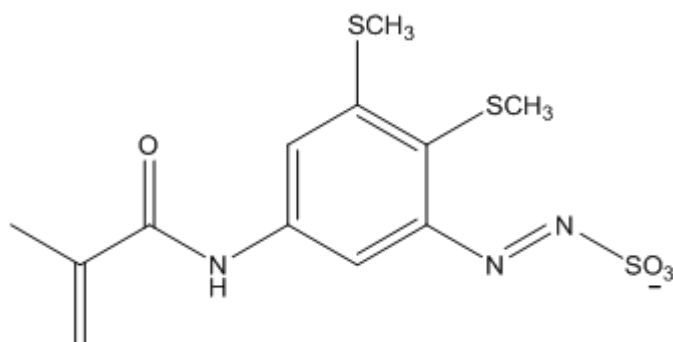


Figure1: schematics of diazenesulfonate

### Computational Details:

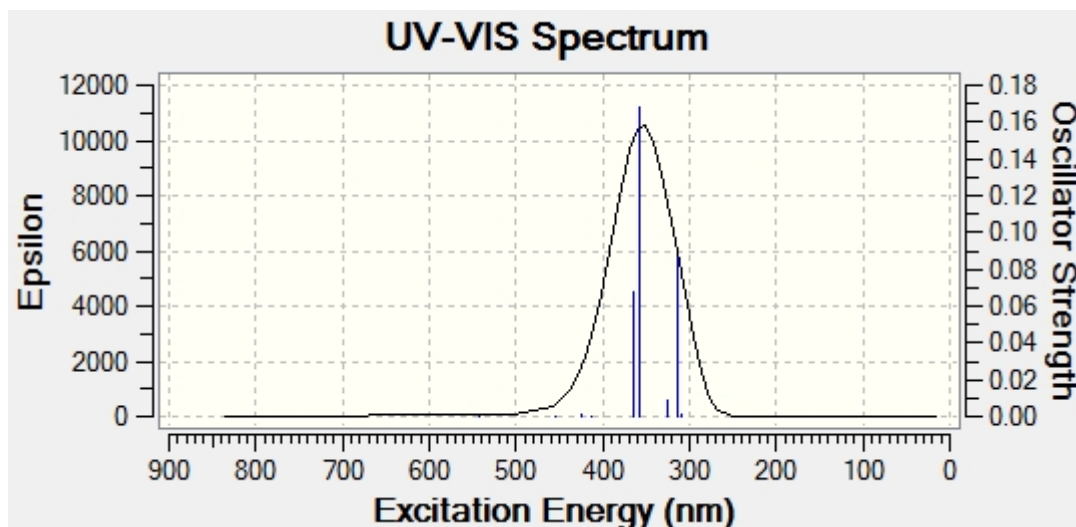
Calculations were done using software Gaussian 98. The (E)-2-(5-methacrylamido-2,3-bis(methylthio)phenyl) diazenesulfonate dye molecule (Figure 1) was optimized by DFT/6-31G (d, p) method in gas phase and Ethanol solvent. The UV-Vis spectra of dyes were computed by using the TD-DFT/6-31G (d, p) method in gas phase and Ethanol solvent.

### Results and Discussion

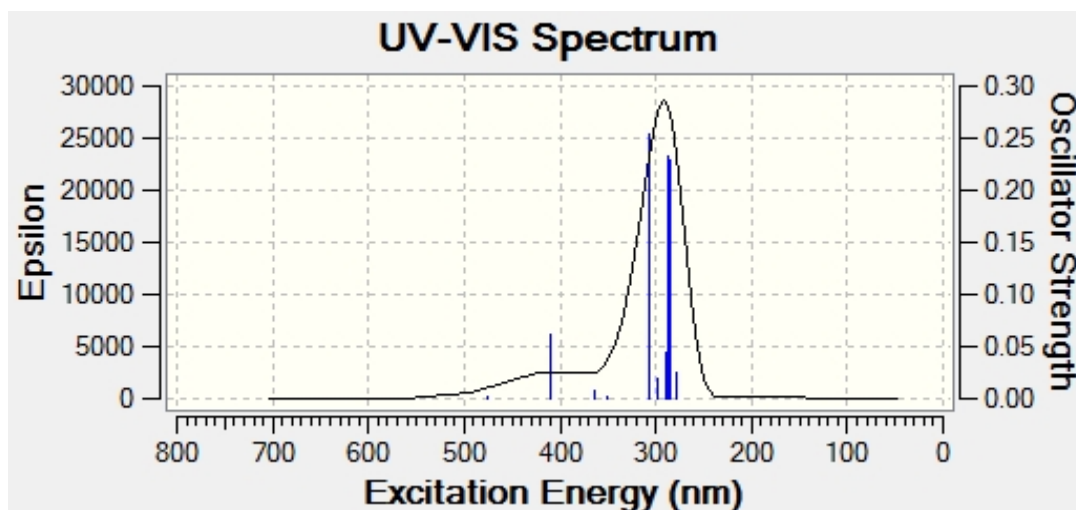
A calculation on the (E)-2-(5-methacrylamido-2,3-bis(methylthio)phenyl) diazenesulfonate dye molecule in gas phase and Ethanol solvent is shown in the diagram 1. According to table 1, the solvent affect on dye structure and optical properties. The UV-vis spectra of the dyes in ethanol have a red shift in compared with gas phase.

Table1: UV-Vis spectra of diazenesulfonate

|                |                            |        |        |        |        |
|----------------|----------------------------|--------|--------|--------|--------|
| <b>Gas</b>     | <b>UV-Vis(nm)</b>          | 364.57 | 358.57 | 326.43 | 314.05 |
|                | <b>Oscillator strength</b> | 0.0680 | 0.1677 | 0.0083 | 0.0915 |
| <b>Ethanol</b> | <b>UV-Vis(nm)</b>          | 409.21 | 307.49 | 288.93 | 286.32 |
|                | <b>Oscillator strength</b> | 0.0614 | 0.2542 | 0.0441 | 0.2324 |



a)



b)

Diagram 1: UV-Vis spectra of diazensulfonate: a) Gas phase b) Ethanol solvent

### Reference:

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- [2] E. Galoppini; “Linkers for anchoring sensitizers to semiconductor nanoparticles”; Coordination Chemistry Reviews 248, 1283–1297, 2004