



دانشگاه علوم پزشکی زابل



SEMINAR OF CHEMISTRY AND ENVIRONMENT

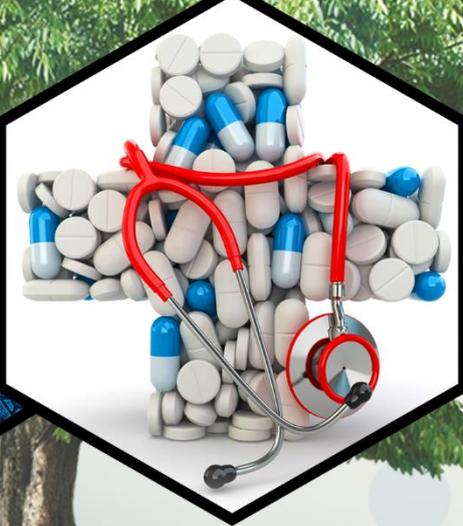


کتابچه

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ششم



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Steric Effect in Ancillary Ligand on Cyclometalated Ruthenium (II) Sensitizers in Dye Sensitized Solar Cells

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Abstract

One of the greatest challenges in energy conversion is replacing fossil fuels with renewable energy sources to reduce negative environmental impacts. Due to high cost of common fuels and their greenhouse effect, the Sun plays a strategic role¹ that can be exploited as solar cell. Dye-sensitized solar cell (DSSC) is a real solution for photovoltaics.² In DSSC technology, photosensitizer dye plays a key role.³ with the aim of increasing the efficiency of DSSC, cyclometalated ruthenium (II) complexes were designed as sensitizers. Notably, our goal is to compare the studied dyes with common sensitizer, N3. Electronic structure of target dyes was optimized using DFT with inclusion of GGA and DZ basis set. For efficient charge injection, generally, the electron cloud should situate close to the supporting semi conduction oxide in excited state. Two derivatives of FT67 dye, 4 methyl and ethyl substituted complexes, were selected, geometry optimized, and compared with N3 as a reference dye in literature. It is interesting that the results show band gap is in excellent agreement with literature. It demonstrates that the dyes are suitable for injection by light. In addition, excited state oxidation potential (ESOP) should be close to semiconductor's conduction band. In the case of target dyes, ESOP of the ethyl derivative dye is nearer to TiO₂ conduction band as well as being distributed on the whole of molecule, Figure 1. In conclusion, it may be proposed that the latter improves the efficiency of DSSC as its electron density is higher than the former.

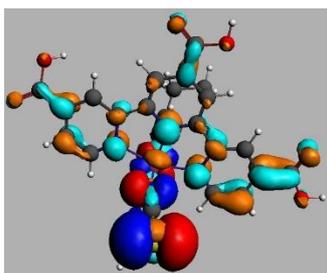


Figure 1. Pictorial representation of HOMO and LUMO of studied dyes determined with DFT at GGA-B3LYP/DZ level of theory.

Keywords: *Cyclometalated Ruthenium (II) Sensitizer; Dye Sensitized Solar Cells*

References:

1. A. Colombo, C. Dragonetti, A. Valore, C. Coluccini, N. Manfredi and A. Abbotto, *Polyhedron.*, 2014, 82, 50.

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