

Effect of Various Auxiliary Acceptors on the Optical and Photovoltaic Properties of a D-A'- π -A Sensitizing Dye. DFT and TD-DFT Study

Manal GOUDJIL¹, Djaffar KHEFFACHE^{1,2}, Maammar REKIS¹

¹Theoretical Chemistry and Computational Photonics Laboratory, Faculty of Chemistry, USTHB, BP 32, Algiers, 16111, Algeria.

²Chemistry Department of the Faculty of Sciences, University M'Hamed Bougara (UMBB), 35000 Boumerdes, Algeria

*Corresponding author

ABSTRACT

The introduction should be simple and easy to understand. Our theoretical study aims to modulate the electronic and photovoltaic properties of a sensitizing dye developed by Marder's team [1] having a D-A'- π -A configuration [1]. To achieve this goal, we examined the effect of various auxiliary acceptors "A" on the spectroscopic and photovoltaic properties of the reference dye [1]. Computational tools based on density functional theory "DFT" and its time dependent variant "TD-DFT" were implemented to determine the optoelectronic and photovoltaic characteristics of the series of sensitizing dyes considered in this study. The optoelectronic and photovoltaic properties including absorption spectra, energy levels (HOMO and LUMO), light harvesting efficiency (LHE), electronic injection driving force (ΔG_{inj}), dye regeneration energy (ΔG_{reg}), and open circuit voltage VOC were determined theoretically to identify the right sensitizer dyes for photovoltaic use.

Keywords: DSSC; Auxiliary acceptor; TD-DFT; UV-visible.

Acknowledgments

Authors can acknowledge any person, or funding agency that has made a significant contribution to the work.

References

- [1] Gao, Y., Li, X., Hu, Y., Fan, Y., Yuan, J., Robertson, N., Hua, J., Marder, S. R. (2016). *Journal of Materials Chemistry A*, 4(33), 12865-12877.

