

Accepted Manuscript

Computational modelling on donor configuration for wide solar energy capture

V. Mohankumar, M. Senthil Pandian, P. Ramasamy

PII: S0167-577X(18)30321-5
DOI: <https://doi.org/10.1016/j.matlet.2018.02.107>
Reference: MLBLUE 23933

To appear in: *Materials Letters*

Received Date: 17 January 2018
Revised Date: 20 February 2018
Accepted Date: 21 February 2018



Please cite this article as: V. Mohankumar, M. Senthil Pandian, P. Ramasamy, Computational modelling on donor configuration for wide solar energy capture, *Materials Letters* (2018), doi: <https://doi.org/10.1016/j.matlet.2018.02.107>

This is a PDF file of an unedited manuscript that has been accepted for publication. As a service to our customers we are providing this early version of the manuscript. The manuscript will undergo copyediting, typesetting, and review of the resulting proof before it is published in its final form. Please note that during the production process errors may be discovered which could affect the content, and all legal disclaimers that apply to the journal pertain.

Computational modelling on donor configuration for wide solar energy capture

V. Mohankumar, M. Senthil Pandian, P. Ramasamy*

SSN Research Centre, SSN College of Engineering, Chennai - 603 110, Tamil Nadu, India

Abstract

The structural and electronic properties of newly designed organic dyes have been examined by means of density functional theory (DFT) and time-dependent density functional theory (TD-DFT). The ground state molecular structures of the designed dyes are fully optimized by DFT calculation in the gas phase. Electronic absorption characteristics are predicted by the TD-DFT calculation. The calculated electronic absorbance spectrum shows red shift if the donor is doubled. The highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO) energy gap were decreased. The electronic and optical properties of the donor modified sensitizers were investigated by DFT and TD-DFT methods for dye sensitized solar cell (DSSC) application.

Keywords: Solar Energy Materials; Simulation and Modelling; HOMO-LUMO; DSSC; Light Harvesting Efficiency; Density Functional Theory.

*Corresponding author

Email: ramasamyp@ssn.edu.in

Fax: +91 44 2747 5166, Mobile: 9283105760

Download English Version:

<https://daneshyari.com/en/article/8013839>

Download Persian Version:

<https://daneshyari.com/article/8013839>

[Daneshyari.com](https://daneshyari.com)