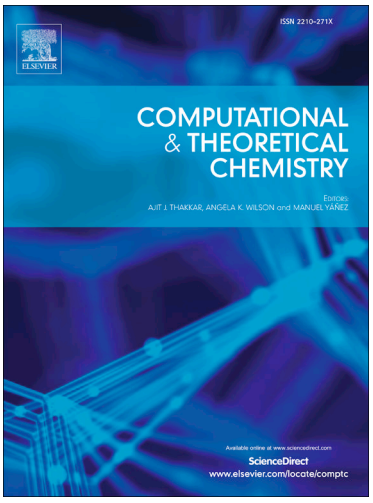

Tuning of some novel triphenylamine-based organic dyes for their potential application in dye-sensitized solar cells: A theoretical study

Rakesh Dutta, Surajit Kalita, Dhruba Jyoti Kalita

PII: S2210-271X(18)30536-X
DOI: https://doi.org/10.1016/j.comptc.2018.09.003
Reference: COMPTC 12341

To appear in: *Computational & Theoretical Chemistry*

Received Date: 15 February 2018
Accepted Date: 4 September 2018

Please cite this article as: R. Dutta, S. Kalita, D.J. Kalita, Tuning of some novel triphenylamine-based organic dyes for their potential application in dye-sensitized solar cells: A theoretical study, *Computational & Theoretical Chemistry* (2018), doi: https://doi.org/10.1016/j.comptc.2018.09.003

Tuning of some novel triphenylamine-based organic dyes for their potential application in dye-sensitized solar cells: A theoretical study

Rakesh Dutta[a], Surajit Kalita[a], Dhruba Jyoti Kalita[a,*]

[a]*Department of Chemistry, Gauhati University, Guwahati-781014, India*

Abstract

Here, we have studied the structural and optoelectronic properties of three series of TPA-based dyes viz. TPA-BBTA, TPA-BTA and TPA-NBT by using density functional theory (DFT). The study is performed by introducing different electron-donating and electron-withdrawing substituents to the TPA-based dyes. Based on the optimized geometries, the relative energy alignment of the frontier molecular orbitals (MO) has been analyzed. The photoelectron spectra and photovoltaic properties have also been investigated with the TDDFT approach. Our study reveals that the dyes substituted with the $-N(CH_3)_2$ and $-OC_2H_5$ groups will show maximum photovoltaic efficiencies along with low Δ_{H-L} values compared to the other substituted dyes. As a result, these dyes will act as potential candidates for fabrication of dye sensitized solar cells (DSSCs).

Keywords: Triphenylamine, Optoelectronic properties, Dye sensitize solar cells, DFT, TDDFT, Light harvesting capacity.

1. INTRODUCTION

Dye sensitized solar cells (DSSCs) have attracted remarkable interest academically and commercially in recent years owing to their low economic and environmental cost for conversion of solar energy into electrical energy with high efficiency [1, 2, 3, 4, 5, 6, 7, 8]. The organic dyes and the mesoporous

*Corresponding author

Email address: dhrubajyoti.kalita@gauhati.ac.in (Dhruba Jyoti Kalita)