

## Accepted Manuscript

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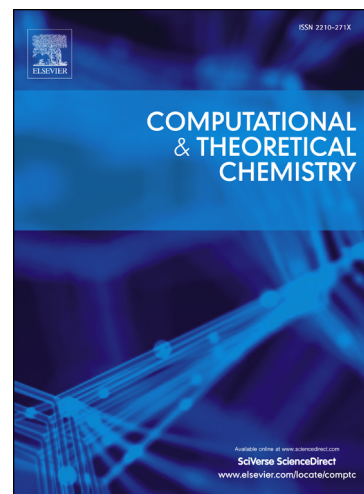
PII: S2210-271X(15)00217-0  
DOI: <http://dx.doi.org/10.1016/j.comptc.2015.05.020>  
Reference: COMPTC 1827

To appear in: *Computational & Theoretical Chemistry*

Received Date: 7 September 2014  
Revised Date: 22 May 2015  
Accepted Date: 24 May 2015

Please cite this article as: A. Mahmood, M.H. Tahir, A. Irfan, A.G. Al-Sehemi, M.S. Al-Assiri, Heterocyclic azo dyes for dye sensitized solar cells: A Quantum chemical study, *Computational & Theoretical Chemistry* (2015), doi: <http://dx.doi.org/10.1016/j.comptc.2015.05.020>

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## Heterocyclic azo dyes for dye sensitized solar cells: A Quantum chemical study

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### Abstract

This study was carried out to design heterocyclic azo dyes for dye sensitized solar cells. Quantum chemical calculations were performed to determine the open-circuit photovoltage ( $V_{OC}$ ), and to quantify the parameters such as the light harvesting efficiency, the electron injection efficiency associated with the short-circuit photocurrent density ( $J_{SC}$ ). All the dyes showed absorbance in visible region (502-521 nm) with high oscillator strength ( $f$ ) (0.473-0.961) and light harvesting efficiency (LHE) (0.663-0.891). After binding to titanium oxide, all dye showed slightly red-shifted absorption (521-527 nm) with improved oscillator strength ( $f$ ) (0.573-0.991) and light harvesting efficiency (LHE) (0.733-0.898). There is high probability that these dyes will show larger  $J_{SC}$  due to high driving force for electron injection. These dyes also showed high  $V_{OC}$  (1.037-1.128 eV). These results indicate that heterocyclic azo dyes will show better light to power conversion efficiency in DSSCs due to high  $J_{SC}$  and  $V_{OC}$ . These theoretical criteria would be useful to design and fast screen other organic dyes, specifically for chemically similar dyes.

**Keywords:** Organic dyes, Dye sensitized solar cells, heterocyclic azo dyes, Density functional theory, efficiency.

### 1. Introduction

Dye sensitized solar cells (DSSCs) have gotten increasing attention as potential alternatives due to their efficient conversion of solar energy to electricity at a low cost [1-4]. In past two decades

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