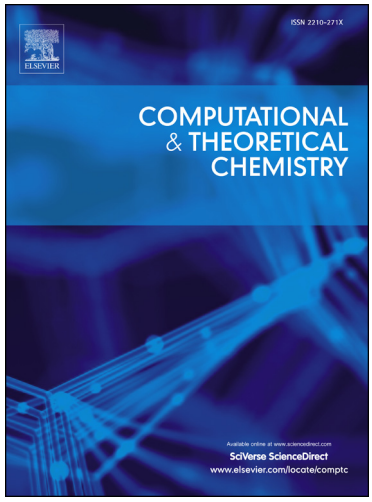

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Heterocyclic azo dyes for dye sensitized solar cells: A Quantum chemical study

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Abstract

Thisstudy 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 showlarger J_{SC} due to high driving force for electron injection. These dyes also showed high V_{OC} (1.037-1.128eV).These results indicate that heterocyclic azo dyes will show better light to power conversion efficiency in DSSCsdue high J_{SC} and V_{OC}.These theoretical criteria would be useful to design and fast screen other organic dyes, specificallyfor chemically fairly 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