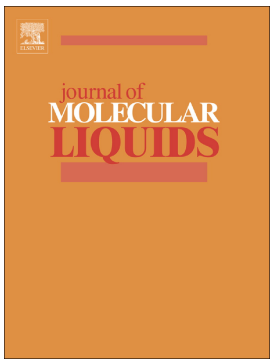

Study of solvent effect on thermodynamic stability and electron efficiency of MZ-341 dye

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Study of solvent effect on thermodynamic stability and electron efficiency of MZ-341 dye

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Abstract

Photo physical and thermodynamic properties of D-π-A organic dye, MZ-341(4-[4-(diphenylamino)phenyl]-7-oxo-7Hbenzimidazo[2,1-a]benzo[de]isoquinoline-11-carboxylic acid), have been investigated for ground and excited states, in order to indicate the different effects of solvent on it as an organic sensitizer in Dye-sensitized Solar Cells (DSSCs). Calculations were performed with Density functional theory approach (DFT) and Time-dependent Density functional theory (TD-DFT) in three different solvents, including water, acetonitrile and carbon tetrachloride. In this work solvation free energy, electron transfer during excitation, Q factor, dipole moment, electronic absorption spectra, recombination (ability of charge injection), life time of excited states, intramolecular bond lengths, light harvesting energy (LHE) by dye and exciton binding energy (EBE) were investigated for ground and excited states. The analysis indicates that amount of intramolecular charge transfer is less in more polar solvents than other solvents. Due to the change in charge distribution during excitation, changes in the value and orientation of the dipole moment and Q factor are generated so it is recognized in more polar solvents; dipole moment and Q factor are higher. Our results showed that solvent also have effect on solvation free energy parameter ($\Delta G_{solvation}$) and consequently the stability of dye so it has been investigated that acetonitrile is the best solvent for use with MZ-341 dye due to the electron and thermodynamic properties.

Key words: Solvation free energy (ΔG), Time-dependent Density functional theory (TD-DFT), Dye-sensitized solar cell (DSSC)

1. Introduction

Third generation of solar cells, are DSSCs[1], which are more efficient than other conventional photovoltaic devices [1] .One of the most important part can improve efficiency of solar cells, is electrode. Aung Ko Ko et al have studied the impact of using carbon nanotubes (CNTs) , graphite and carbon black as working and counter

[1] Dye sensitized solar cells