Theoretical study on C9131 group of dyes for dye-sensitized solar cells - the effect of different solvent and different ligand groups

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INTRODUCTION

The search for efficient, low-cost and metal-free solar cells has aroused a great interest of researchers in dye sensitized solar cells. Since it is the dye that absorbs the light, generates and transports the charges, studies have focused on new conjugated organic dyes.[1,2] In this work, a class of organic dye, namely C9131, with variations in donor and acceptor groups (Figure I), has been theoretically studied and their photophysical properties has been evaluated.

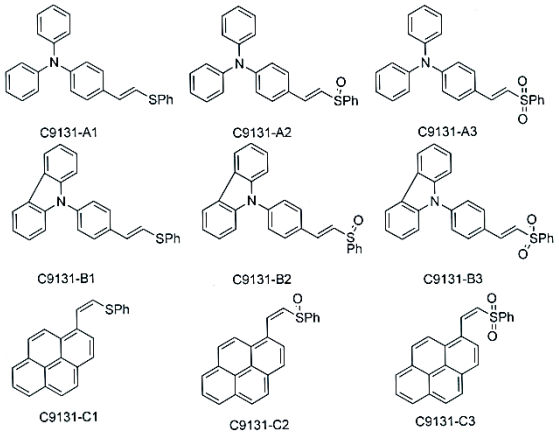

Figure I. Structures of C9131 derivatives.

METHODS

Time-Dependent Density Functional Theory (TD-DFT) was used to study the photophysical behavior of the molecules presented in Figure I, in the ground (S_0) and excited state(S_1). CAM-B3LYP functional was used at cc-pVDZ level for the optimization of S_0 and S_1, and using jun-cc-pVTZ basis set for determination of the wavelength and oscillator strength of the absorption and emission. Compared to experimental data, this level of theory has described correctly these systems. The effect of solvent was evaluated by the PCM model, with acetonitrile, dichloromethane, 1,4-dioxane and ethanol as solvents.

RESULTS AND DISCUSSION

The solvent effect can be seen when comparing the difference between wavelengths of the same molecule. Blueshifts at the absorption and redshifts on the emission have been noted on all of the molecules as the solvent dielectric constant increases. Similar effects can be observed as the donator and acceptor group is changed. Comparing the change of the donator group, redshifts can be observed as the group becomes more rigid. Raising the acceptor group polarity causes redshifts to occur at the wavelength of absorption and blueshifts on the emission. These shifts can be explained as these changes vary the localization of HOMO and LUMO, which influences directly on the molecule dipole moment.

CONCLUSIONS

The positions of HOMO and LUMO and the variation in dipole moment is a strong indication for charge transfer, as it characterizes the conditions for a molecule to obtain the push-pull effect, placing C9131 and its derivatives on the list of possibilities as sensitizers for solar cells.

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