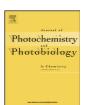


Contents lists available at ScienceDirect

## Journal of Photochemistry and Photobiology A: Chemistry

journal homepage: www.elsevier.com/locate/jphotochem



# Coumarin dye with ethynyl group as $\pi$ -spacer unit for dye sensitized solar cells



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#### ARTICLE INFO

Article history: Received 20 March 2015 Received in revised form 8 May 2015 Accepted 16 May 2015 Available online 21 May 2015

Keywords:
Coumarin dyes
Alkyne bridge
Dye-sensitized solar cells
ElS analysis
Charge recombination
Dye aggregation

#### ABSTRACT

**C1-LEN** coumarin dye, containing an ethynyl conjugated bridge was tested as a new chromophore for dye-sensitized solar cells (DSSCs). Investigation on the relationship of dye structure, optical properties, electrochemical properties and performance of DSSCs is described. The **C1-LEN**-sensitized solar cells showed an overall conversion efficiency of 2.2% ( $J_{SC}$  = 6.11 mA/cm<sup>2</sup>, $V_{OC}$  = 547 mV, FF = 0.66), which corresponds to 68% of N719-based device efficiency, fabricated under similar conditions. Electrochemical impedance spectroscopy (EIS) analysis reveals that charge recombination at the nanocrystalline TiO<sub>2</sub>/ dye/redox electrolyte interface is similar for **C1-LEN** and N719 sensitized solar cells, i.e., charge recombination is not the factor limiting the performance of **C1-LEN** device.

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### 1. Introduction

Organic chromophores for dye sensitized solar cells (DSSC) have drawn the attention of many research groups in the last decade. The wide variety of structures and easy modification of organic dyes provides potential for molecular design, with the introduction of substituents onto the chromophore skeletons allowing control of not only their photophysical and electrochemical properties, but also of their stereochemical structures. Donor– $\pi$ –bridge–Acceptor (D– $\pi$ –A) system is the basic feature for most metal free organic dyes because an efficient electron transfer from donor to acceptor can happen upon photo–excitation of the sensitizer [1,2].

A lot of studies have focused on conjugated bridges such as vinyl, phenyl and thiophenyl, but only few focuses on the influence of a triple bond as a  $\pi$ -spacer unit in the concept of D- $\pi$ -A structure [3–7]. The alkyne  $\pi$ -bridge has been utilized for conjugated donor–acceptor systems because it is a rigid and straight for conducting electrons and at the same time reduces charge recombination [4,5]. Based on reported studies [6], a triple

\* Corresponding author. Tel.: +351 210924600. E-mail address: mjoao.brites@lneg.pt (M.J. Brites). bond geometrically close to the electron donor moiety is more electronegative than a double bond. This weakens the electron-withdrawing ability of electron acceptor because of the opposite dipole moment of triple bond and electron acceptor, resulting in a blue-shift in the absorption spectra. However, changing the position of the triple bond closer to the electron acceptor will strengthen the electron-withdrawing ability of the electron acceptor because of the identical dipole moment of triple bond and electron acceptor, resulting in a red-shift in the absorption spectra.

Recombination of injected electrons in the conduction band (CB) of  ${\rm TiO_2}$  with dye cations and triiodide ( $I_3^-$ ) ions in the electrolyte, leading to lower short-circuit current densities ( $J_{\rm SC}$ ) and open-circuit voltage ( $V_{\rm OC}$ ), depends strongly on the molecular structure of the dye sensitizer and the molecular orientation and arrangement of the dyes on the  ${\rm TiO_2}$  surface. The most effective strategy to retard charge recombination between the injected electrons and the dye cations is the formation of a wide spatial separation between the moieties with positive charge density on the excited dye and the  ${\rm TiO_2}$  surface and it seems that preventing the dyes from lying on the  ${\rm TiO_2}$  surface is a key consideration [1,8,9]. Charge recombination between injected electrons in the conduction band of  ${\rm TiO_2}$  and  ${\rm I_3}^-$  ions in the electrolyte can be