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ORIGINAL PAPER

Nile red based dye D–π–A as a promising material for solar cell applications

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Abstract

A recently reported Nile red (NR) dye conjugated with benzothiadiazole species paves the way for the development of novel organic-based sensitizers used in solar cells whose structures are susceptible to modifications. Thus, six novel NR structures were derived from two previously developed structures in laboratories. In this study, density functional theory (DFT) calculations and time-dependent DFT (TD-DFT) were used to determine the optoelectronic properties of the NR-derived moieties such as absorption spectra. Various linkers were investigated in an attempt to understand the impact of π-linkers on the optoelectronic properties. According to the findings, the presence of furan species led to the planarity of the molecule and a reduction in the band gap between the LUMO and the HOMO. Each one of the aforementioned molecules exhibited great delocalization of π-electrons. Based on the TD-DFT calculations, two furans had the highest value for the red-shift. There is an excellent correlation observed between the computed optoelectronic properties and calculated HOMO-LUMO gaps. In conclusion, the current work aimed at clarifying the impact of π-linkers on the photophysical properties of the NR-derived moieties. Also, the current study provided useful insights into the development of novel species used in optoelectronic devices.

Keywords Nile red · Benzothiadiazole · Optoelectronics · Photophysical properties

Introduction

Recently, fossil fuel reservoirs have been depleted due to the rise in the population and there is thus a desperate need for alternative energy sources. Consequently, researchers have focused on alternative sources of energy (Graetzel et al. 2012; O'Regan and Grätzel 1991; Fan et al. 2021, 2022; Cai et al. 2022; Zhang et al. 2016; Tong et al. 2016; Gao et al. 2021a; Said et al. 2022). Trapping the sun's energy using solar cells has attracted considerable attention since it is highly efficient, it emits no pollutants and it is cost-effective (Nozik and Miller 2010; Brédas et al. 2009; Ji et al. 2017; Wang et al. 2018a, 2021, 2018b; Gong et al. 2022; Yang et al. 2022). The solar cells developed by incorporating metals such as Zn–porphyrin (Karthikeyan and Lee 2013), Co(II/III)tris-bipyridyl (Lu et al. 2013), and Ru(II)polypyridyl

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