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Exploring ethynyl-based chalcones as green semiconductor materials for optical limiting interests

Abstract

The fabrication of molecular electronics from non-toxic functional materials which eventually would potentially able to degrade or being breaking down into safe by-products have attracted much interests in recent years. Hence, in this study, the introduction of mixed highly functional substructures of chalcone (–CO-CH=CH–) and ethynylated (C≡C) as building blocks has shown ideal performance as solution-processed thin film candidatures. Two types of derivatives, (MM-3a) and (MM-3b) repectively, showed a substantial Stokes shifts at 75 nm and 116 nm, in which such emission exhibits an intramolecular charge transfer (ICT) state and fluoresce characteristics. The density functional theory (DFT) simulation shows that MM-3a and MM-3b exhibit low energy gaps of 3.70 eV and 2.81 eV, respectively. TD-DFT computations for molecular electrostatic potential (MEP) and frontier molecular orbitals (FMO) were also used to emphasise the structure–property relationship. A solution-processed thin film with a single layer of ITO/PEDOT:PSS/MM-3a-MM-3b/Au exhibited electroluminescence behaviour with orange and purple emissions when supplied with direct current (DC) voltages. To promote the safer application of the derivatives formed, ethynylated chalcone materials underwent toxicity studies toward Acanthamoeba sp. to determine their suitability as non-toxic molecules prior to the determination as safer materials in optical limiting interests. From the preliminary test, no IC50 value was obtained for both compounds via 3-(4,5-dimethylthiazol-2-yl)-2,5-diphenyl-2H-tetrazolium bromide (MTT) assay analysis and molecular docking analysis between MM-3a and MM-3b, with profilin protein exhibited weak bond interactions and attaining huge interaction distances.

Keywords

Acanthamoeba sp.; FMO; Non-toxic; Push-pull; Spectroscopy