2020-01-01

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Elsevier Inc.

https://doi.org/10.1016/j.jmgm.2019.107457

Lawsone isomers, lawsone ether and bilawsone for dye-sensitized solar cells applications: DFT and UV–Vis studies

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DOI:

https://doi.org/10.1016/j.jmgm.2019.107457

Abstract

Structural and optoelectronic properties of lawsone (L), lawsone ether (LE) and bilawsone (BL) were studied theoretically using the DFT and time-dependent DFT methods with hybrid functional B3LYP5 and 6-311G (2d,p) basis set. For the monomer lawsone molecule, isomerization reaction between two rotational isomers was analyzed based on a thermodynamic approach. The electronic spectra of the dyes molecules in a vacuum and solvents (DMSO and CH2Cl2) were computed. The maximum wavelengths were found at 355–408 nm for the LE and 350–448 nm for BL that indicated bands shift to visible range compared to L (340 nm). The UV–Vis spectra of the L and BL were measured experimentally in DMSO solution. For the BL, a broad and intensive band was observed in a visible region at 452 nm that apparently would favour sensitizing ability of the dye. The optoelectronic properties of the LE and BL showed them as more promising candidates for DSSCs applications compared to the individual lawsone dye.

Keywords

Lawsone isomers, Lawsone ether, Bilawsone, Dye-sensitized solar cells, UV–Vis/vibrational spectra, DFT/TD-DFT