Int. J. New. Chem., 2022, Vol. 9, Issue 1, pp. 36-52.

International Journal of New Chemistry

Published online in http://www.ijnc.ir/

Open Access

Print ISSN: 2645-7236

Online ISSN: 2383-188x

Article Type (Original Research Article)

Design and TDDFT Study of The Novel Structures Similar to BODIPY with Prominent Fluorescence Properties

Ali Bodaghi [1,*] and Hamid Reza Shamlouei [2]

[1] *Department of Chemistry, Tuyserkan Branch, Islamic Azad University, Tuyserkan, Iran*

[2] *Department of Chemistry, Lorestan University, Khorramabad, Iran*

Received: 2019-11-01 *Accepted: 2020-02-15* *Published: 2021-10-28*

ABSTRACT

Functional dye is a new term in the field of dye chemistry which has been specifically designed for high-technology applications such as solar cells, photochromic dyes, liquid crystal, electrophotography, fluorescent sensors and photodynamic therapy. BODIPY and its derivatives as organic fluorophores have optical properties and can be used as potential sensors in various applications for biotechnological, industrial and medical purposes. In this research, a group of a new fluorescent indicators based on BODIPY structure were designed which have been composed from two seven-membered rings including Al or B atoms that has been connected with methine bridge complexed with NH_2 or PH_2 center. The geometries, optical properties and electronic structures of various designed molecules were studied using time-dependent density functional theory (TDDFT). The results of the calculations showed that the new designed structures are stable and highly optically active with considerable quantum yield (Φ) absorption and emission as if is promising candidates for hi-tech different applications.

Keywords: BODIPY; Computational; Conjugated System**;** Fluorescence; Functional dyes; Optical Properties; TDDFT

***Corresponding Author: Tel.: +988134921629 and +989183535131; E-mail: alibodaghi@ymail.com**