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Computational Study on Optoelectronically Important Novel 1,3,4-Oxadiazole Chromophore

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Abstract

In this work, we report on computational studies of a novel optoelectronically important chromophore 2-(4-((E)-2-(5-((E)-4-(5-(4-tert-butylphenyl)-1, 3, 4-oxadiazol-2-yl) styryl) thiophen-2-yl) vinyl)-5-(4-tert-butylphenyl) 1, 3, 4-oxadiazole (3TPO). Density functional theory (DFT) and time dependant density functional theory (TD-DFT) computations were carried out to demonstrate various intramolecular interactions that cause the stabilization of the compound leading to its optoelectronic applications. The solvation effects were tested using integral equation formalism for the polarizable continuum model (IEF-PCM) model. The highest occupied molecular orbital energy (HOMO), lowest unoccupied molecular orbital energy (LUMO), the energy gap, ground and excited state dipole moments, chemical hardness (η), softness (σ), electronegativity (χ) and chemical potential (μ_c) were estimated with the help of frontier molecular orbitals. It is observed that the experimental results agree well with the computed values.

Keywords: DFT and TDDFT, FRET, Oxadiazole, Salvatochromism, ZnSe/ZnS QDs.

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