Revising the formation and electronic properties in flavylium derivatives. A theoretical tandem towards optimized DSSCs

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Abstract
We attempted to describe a set of flavylium derivative molecules through quantum density functional methods, which may lead to a better understanding of the physicochemical properties of these organic systems. Consequently, such empirical and hypothetical flavylium compounds have a suitable route to obtain their molecular structures. The role of optical transitions in the benzopyrylium derivatives is understood as an electronic communication between the benzopyrylium (A,B-ring) and substituent (C-ring) moieties, and the obtained results are promising for the novel design of new solar cells based on their optical properties. In this framework, optical properties were analyzed in their ground and excited states using time-dependent density-functional theory (TDDFT) methodologies. In this sense, the wavelength of maximum absorbance (λ_{max}) red shift that is observed could contribute towards enhanced applications. Furthermore, the emission pathway obtained was in agreement with the experimental results. Our results provide interesting insights for new experimental assemblies of heterocyclic flavylium compounds and their performance could contribute to optimized dye sensitized solar cells (DSSCs). Furthermore, the main bonding characteristics involved in the formation of these interesting compounds were investigated by taking advantage of the energy decomposition analysis-natural orbital for chemical valence (EDA-NOCV), thus enabling the elucidation of the energy components and their chemical nature through a detailed bonding picture.

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