Optical and electronic properties of benzopyrylium derivatives. Theoretical-experimental synergy towards novel DSSCs devices

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Here, we discuss the formation of several heterocyclic benzopyrylium compounds via joint experimental-theoretical efforts, in order to obtaining a better understanding of the diverse properties of these interesting organic species. Our results suggest these benzopyrylium dyes as interesting sensitizers in the novel design of new solar cells from the basis of their optical properties and pH-dependent characteristics. The role of aromatic stability of the pyrylium compounds in the obtained properties is discussed in terms of both NBO and analysis of the induced magnetic field toward the isotropic respond. Furthermore, optical properties were analyzed in the framework of TD-DFT methodologies. Noteworthy changes in red-shift and absorptions ?max are observed that contribute toward the interesting DSSCs applications. Additionally, the emission profile of 2a derivative was obtained in agreement to both theoretically and experimental strategy. We expect that our results can be informative for further development of heterocyclic benzopyrylium compounds and their application in DSSCs devices.