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Abstract

The photophysical properties and photochemistry reactions of 2-(2-Hydroxy-phenyl)-4(3H)-quinazolinone (HPQ) system in different solutions are studied by using density functional theory (DFT) and time-dependent density functional theory (TDDFT) methods. Our theoretical investigation explores that an ultrafast barrier-free excited state intramolecular proton transfer (ESIPT) process occurs and the configuration twisting is found in the electronic excited state. In the polar protic methanol solution, the hydrogen-bonded complex composed by HPQ and