Title : Photophysical Properties and Relief of Excited-State Antiaromaticity upon Proton Transfer of 2-(2'-Hydroxyphenyl)benzothiazole and its Derivatives

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ABSTRACT

Fluorophores undergoing excited-state intramolecular proton transfer are known to exhibit notably redshifted emission wavelength with respect to their absorption wavelength. Consequently, they suffer less from self-absorption and are of interest in applications requiring photon down-conversion, such as fluorescent probes, sensors, and organic light-emitting diodes. In addition, previous studies indicated that excited-state intramolecular proton transfer is driven by excited-state aromatization, which manifests as relief of excited-state antiaromaticity for Hückel-aromatic fluorophores. In this work, effects on photophysical properties, exothermicity upon excited-state intramolecular proton transfer, and excited-state antiaromaticity arising from strategic mono-substitutions of 2-(2'-hydroxyphenyl)benzothiazole were theoretically investigated. In addition, links between exothermicity and relief of excited-state antiaromaticity, were highlighted. The author hopes this study will provide insights towards data generation and screening for machine-learning-based approaches on theoretical studies of excited-state intramolecular proton transfer-based fluorophores.

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