## Influence on photophysical properties of (de)protonation of phenol-substituted diazine chromophores: experimental and theoretical studies

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In recent years, lighting has become more and more energy consuming, now reaching 20% of the global electricity consumption. Thus, there is need to properly design new environment friendly lighting devices and organic light emitting devices (OLEDs), in particular White OLEDs (WOLEDs), are more relevant than ever.<sup>1</sup> The major issue is that obtaining white light is not an easy task, and is in most cases achieved by using multilayer devices or a combination of different emissive molecules.<sup>1,2</sup> In this contribution, we present an innovative way of obtaining white light emission by modulating the protonation<sup>3,4</sup> and deprotonation of organic fluorophores.

To this end, a series of 8 push-pull phenol substituted diazine derivatives has been designed by varying the nature of the acceptor diazinic heterocycle (pyrimidine/pyrazine) to be protonated and of the linker moieties (thienylene, vinylene, thienylenevinylene, vinylphenylene). The photophysical investigation of this series of compounds in solution showed a systematic bathochromic shift of the emission compared to the neutral form, not only upon the protonation, but also after deprotonation. Extensive Density Functional Theory (DFT) and TD-DFT calculations were performed to rationalize this behavior and understand the impact of (de)protonation on the different optical transitions characteristic of this family of fluorophores. Such computations showed that the (de)protonation impacts not only the energies of the vertical transitions, but also the nature of these transitions, with a significant increase in the Intramolecular Charge Transfer (ICT) character of the (de)excitations. Furthermore, playing with the nature of the diazinic moiety and the linker in the push-pull skeleton allows to fine tune the emission wavelength of the two forms and reach a complementary emission in solution.

To the best of our knowledge, modulation of the emission by deprotonation has not yet been reported as an alternative strategy for obtaining white light emission. Our experimental and theoretical results on the phenol-substituted diazinic chromophores demonstrate that this approach proves successful, at least in solution. Thus, it opens a new route for the design of efficient WOLEDs and shall prompt further investigations up to device fabrication.

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