Master's Thesis

is available in the Trimmel Group:

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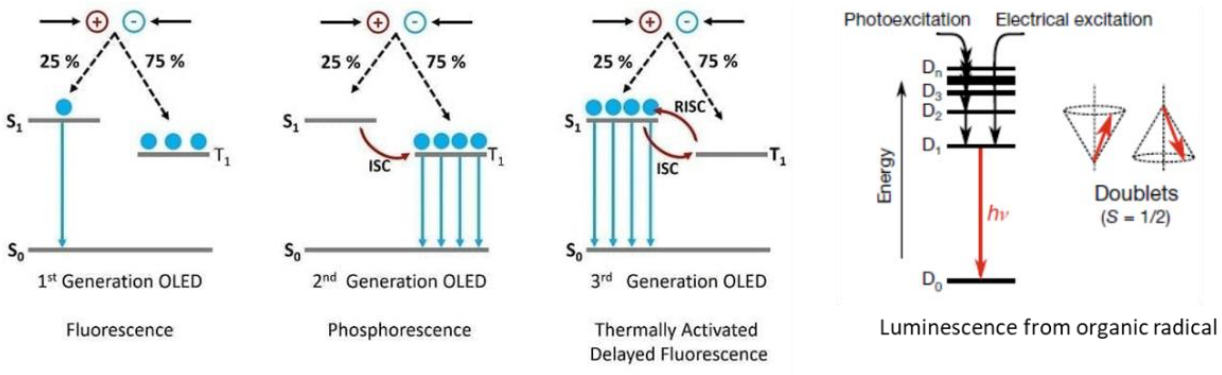
Synthesis of luminescent organic radicals for OLEDs

Context: Open-shell organic radicals are attractive in material science and various areas due to their fundamental structures and unique physicochemical properties. However, the intrinsic instability arising from their incompletely satisfied valency hinders further development. In these decades, in-depth studies on structure-stability relationships proved the possibility to prepare persistent and even stable organic radicals, which have been successfully applied in various functional devices.



Objective: Until now, there are a very limited number of examples of organic luminescent radicals, like perchlorotriphenylmethyl (PTM), tris(2,4,6-trichlorophenyl) methyl (TTM), and dithiadiazolyl (DTDA) radicals.[1] These radicals show emission mainly in the red to NIR region (600-750 nm) with poor to moderate quantum yield in the solid state with broad emission range, resulting OLEDs with low color purity. A stable non-luminescent radical (TAntM) was earlier developed by Kubo et al.[2] Inspired by this result, we envision the synthesis of highly emissive and stable radicals based on the TAntM core. Firstly, we will introduce multiple fluorine/chlorine substituents in the core to make it more electron-deficient. This change in the electronic configuration of the radical will lead to a SOMO-HOMO inversion, i.e., SOMO lies below the HOMO; resulting in a non-Aufbau radical. Secondly, we will incorporate tetraphenylethylene and pyrene as substituents in order to confer aggregation-induced emission (AIE) in the solid state. These bulky groups also will provide a certain degree of shielding of the radical from the outside environment and so increase stability. Later, we will perform preliminary spectroscopic studies (UV-Vis and Fluorescence) of the molecules both in the solution and solid state.

Requirements: Bachelor's in Chemistry (multi-step organic synthesis experience)
Start of the work: As soon as possible

1. Z.X.Chen et al., *Chem* 2021, 7, 288
2. T. Kubo, et al., *J. Am. Chem. Soc. 2011,* 133, 14240