

Stable organic radicals capable of thermally activated delayed fluorescence – multi-purpose materials for optoelectronic applications

Organic radicals are a specific class of chemical compounds that contain at least one unpaired electron. They are extremely desirable materials due to their unique spectroscopic properties, especially the absorption and emission of radiation in the ultraviolet, visible and infrared (UV-Vis-NIR) ranges. However, the presence of an unpaired electron raises stability problems and increases the reactivity of such compounds, which significantly limits their use in the design of modern optoelectronic devices, such as OLEDs or organic photovoltaic cells (OSCs). On the other hand, it is the unpaired electron that is responsible for good conductivity and creates the possibility of creating the first quantum computers and molecular magnets. Therefore, an extremely important challenge for modern materials chemistry is to develop a strategy for designing stable organic radicals.

Luminescent organic compounds are ubiquitous in both natural and everyday settings, showcasing a fascinating phenomenon wherein radiation is emitted due to the release of excess energy previously absorbed. This emission occurs through various mechanisms. The most prevalent form is classic fluorescence (PF - prompt fluorescence). However, limitations stemming from the statistical distribution of electron spin during excitation have necessitated exploration into alternative mechanisms of radiation emission. One such mechanism is thermally activated delayed fluorescence (TADF). This phenomenon employs the ability to convert excited state electrons – excitons – between two multiplet states – singlet and triplet, thus paving the way to 100% emission efficiency. In order for a molecule to exhibit TADF, it must not be planar, which is related to the location of the electron density of the HOMO and LUMO levels in different places of the molecule. This implies the large size of such structures and makes it possible to use them to control interactions in the solid phase.

The proposed solution assumes the creation of a hybrid molecular backbone that combines a PF/TADF-exhibiting entity with a radical. The first of the subunits will ensure the stabilization of the radical center and enable the fine-tuning of the optical response. In turn, the inclusion of a radical in the system will significantly increase the efficiency of fluorescence and conductivity. The obtained set of hybrid compounds of the PF/TADF-radical type will allow to determine how individual structural modifications of both subunits affect changes in the observed properties and reactivity. For this purpose, standard analytical methods will be used, such as NMR/EPR spectroscopy, UV-Vis-NIR spectroscopy or fluorometry. Based on these initial studies in solutions, the most promising radical materials will be selected, which will then be subjected to more specialized measurements using solid-state compounds. Such experiments mainly include time-resolved emission spectroscopy, transmission spectroscopy and X-ray measurements. In the last stage, the tested radical systems will be used to build prototype optoelectronic devices selected on the basis of spectroscopic characteristics.

The proposed concept will allow to obtain multifunctional materials for use in the most modern optoelectronic devices. The development of this field is closely related to the search for alternative solutions for light sources (e.g. OLED), as well as more reasonable management of energy resources, with particular emphasis on renewable energy sources (e.g. solar energy). That is why it is so important to search for new, unconventional solutions that will improve both the comfort of life and care for the environment in the long term.