Humankind activity changes our planet, and rates of these changes increase in geometric progression. There is a good chance that in a few decades due to the dominating philosophy of a "throw-away society" together with fast development of various technologies, growing number of "one-season" electronic devices, tons of used batteries etc., the problem of waste utilization will become of the utmost importance. Highly expensive and technologically complex utilization procedures are usually due to the use of inorganic materials, mainly those containing toxic heavy metals. On the other hand, organic materials offer lots of benefits, most importantly low cost of production and utilization, broad availability, low toxicity and biocompatibility. The sooner inorganic heavy-metal materials will be replaced by the organic ones the better.

The organic light emitting diode (OLED) technology represents one of the most fascinating and highly promising example of application of organic materials in electronics. In spite of the name "organic", the key elements of commercially available OLEDs still contain an emitter with heavy metal. This project will focus on the investigations of thermally activated delayed fluorescence (TADF) phenomenon, which application in OLEDs is believed to be the most promising way to replace heavy-metal emitters by the all-organic ones. In OLEDs, TADF enables efficient transformation of "dark" triplet excitons to the singlet ones, which produce light. Currently, there are two fundamental problems which impede further development of TADF OLEDs: low stability and efficiency of deep-blue diodes and lack of universal model describing key parameters of organic TADF emitters. These problems are tightly connected: without clear understanding of the phenomenon, it is hard to find the best solution for its application.

Despite high world-wide scientific interest in TADF, the photophysical models developed before describe only selected parameter(s) of limited emitters in very specific conditions. Still, current molecular design rules strongly rely on such models. They all follow the selection rule known for almost a hundred years, stating that transitions between the electronic states with the same nature but different spin are forbidden (spin-flip transitions). In reality, this means that such transitions take milliseconds or even seconds, which is too slow for OLED applications.

Thorough analysis of literature reports and our preliminary investigations of one of the most popular TADF emitter evidence that previous models are not applicable. This compound not only breaks the spin selection rule, but also undergoes the above mentioned forbidden spin-flip transitions around million times faster than expected! This conclusion is quite surprising, and we need to check if it can be generalized for other emitters. To improve the "all-organic" OLED technology and make a step towards the solution of deep-blue-OLED problem, we should first understand if other state-of-the-art blue TADF emitters also break the spin selection rule. By means of joined experimental and theoretical investigations in various conditions and temperatures the first aim of this project will be realized: to develop a universal model, describing key parameters of the best TADF emitters and further provide suggestions on how to create an ideal TADF emitter.

However, forbidden or not, the advantageous spin-flip transitions should be accelerated in TADF emitters, especially in the blue ones. For this reason, the next aim of this project is to investigate the effect of cheap and abundant non-toxic heavy atoms on the deep-blue organic TADF emitters. Realization of the second aim is a search for the golden mean between organic TADF materials and heavy-metal ones to solve the problem of deep-blue OLEDs. To do so, cheap and abundant heavy halogens and chalcogens will be introduced into the best TADF emitters. The investigations of such hybrid emitters should answer the following questions: how the presence of heavy atoms influences the advantageous spin-flip transitions? Which elements and how can be used for improvement of blue emitters? Which negative factors accompany introduction of heavy atoms?

Realization of both aims of the project is tightly connected. The universal TADF model will enable better understanding of the investigated processes, while its application to the emitters bearing cheap and abundant non-toxic heavy atoms will help to verify basic conclusions of the model and hopefully find a promising route for improvement of OLED technology.

The project plan includes investigations using modern methods of organic chemistry, steady-state and time-resolved electronic spectroscopies, and quantum-chemical calculations.