

Abstract

With the development of technology, electronic devices have become relevant element in activity of modern human, accompanying him in most areas of his life. Commonness of mobile phones, tablets and computers is the best proof of this. The operation of many of them is based on use of materials, that are able to emission of light when external energy is applied, which take place for example, in displays. The macroscopic features of such light-emitting devices, such as color, brightness or stability, depend on the type of chemical compounds (emitters) used and their photophysical properties at the molecular level. Thanks to the knowledge gathered so far, the currently designed emitters show very good parameters, and the lifetime of devices made of such compounds is not a limitation in their functionality.

The problem is that the key components of all commonly available optoelectronic devices are made of inorganic or hybrid compounds, containing in their structure heavy metals such as iridium, platinum, rare earths, etc. The limited access of these elements, depending on geographical, political and economic factors, is one of the key reasons why the production cost of these devices is very high. What is more, the toxicity of transition metals disqualifies such materials from some application and complicates the methods of their waste management. With respect to this, investments devoted to implementation of less harmful and more accessible materials are one of the current leading scientific directions and a well known research and development priority. Unfortunately, fabrication of friendly organic materials technology has not reached the sufficient level required by the industry. The low efficiency and stability of pure organic compounds remain currently the main problems, because of which replacement of the key elements with their organic analogs have failed so far. Especially, it is true for light-emitting materials, which are the subject of this dissertation.

The doctoral thesis is devoted to photophysical and photochemical investigations of selected organic light-emitting compounds, with high applicative potential in optoelectronic devices. The fundamental aim of this work is to understand the mechanisms of photoinduced processes occurring in excited state, which determine emission efficiency and photostability of emitters.

First part of this work is based on description of performed investigations of 2'-hydroxychalcones derivatives, which show excited-state intramolecular proton transfer (ESIPT) and aggregation induced emission (AIE). Despite showing attractive photophysical features, these compounds are extremely unstable and can easily undergo photoinduced processes, leading to formation of molecules without beneficial emissive properties. Since stability is a crucial parameter determining the possibility of using compounds in optoelectronics, described research here provides detailed knowledge about the mechanism of photodegradation taking into account individual stages and ways to control it.

By using conventional experimental methodology and advanced theoretical tools, description of six-stage phototransformation has been made, including proton transfer, s-cis – s-trans isomerization and cyclization processes. The collected data and undertaken attempts unambiguously prove, that photodegradation can be stopped at its early stage, therefore it could facilitate the implementation of this (and similar) compounds in devices in the near future.

Second part of dissertation concerns organic emitters with thermally activated delayed fluorescence (TADF), being currently relatively young, but dynamically developed class of objects, mainly devoted to application in OLED industry. Presented research here is focused on solving problem in TADF compounds, related to slow reverse intersystem crossing (rISC). At the moment, red and blue emitters are strongly demanded, thus they are the subject of presented research. More precisely, the concept of improving the photophysical properties of blue and red TADF emitters based on introducing well accessible heavy atoms (HA) into their structure was experimentally verified. It assumes that incorporation of HA can enhance spin-orbit coupling (SOC) and will accelerate conversion of triplet excited states into singlet ones, from which efficient electroluminescence can occur. Based on performed photophysical measurements and thanks to originally developed analysis methodology it was evidenced that so called heavy-atom effect in some specific cases can have a positive impact on luminescent parameters of modified compounds. By using detailed theoretical calculations correlated with experimental observations, the mechanism of TADF was revealed with identification of most important factors that affects its efficiency.