Chemistry in the World of Physics. How to Unify the Knowledge and Get Efficient OLEDs.

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The discovery of electroluminescence of organic molecules is one of the ground-breaking and promising breakthroughs in the last century. Owing to it and to the progress in the field of organic electronics over the last half-century, nowadays, we are surrounded by organic light-emitting diodes (OLEDs) products. In addition to lightness, flexibility, and low production cost, the major advantage of using organic emitters for OLEDs is the possibility to tailor their properties by designing and modifying their molecular structures. From the viewpoint of emission mechanisms, there are two types of emitters: fluorescence and phosphorescence emitters. Fluorescence emitters are the first generation of electroluminescence emitters for OLEDs, but they are fatally restricted by the upper limit of internal quantum efficiency (IQE) of 25%, due to spin-statistics. The second-generation emitter, phosphorescence emitters, are more efficient and for this reason, are commonly used in OLED-based displays. However, nothing is perfect: phosphorescence emitters that are currently used in organic electronics are organometallic complexes comprising of very expensive and rare heavy metals such as Ir and Pt. To overcome this problem, the search for all-organic TADF (Thermally Activated Delayed Fluorescence) emitters is conducted.

Herein I present a new approach to the design of metal-free organic thermally activated delayed fluorescence emitters for organic light-emitting diodes. I present different aspects of modification of molecule structure in order to increase efficiency. Even by simple electrochemical modification, it's possible to change the energy levels in order to decrease the singlet-triplet energy gap. The subtle tunning of the energy difference between the singlet and triplet excited states allows for tailored emission properties of thermally activated delayed fluorescence and its efficiency. Finally, depending on the molecule and its host environment interaction, we may change the emission and increase efficiency. All presented steps will give an insight into broad possibilities of tailoring OLED emitters.