

## **Hund's Rule Violating Molecules as Precursors of New Optoelectronic Materials**

Organic light emitting diodes (OLEDs) have become of considerable interest for both academic research and industry due to their unprecedented advances in display and lighting technology. OLED displays possess several advantages over the existing liquid crystalline displays (LCDs), such as improved picture quality, low weight, fast response time, wide viewing angles, thinness, and a wide range of emission colors due to structural variability of organic materials. The possibility of fabricating OLEDs on flexible substrates is a strong advantage in several applications of displays and lighting products. The main weakness of OLEDs is the generally low luminescence efficiency.

The reason of this is related to the so-called Hund's Rule according to which in organic molecules the (non-luminescent) triplet excited state is energetically located below the (luminescent) singlet excited state. Because according to spin statistics, the recombination of charge carriers generated by voltage in optoelectronic materials produces singlet and triplet excitons in the ratio 1:3, the luminescence quantum yield of such materials cannot nominally exceed 25%. The ideal organic molecule for construction of OLED should possess highly emissive singlet state lying below the triplet state. Unfortunately, until recently, no stable Hund's Rule violating organic molecule was known. The first stable organic molecules with such property discovered by the applicant and coworkers in year 2019 breaks a ground for creation of a new generation of organic optoelectronic materials and allows in principle to achieve 100% yield of electron to photon conversion in OLEDs.

The primary research goal of the current project is to perform extensive computational explorations of the novel class of molecular systems exhibiting the singlet-triplet inversion in order to understand fundamental mechanisms responsible for the phenomenon and to determine electronic and nuclear factors that govern the phenomenon. Provided that such molecules with appreciable fluorescence rates can be found, they will become the next (forth) generation of OLED materials.