Organic light-emitting diode (OLED) technology is widely known from everyday life and used electronic devices such as TVs, computers, smartphones. It is a valuable technology that significantly affects the quality of electronic devices usage through image quality, weight, and efficiency. It is based on organic compounds that have the ability to emit light. There are many of such compounds, and they are divided depending on the emission mechanism. The oldest groups of OLEDs are the first- and second-generation emitters, based on the emission mechanism via fluorescence or phosphorescence - both processes are the result of prior exposure of the substance to light or another type of radiation. In later, more advanced technologies, electrons excited to the triplet state - i.e. the dark state from which light emission is not possible - are excited, for example thermally, as in the case of third generation emitters, to higher singlet states - i.e. bright states from which light emission occurs. Dopants are also used - this is the fourth generation - which increase the efficiency of the mechanisms used on third generation molecules. Nevertheless, it is the low efficiency that is the biggest problem of all four generations of OLEDs.

The source of this low efficiency is the configuration of states resulting from Hund's principle. It says that the first excited state in the system is a triplet. Majority of excitons just before relaxation to the ground state, as a result of relaxation from higher states, remain in the first excited state, the dark state, the emission of which cannot occur during relaxation to the ground state. A certain part of excitons relaxates to the ground state from higher bright states, but this is a relatively small part - in the most favorable case, 25% of all excitons. This means that at least 75% of the excitons remain unavailable for emission.

However, there are systems that violate Hund's rule - this is the fifth generation of light-emitting systems, called INVEST (inverted singlet-triplet gap) molecules. In their case, the first excited state is the singlet state, which is a bright state. Thanks to this inversion, the situation changes completely. Theoretically, it is possible that up to 100% of the excitons will be available for the emission process. No previous generation of OLEDs is able to provide similar results, which is why INVEST systems are currently the most promising development perspective in this field.

These systems and the research conducted on them still have some problems. This is a new topic, still being researched, because only in the last few years has the existence of this type of molecules been confirmed. For this reason, it is still unclear how to build this type of systems to ensure state inversion. However, this problem can be solved by proposing a model for pre-screening, i.e. quick and cheap calculation of ST gaps in large sets of systems. This is one of the problems addressed in the project - creating a model based on the time-dependent density functional theory (TD-DFT) and a correction calculated from perturbation theory, which will allow for quick and cheap calculations of ST gaps for a large number of systems with the accuracy of reference methods such as coupled-cluster.

However, this is not the only aspect that seems important from the point of view of OLED technology. Oscillator strength is a quantity that determines the intensity of emissions from a given state. Unfortunately, INVEST systems have relatively small oscillator strengths, which makes them additionally difficult to examine. Additionally, research in this area is practically not conducted. Therefore, the second goal of the project will be to propose a theoretical model that will allow obtaining accurate oscillator strengths for INVEST systems.

These types of models may constitute a milestone in the development of OLED technology, providing easier access to structures that potentially meet the conditions suitable for the emitter. Thanks to accurate, fast computational methods, the costs associated with the synthesis and testing of INVEST compounds can also be significantly reduced by the ability to easily isolate appropriate candidates. Moreover, the model proposed in the project could be incorporated in machine learning for the purpose of predicting or even designing new molecules. All that makes the proposed model a very promising tool also in the area of material development, not only in theoretical chemistry itself.