Modular, cyclazine-based polyclic aromatic hydrocarbons (PAHs): robust materials for optoelectronic applications

In an era of dynamic technological development, sustainable energy management becomes a global problem in a way that systematically strives to reduce its consumption. Bearing in mind that the energy consumption of commonly used photovoltaic devices (smartphones, tablets, displays) constitutes more than 20% of total electricity consumption, it is necessary to develop new technologies and search for novel, less energy intensive photoactive materials. Designing and manufacturing of such systems can allow for more efficient energy storage and processing.

Electroluminescence is a process that allows the conversion of electric energy into light with a specific color and intensity. The practical use of photoluminescence and electroluminescence processes involves organic materials that exhibit as strong emission properties as light emitting diodes. These materials can produce a considerably high contrast and high quality images, which are required in modern displays. Commercial emitters are based on photosensitive heavy metal complexes (Iridium, Platinum). Application of their rarely available salts not only increases production costs, but also has negative environmental effects relating to pollution during extraction and their disposal. These two unfavorable parameters, from the viewpoint of further dynamic technological development of technology, have given a boost towards the search for new, photosensitive thermo- and photostable organic structures, which may play the role of photoactive layers in a wide range of optoelectronic devices.

The aim of the project is to understand the relationship between the structure of the proposed nanoarchitectures and their optoelectronic properties, which can effectively solve the above problems. The tool to solve this problem is molecular engineering in the form of precisely controlled advanced organic chemistry. It will be used to create a collection of new "tailor-made" nanographene architectures, comprising not only carbon and nitrogen atoms but also, bringing absolute novelty to the project, precisely located boron atoms (both inside the molecule and on its periphery). In order to achieve the intended goal, it is planned to use chemical building blocks (specific "Lego bricks") in the form of pyrrolomonoimide derivatives as well as their extended analogues, cyclazines. These allow the creation of precisely fused aromatic rings (increasing resistance to thermal stimuli) with a strictly defined size and shape, as well as matched topology of heteroatoms, e.g. nitrogen, which leads to the formation of PAHs (polycyclic aromatic hydrocarbons) that are expected to exhibit the desired thermo and photostability. In the next stage, incorporation of boron atoms would be carried out, which should enable systematic determination of the role of both *so-called* dopants (nitrogen and boron atoms) and their effect on the unique photophysical properties of designed systems. The use of molecular engineering in the proposed project strategy can tangibly affect the absorption and emission characteristics of the architectures discussed here and result in elongation of their lifetime in the excited state. Both of these requirements should allow the practical implementation of designed molecules as elements of a new class of high performance emitters with high thermal stability.

The materials discussed here, constructed solely on the organic structure of coronenes, can be employed in modern OLED materials. There is not only a real chance to increase the quality and contrast of the displayed image, but to eliminate emitters based on toxic heavy metal complexes currently utilized. These nano-architectures can also contribute to the further effective miniaturization of new and highly efficient devices that most often have sizes on the nanometer scale.