Photosensitive diodes have been the subject of intensive work in scientific and industrial research centers for many years. Devices built using light-sensitive diodes, such as photodiodes and photovoltaic cells, are used as light intensity sensors in signal receivers in fiber optic lines and in opto-isolators, and as photovoltaic cells for converting solar energy into electricity, respectively. In addition, devices built from organic materials can be flexible, opening up the prospect of new large-scale applications.

Organic photodiodes and solar cells contain a photosensitive layer made of two materials mixed together, with electrons (n-type electron-acceptor semiconductor) easily moving in one and holes (p-type electron-donor semiconductor) in the other. These semiconductors mixed together form a volumetric donor-acceptor heterojunction with a very extensive contact area. The operation of the solar cell is based on the absorption of light quanta by the semiconductors, which causes electron excitation of the molecules. Excitons are transferred to neighboring molecules until they decay into free holes and electrons near the interface of acceptor and donor materials. The resulting charge carriers move toward the electrodes, with electrons moving in an n-type semiconductor and holes in a p-type semiconductor. The accumulated holes near the anode and electrons near the cathode produce a potential difference called the open circuit voltage of the photovoltaic cell. When a receiver is connected to the cell, the moving holes and electrons in the cell induce current flow in the receiver. If the electrodes of the cell are short-circuited to each other, we have a photodiode, in which the light-induced current flow is proportional to the power of the light.

The high efficiency of light-to-current conversion in organic photodiodes and photovoltaic cells depends primarily on: the type of materials used to produce thin films, which should exhibit good hole and electron conductivity; the exciton dissociation efficiency at the donor-acceptor interface; and the morphology of the thin films produced. A strong photovoltaic effect in the bulk heterojunction will occur when the following requirements are met: 1) the phases of the donor and acceptor material will form a network of interpenetrating molecular structures, with the acceptor having the best possible contact with the cathode and the donor with the anode, 2) the domains of the heterojunction structure, filled with donor or acceptor material, must be small enough so that the excitons moving chaotically have a chance to reach the junction, 3) the domains of the donor and acceptor materials must not be separated from each other, because the transport of holes and electrons toward the electrodes would be greatly impeded, which would significantly reduce the intensity of the light-induced current.

In order to obtain the optimal molecular structure of a volumetric heterojunction layer, a lot of time-consuming experimental research must be carried out. Computer simulations can also be carried out, which are a suitable tool for studying such issues. Properly selected and properly applied computational methods make it possible to find the optimal parameters of the process of forming macromolecular layers of semiconductor mixtures and to relate the morphology of such materials to their properties concerning the transfer of excitons and electric charges. The combination of experimental and simulation methods saves the duration of research and significantly reduces its cost.

The project plans to produce organic photodiodes and photovoltaic cells with bulk heterojunctions. Using a number of experimental methods, the morphology of layers and electro-optical properties of cells, as well as conductivity and photogeneration, capture and recombination of charge carriers will be examined. Comprehensive simulations are also planned, taking into account all stages of the production and operation of heterojunction layers, from generating the molecular structure of the interpenetrating donor and acceptor materials, to full analysis of the photovoltaic effect, taking into account phenomena occurring in real devices, such as the absorption of light quanta and the formation of excitons, diffusion and decay of excitons near the p-n junction into free electrons and holes, trapping and recombination of charge carriers. Simulations will be carried out using modern and efficient methods of molecular dynamics and quantum computing.