ABSTRACT

In recent years, there has been tremendous progress in the synthesis of organic electroactive compounds, which has contributed to their commercial applications in various optoelectronic devices, such as light-emitting diodes, field-effect transistors, or dye-sensitized and bulk-heterojunction solar cells. However, intensive work is still being carried out to obtain organic materials with the most favorable properties and enable the least complicated industrial production of optoelectronic devices at low costs.

This doctoral dissertation is a part of the research field and the development of solution-processable and stable compounds that can transport positive charges. The work discusses the studies' results of four groups compounds' selected properties, namely: (i) azomethinoimides, (ii) azomethines, (iii) oxetanes with carbazole structures, and (iv) compounds containing fluorene or carbazole as a core.

The work aimed to analyze their thermal, absorption properties in the UV-Vis range, photoluminescence, and electrochemical properties, as well as to determine the ability to transport positive charges, which was verified in inorganic-organic, i.e. perovskite solar cells. Thermal stability and temperature changes during phase transformations of the tested compounds were analyzed based on TGA and DSC thermograms. The photophysical properties were examined based on measurements of the solution's absorption, emission, quantum yield, and fluorescence lifetimes, considering the influence of the solvent polarity and concentration, as well as in a solid form. The energies of the HOMO and LUMO boundary orbitals and energy band gaps were estimated from the oxidation and reduction potentials obtained from electrochemical measurements carried out using cyclic voltammetry. The compounds were used as organic layer in cells with the FTO/b-TiO₂/m-TiO₂/MAPbI₃/compound/Au structure, whose photovoltaic parameters (short-circuit current, open circuit voltage, fill factor, and efficiency) were determined from the current-voltage characteristics. Photovoltaic (PV) parameters were analyzed in relation to the parameters of the produced reference cells without an organic layer. Attempts were also made to explain the impact of the used compounds on the PV parameters of the constructed cells, taking into account their impact on the UV-Vis absorption range, the roughness coefficient from AFM measurements, and for selected ones, the PL intensity and contact angle of FTO/b-TiO₂/m-TiO₂/MAPbI₃/compound to structures without an organic layer. The determined HOMO energies of the tested compounds concerning the perovskite valence band were also analyzed.

The most promising compounds as the *p*-type semiconductors for optoelectronic devices were: azomethine with a central triphenylamine group, imine with a morpholine structure, and naphthalene azomethinoimide with a triphenylamine group, for which a multiple increase in cell efficiency was found compared to the reference cells. The azomethinoimide with $-C \equiv C$ ethvlcarbazole substituents did not show electroactivity and oxetane with because the efficiencies of the cells in which they were used were lower or at the level of the reference cell. Some of the tested compounds, i.e. oxetane with naphthalene substituents and oxetane with triphenylamine were characterized by high photoluminescence quantum yields in solution and were emissive in the form of a layer, which may indicate the possibility of using them as components of active layers in light-emitting diodes.