Summary of doctoral thesis

Synthesis and semiconductor properties of the heterocyclic systems for applications in sensor devices

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Heterocyclic compounds due to the conductivity and electroluminescent properties are used in modern electronic devices, including the light-emitting diodes (OLED PLED, WPLED AMOLED), organic field effect transistors (OPV) solar cells (DSSC, OPVC) and sensor devices. The efficiency of the optoelectronic devices depends mainly on the structure of organic compounds used in their construction. Although there are many well-known conductive materials, they are characterized by an unsatisfactory physicochemical parameters (i.a. stability, solubility, quantum yield). Therefore, it is fully justified to continue research aimed at seeking new heterocyclic systems used in various sectors of economy.

The research problem undertaken in the doctoral dissertation is the synthesis of new derivatives systems such as tetraphenylsilane, dithienosilole and anthracene selected on the basis of the quantum-chemical study made according to the Density Functional Theory (DFT) by using the functional hybrid B3LYP in database function cc-pvdz and according to the method of Time Dependent Density Functional (TD-DFT). In this part of the dissertation the special attention is paid on the energy levels of orbitals HOMO/LUMO, the value of ionization potential and width of band gap which

affects the conductive properties of the system. An important aspect of the research is also the analysis of the physicochemical properties of the obtained compounds, including the characteristic of UV-Vis spectra, fluorescence and cyclic voltammetry. The end result of the research is to obtain stable systems for the application in thin-film optoelectronic devices. The polymers deposited on the surface of the electrode serves as an electrons relay in miniature sensor systems. The application of such solutions (in situ) has a variety of advantages which are as follows: the lack of need for sample pretreatment, high selectivity and accuracy of measurement, broad spectrum of activity, as well as short response time, ease of use and low operating costs.