In recent years, computer simulations have become a popular research tool. They are used in many fields of science from medicine through economics to material engineering. For computer simulation methods to be successfully used in materials engineering to design modern, functional materials, it is necessary to develop suitable computational models and methodologyy of proceeding. It is required that simulation works are to reflect physical phenomena taking place in the real world, and the results obtained are comparable to experimental data, which is not easy, since the values measured in the experiment are not the parameters that result from quantum chemical calculations at the atomic level. On the other hand, computer simulations allow the prediction of material properties without the necessity of its synthesis, explaining the choice of components, so that their physical parameters facilitate finding the desired composites.

The objective of the smaller project is to develop a methodology of proceeding and to create a computational model that allows the prediction of linear and nonlinear optical properties of composite materials at the level of polymer and NLO active molecules. Such cured thin film materials can be used for optical recording of information and holography as well as for the construction of electro-optical elements, switches, displays and laser generators. However, to talk about the practical use of these materials, it is necessary to examine and describe the mechanisms of physical phenomena in them.

The utility of polymer composite materials for NLO applications depends on the polarization of organic molecules in the matrix, hence on the orientation of the chromophores in space. Therefore, it is necessary to place the molecules in the polymer matrix, to arrange them by the corona poling method, and to cure the composite in the thin film form. The polymer matrix significantly changes the optical properties of the chromophores in comparison with the properties of the isolated molecules. The change of the composite optical properties in relation to the isolated components is a very interesting issue in the process of production of thin films with high NLO performance. Conducted experimental research starting with the synthesis of the layers to examine their optical properties such as UV-vis absorption and the phenomena of second and third harmonic generation provide a description of the electronic and optical properties of composite structures as bulk material.

Computer simulations conducted by the methods of molecular dynamics and quantum-chemical calculations describe the physical processes taking place in the material at the atomic level. Creating a computational model, which through polarizability and hyperpolarizability simulations defines linear and nonlinear optical susceptibilities, will allow to design modern materials with the use of quantum-chemical and molecular-dynamic methodologies. For this purpose, it is necessary to model the structure of the NLO molecule active in the polymeric environment while maintaining the thin-layer parameters of the solid, to calculate the microscopic properties of the optical components, to apply the discrete local field methodology to calculate the optical properties of the composite material. Comparison of experimental values with the results of calculations will verify the correctness of the applied calculation model and determine the interactions of the components. The proposed multipole interaction model between the composite molecules will be verified.

In conclusion, the project implements experimental and theoretical research to determine the effect of polymer matrix on the change of linear and nonlinear optical properties of thin-film composite materials of the "guest-host" type. PMMA, PVK and PC polymers are used as matrices, while active molecules are *push-pull* chromophores having electron donor and acceptor groups. Experimental research will be used to validate the proposed theoretical models. Typically, theoretical studies of molecules analyze their optical properties in a vacuum or in a solvent. The proposed project presents a modern approach to the analysis of optical properties of NLO molecules active in the thin polymer layer.