Summary of PhD thesis entitled "**Molecular modeling study of self-assembling phenomena of hybrid systems**" defended by Chem. **Mercore (married Epure) Elena-Luiza**, doctoral advisor Prof. Dr. Eng. **Nicolae Hurduc**

The PhD thesis follows a modern direction, namely, molecular modeling and simulation of some properties. Molecular modeling, providing nanoscale information related to the organization of the chemical systems, is a complementary alternative to the traditional methods of characterization. The originality of the thesis is reflected in the investigation of the supramolecular ordering of hetero-organic systems, in various phase states. The modeling studies were performed by using Materials Studio and GROMACS software.

The performed simulations followed, among other things, the organization of the azobenzene and nucleobases-functionalized polysiloxane systems in a solid state. In these studies, polysiloxane was selected because it is biocompatible and has some very special properties (high chain flexibility, hydrophobicity, low glass transition temperature, high thermal stability). The materials were synthesized to be used for immobilization and laser nano-manipulation of the biomolecules. The PhD thesis addresses the issue of supramolecular organization and reorganization phenomena, due to the photo-isomerization process of azobenzene groups from the polysiloxane side chain. Modeling these systems presented some problems, such as those related to the judicious choice of the starting conformations, the building of the systems in the condensed phase, the choice of the force field, the selection of simulation conditions to accurately describe the electrostatic interactions at large distances, etc. The validation of the calculation procedures was done by comparing the theoretical results with the experimental ones. Mechanics and molecular dynamics simulations allowed the obtainment of information about the internal structure of the material and the surface ordering of the films, helping to clarify questions about the interaction of DNA with azopolysiloxane film surfaces. The simulations have revealed that the morphology of the systems depends on the polymer type (flexible/rigid), the nucleobases type existing in the side chain (hydrogen bond strength), and their proportion towards azo groups.

Another goal of this thesis was to study the phenomena of micellar assembly of amphiphilic azo-polysiloxanes modified with tertiary amines, using the molecular dynamics technique. Depending on the chemical structure of these amphiphilic polymers, the micelles can form intermicellar clusters, which is a very rare organization system. This mode of organization of the amphiphilic azo-polysiloxanes has not been reported before in the literature, this study being carried out for the first time. Due to the limitation of computing resources necessary for the Materials Studio software, the GROMACS software was also used, requiring geometric parameterization of hetero-organic systems. While some atomic parameters can be transferable between different types of structures, the atomic charges will depend on the molecular composition and conformation. For this reason, the attention has been focused on finding non-transferable atomic parameters and, in particular, EPS partial charges through CHELPG procedure. It is noted that the azobenzene-type segments were not previously parameterized. The built model very well reproduces the actual behavior observed in the studied systems.

The thesis also analyzes the ordering processes of the hybrids or small molecular organic compounds (mesogens with ferrocene groups and asymmetric/symmetric substituted oxadiazoles) in the liquid crystalline phase. The simulations were focused on the correlation between the experimental results related to the ability of the compounds to generate mesophases and the theoretical principles of soft-hard control of the liquid crystals. Ab initio data brought extremely useful information regarding molecular geometry and electronic distribution, since no crystallographic experimental data for these systems have been reported in the literature.