Summary of PhD thesis entitled "**Molecular modeling study of self-assembling phenomena of hybrid systems**" defended by **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 chemical systems, is a complementary technique to the traditional methods of characterization. The originality of the thesis is reflected in the investigation of supramolecular ordering of hetero-organic systems, in various phase states. The modeling studies were performed using Materials Studio and GROMACS software.

The simulations explored, among other things, the organization in solid state of azobenzene and nucleobases-functionalized polysiloxane systems. In these studies, the polysiloxane was selected due to its biocompatibility and 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 biomolecules. The PhD thesis addresses the issue of supramolecular organization and reorganization phenomen that take place as a result of the photo-isomerization process of azobenzene groups from the polysiloxane side chain. Modeling these systems presented some challenges, such as those related to the judicious choice of the starting conformations, the construction of systems in condensed phase, the appropriate force field, the selection of simulation conditions to accurately describe the electrostatic interactions at large distances etc. Validation of the calculation procedures was accomplished by comparing theoretical results with the experimental ones. Mechanics and molecular dynamics simulations allowed obtaining information about the materials internal structure and the molecules ordering of the film surface, helping to clarify questions about the DNA - azo-polysiloxane film surfaces interaction. The simulations have revealed that the systems morphology depends on the polymer type (flexible / rigid), on the nucleobases type from the side chain (hydrogen bonds strength) and their proportion relative to 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 inter-micellar clusters, which is a very rare organization system. This mode of organization of the amphiphilic azo-polysiloxanes has not been previously reported in literature, this studies 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, which required geometric parameterization of the 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 reproducees very well the actual behavior observed in the studied systems.

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