Ionic liquids (ILs) are chemicals that can be classified as salts. Unlike the table salt, however, they are usually liquids at room conditions. This amazing feature is strongly related to chemical structure of molecules forming them. Compared to “traditional” salt which are based on small spherical ions that can be packed very close to each other and form a solid at macroscopic level, ILs’ ions are much bigger and exhibit significant asymmetry. This hinder their ordering at microscale and results in liquid phase formation. Due to their unique chemical nature ILs have been shown to disclose a series of peculiar properties, which make them chemicals more fascinating and desirable compared to traditional inorganic salts or conventional organic solvents. The properties of ILs open numerous perspectives of their possible applications in many areas of science and industry. In particular, ILs (as being salts) basically do not evaporate. This feature make them very attractive for novel cleaner and „greener” processes and product of chemistry. Therefore, by replacing volatile organic solvents affecting the nature, ILs may in near future significantly contribute in changing a general ”image” of chemistry as a branch of life that is very eco-unfriendly.

One of the key advantages of ILs is their diversity. In fact, chemists are now able to synthesize uncountable number of ILs by delicate modifications of the chemical structure. However, experiments and measurements of the properties of ILs are usually time consuming and very expensive, hence due to the time and economical factors are the main obstacles in developing new solutions employing ILs. This is also disadvantageous from the point of view of pure science, since having a lot of ILs available, the scientists and engineers would be able to find mutual relationships between the structure and composition of ILs and their important properties. Given this knowledge, they could then design ILs meeting the criteria of future applications.

Nowadays, such molecular-based design can be performed using advantages of computers, mathematical chemistry and chemoinformatics — relatively new disciplines combining the achievements of mathematics, computer science, statistics and chemistry. In particular, these “big data” of experimental work on ILs, which has been already carried out since the beginning of 21st century, would be processed by using so-called “machine learning algorithms” to create *quantitative* structure-property relationships (QSPRs) for ILs. Having QSPRs, one can perform “in silico” (i.e. very quickly, using computer only) experiments to search for interesting chemical structures of ILs or at least to create some systematic paths for the real experiments. ILs are very complex chemicals, therefore that is important to know which aspects of their chemical structure (types of atoms only, or the way they are connected to each other, or maybe their spatial arrangement, etc.) affect their properties in the most dominant way.

Development and testing (including experimental verification) of the new QSPR models for several key and fundamental properties of ILs (for example, melting point, density, viscosity, solubility in water) is the primary objective and utilitarian aspect of the proposed project. A study of effect of different ways of chemical structure representation is also going to be investigated, first of all to get the scientific society closer to understanding the rules governing the properties of ILs’ in terms of their microscopic characteristics, in consequence to provide new tools that will hopefully boost development of new applications of ILs in many areas of pure and applied science as well as industry.