

Structure and dynamics of water in liquid state has been of great interest for world of science for many years. Opinion-forming Science magazine states question about water structure as one of 125 unanswered, the most important questions for mankind. Water is regarded as an essential substance for life as we know it, it makes 70 % of our body weight. Its anomalous properties (almost 70 anomalies of water behaviour are known) create Earth climate, allow water organisms surviving frostiness, determine water properties as good solvent for many substances. Liquid water properties result from strong molecular interactions – hydrogen bonds, which form three-dimensional network. Despite of many works, we still do not know how H<sub>2</sub>O molecules connect with each other and in what way hydrogen bond structure is changed upon various factors, e.g. organic ions, nanoparticles and others. It is also still unknown if, and possibly in what way, local structure and dynamics translates into water properties in macroscale (effect of structure hierarchy is observed for many known systems, e.g. polymers, proteins, zeolites, composites and others). This project assumes investigations of correlations of changes taking place in water in different time scale (from trillion part of second to scale of thousand part of second) and in different size scale (from single molecules to large groups of them, named clusters). How mentioned earlier, water is universal solvent, its accessibility and low price make it as basis of many contemporary technologies. It is worth to highlight, that water (humidity) strongly modifies properties of many appropriable materials, like building materials: cements, gypsums, wood and wood-based materials, polymers etc. Knowledge about water interactions with different substances and its structure in these materials constitutes serious issue, essential from point of view of many aspects of life.

Metal nanoparticles are example of modern materials, which become more and more popular in daily life. They are used among others, as an additive to textiles, paints or cosmetics giving them antibacterial properties. Increasing amount of applications causes that nanoparticles access our environment in larger amounts. Influence of this kind of substances on water structure and dynamics is an important aspect, which cannot be ignored because of the fact that we do not know migration paths of nanoparticles in ecosphere. Due to limited stability of metal nanoparticles, their superb abilities to penetrate even through small size pores (many of them have ability to penetrate cell walls), as well as aspects connected with environmental protection, knowledge about water – metal nanoparticles interactions seems very significant. Moreover, computer simulations results show the possibility of creation of specific water structures on the metal nanoparticle surface.

Another example of materials in which water plays significant role are ionic liquids. These are salts, which consist of organic substances ions in their chemical structure. Under temperatures close to room-temperature they are in liquid state. Ionic liquids are modern materials. Despite of the fact that their history has more than century, first commercially available ionic liquids appeared not more than 20 years ago. Ionic liquids low stability in the presence of humidity has been a serious problem for many years. Because of their properties, these substances find application in many areas, among others, as a designed solvent or as an electrolyte in the batteries. Presence of water may strongly affects their properties, so that tailoring water content we can fit properties to requirements. Thus, knowledge about water structure and dynamics in these systems and water – organic ions interactions is so crucial.

Studies conducted in the frame of this project will allow taking global look into water structure and dynamics in its pure state, and also in two selected categories of modern functional materials gaining more importance in our daily life.