The subject of the research will be phosphate glasses containing iron and/or aluminium ions as well as glass-ceramic materials resulting from their crystallization. Phosphate glasses are materials of high technological and application importance. They are characterized by relatively low melting point, relatively high coefficient of thermal expansion and higher electrical conductivity compared to conventional silicate glasses. Their high thermal expansion coefficient with low liquidus temperature makes them an attractive material as glass sealants for metal-ceramic connections. On the other hand, phosphate glasses with the addition of Ca have biocompatibility and can serve as dental or bone implants. The addition of rare earths makes them potential materials for optoelectronic and laser applications. Due to the existence of easily hydrating P-O-P bonds, they are used as carriers of micronutrients in modern fertilizers with controlled solubility. On the other hand, phosphate glass is characterized by rather low resistance to environmental factors such as water vapour. Nevertheless, the partial replacement of phosphorus by iron and/or aluminium leads to a significant increase in the water resistance of these glasses. This increase is extremely fast and glass with a content of about 40 mole% Fe_2O_3 is characterized by very high chemical resistance. It is currently considered as a material for binding, in its structure, particularly hazardous forms of radioactive waste containing significant amounts of chlorides and sulphates, which cannot be immobilized by cementation or vitrification in borosilicate glasses.

The research we plan to conduct as part of the project is the analysis of interactions between ions in a solid-state. This leads to a specific ordering of the glass network. This gives the glass specific features**.** Thus, as a project goal, the determination of phosphorus glass network structure from the P_2O_5-Fe_2O_3-Al_2O_3 system was made by experimental research and molecular modelling using classical and quantum molecular dynamics methods.

In the proposed glasses, iron and aluminium ions can play a dual role depending on the coordination number adopted in relation to oxygen. These atoms can, on the one hand, build a glass network and, on the other, be its modifiers. Currently used research methods do not give an unambiguous answer to this question. This causes that there is a whole range of different types of the glass network models. The project envisages proposing a model for the structure of phosphate glasses containing iron and/or aluminium ions by means of detailed experimental studies in combination with molecular modelling. It is planned to conduct a detailed study of the thermal properties of glasses from the P_2O_5-Fe_2O_3-Al_2O_3 system. On this basis, the conditions for their crystallization will be determined. As a result of the crystallization process, a devitrified materials will be obtained. The obtained glass and the devitrified materials will be subjected to structural research using FTIR, Raman, Mössbauer, MAS-NMR and XRD spectroscopy. Their mechanical properties will also be determined by the nanoindentance method. Simultaneously with the experimental research, theoretical simulations will be conducted. In the first place, it is expected to carry out a classic molecular dynamics simulation. For this purpose, on the basis of previous studies on glass crystallization, data on density, mechanical properties, as well as on the basis of literature data, the form and parameters of the potential of interactions between particular ions as well as simulation conditions will be selected. As a result of the simulations carried out, the structure of the glass network of the proposed glasses will be pre-determined. The simulations performed using classical methods will serve as a starting point for the quantum molecular dynamics simulation using the Carl-Parrinello method. As a result, it should lead to a very realistic prediction of the properties of the new glasses based on computer simulations as well as the impact of other additives on them. Simultaneous combination of experimental and theoretical methods in application to amorphous materials gives the project an innovative character.