

The development of modern civilization results in a continuous increase in energy consumption. Therefore, it is necessary to research alternative and ecological sources of energy. A good example of alternative sources of energy are electrochemical devices, such as fuel cells. Fuel cells convert the energy from chemical reactions into electricity and do not produce contamination. Therefore, they are environmentally friendly. One of the most important parts of fuel cells is a ion conductive membrane composed of electrolyte, such as polymer proton conductors. They can transport the smallest type of ions – the ionized hydrogen atoms, protons.

An example of a polymeric material which is a proton conductor is Nafion – currently the most commonly used polymer in the fuel cell technology. Unfortunately, membranes composed of Nafion, have significant drawbacks: they are expensive and difficult to manufacture. Moreover, Nafion can conduct protons only in its hydrated form. Only the presence of liquid water in the matrix built with Nafion allows for proton transport. This limits the operating temperature of the polymer to temperatures below the boiling point of water, below 100 °C. Furthermore, the use of liquid water in an electrochemical device results in its complex construction as the liquid needs to be maintained in the polymer matrix. Moreover, low operating temperature causes the so-called effect of catalyst poisoning, present in a fuel cell, which could be avoided by increasing the operating temperature. This would result in an increase in its durability.

The aim of the project is to obtain and characterize physico-chemical properties of new nanocomposites based on cellulose nanofibers functionalized with different heterocyclic molecules on the surface. The resulting new nanomaterials are expected to be polymeric proton conductors and should have **designed properties**: proton conductivity above the boiling point of water, thermal stability within a wide temperature range, eco-friendliness, and being easy to manufacture.

In order to obtain new nanomaterials, the most common natural polymer will be used – cellulose. Cellulose is the main building material of plants, therefore, it is ecological, available on a large scale and inexpensive. Cellulose nanofibers will be used for the synthesis of novel nanocomposites. Nanoscale materials, that is those whose at least one dimension is 1 to 100 nm, have exceptional properties. Cellulose nanofibers are objects with nanoscale diameters, and whose lengths may reach up to a few micrometers. They have high stiffness and strength, low weight, they are chemically and thermally resistant, and, like other materials in nanoscale, they have a specific surface area wider than their macroscale equivalents.

The polymer matrix consisting of cellulose nanofibers will be functionalized with heterocyclic molecules containing nitrogen atoms, for example, imidazole, as a filler in a nanocomposite. We will use these molecules because of their similarity to water molecules, and as such they are an attractive replacement of water in proton conductors: similarly to water they create hydrogen bonds and can be donors and acceptors of protons. However, they have relevant properties which determine their superiority over water: they have higher boiling point, and, additionally, it is possible to immobilize them in a polymer matrix. **Functionalization of cellulose nanofibers' surface** with different heterocycles will result in obtaining **new nanocomposites** exhibiting proton conductivity and **containing no liquid in their structure**.

In the framework of the project, in order to describe the physico-chemical characteristics of the newly obtained nanocomposites, there will be carried out **a comprehensive study** of their thermal, structural, and electrical properties, as well as molecular dynamics. The conducting properties of the synthesized nanomaterials will be correlated with their molecular dynamics. It will be attempted to find a model that can describe the phenomenon of proton conduction in the new nanocomposites. In accordance with the above, inter alia, the following methods will be used: differential scanning calorimetry (DSC), thermogravimetric analysis (TGA), impedance spectroscopy, infrared spectroscopy (FTIR), and methods of high resolution magnetic resonance spectroscopy in a solid-state (ssNMR).