Producing new materials with strictly controlled properties is extremely important from the application point of view and is currently experiencing enormous development. For scientists, the overarching goal is, however, to understand and quantify the fundamental laws and phenomena that determine such properties. This allows for even better control of the obtained materials and prediction of their properties already at the initial stages of synthesis. Unfortunately, materials with sophisticated properties are often difficult to understand using available tools and require an interdisciplinary and complementary approach to explain the laws that govern them.

One of the class of materials that are extremely popular are polypeptide complexes whose synthesis is based on the mixing solutions of polypeptides with opposite charges. Polypeptides, unlike synthetic polymers that often have a toxic effect, are less harmful, which makes them widely used in medicine and biotechnology, e.g. as gene therapy vectors or drug carriers. By choosing precisely synthesis conditions, we can control the properties of these materials, for example, control the release of drugs from capsules, produce self-organizing materials, or reacting to external stimuli, such as temperature or pH.

Large-scale research covering all phases of synthesis is necessary to understand the reasons for the properties exhibited by new materials. Often, information about how macromolecules, which are the basic building blocks of material, behave in the conditions of synthesis can help us predict some properties of the material. In addition to experimental research, parallel theoretical studies are extremely important. They serve as a complementary tool and allow to obtain information inaccessible to experimental techniques, as well as, quantitative description and in-depth understanding of the investigated processes.

This project aims at complementary theoretical and experimental research on the preparation of polypeptide complexes that will combine the synthesis conditions with the properties of the final materials. This will allow us to predict and control the properties of such materials in a more conscious way.

In the first stage, the authors will focus on determining the relationship between the conditions of the formation process of the complex and the properties of individual polypeptides. Both molecular dynamics modeling with atomistic resolution, as well as a number of experimental techniques will provide information on how the shape, charge and conformation of the molecule changes depending on the pH or ionic strength of the solution.

The next stage of research will be to understand the interaction between oppositely charged polypeptides. The aim of this stage will be to reveal the mechanism and thermodynamics of the process of polypeptide complexation depending on the synthesis conditions, as well as, provide detailed description of the obtained structures and their properties. The main tool will be theoretical modeling supplemented by an isothermal titration calorimetry, which will provide valuable information on the entropic and enthalpic contributions to the complexation process.

The final stage will concern the synthesis and characterization of polypeptide complexes. The research aims at determining the changes in mechanical and thermal properties caused by different synthesis conditions. This will provide information on the effect of the effective charge of the molecule and its conformation on the macroscopic properties of the complexes. Correlation between the results obtained for polypeptide complexes and the fundamental properties of single molecules will be an extremely useful predictive tool.

Such innovative and multi-stage approach, combining theoretical modeling and experimental research, carried out in cooperation with leading foreign centers in Finland and USA, will allow for an in-depth understanding of these extremely interesting and promising materials.