Hydrogen is currently a gas which is widely used in various fields of industry, science, and medicine. For example, it is a key reagent used in hydrogenation reactions in the synthesis of many pharmaceutical ingredients. Hydrogen is also increasingly attracting attention as an eco-friendly fuel because its combustion results in the production of water. It is predicted that hydrogen will play an increasingly important role in the energy sector in the near future. Another important application of hydrogen is its role in nuclear magnetic resonance (NMR) spectroscopy and magnetic resonance imaging (MRI). Because of its unique physicochemical properties, hydrogen significantly improves the sensitivity of NMR and MRI.

One of the most interesting features of hydrogen is its occurrence in two forms orthohydrogen and parahydrogen. Specifically, a hydrogen molecule (H_2) consists of two hydrogen atoms, and each atom's nucleus, being a proton, has a unique property called spin. Associated with the nuclear spin is a magnetic moment, which can be imagined as a small bar magnet. The spins of the two nuclei in a hydrogen molecule can be aligned in the same direction, forming orthohydrogen, or in opposite directions, forming parahydrogen. These two forms of hydrogen have completely different physicochemical properties and do not spontaneously convert into each other. Such a conversion is possible only in the presence of an appropriate catalyst. Although the hydrogen molecule has been known to humanity since the 17th century, and almost everything is known about it today, it was relatively recently discovered that certain catalysts can convert parahydrogen into orthohydrogen in such a way that the orthohydrogen molecule's spectrum in NMR spectroscopy has a previously unseen shape (PNL - Partial Negative Line). The formation of such a spectrum does not conform to the current understanding of the orthohydrogen molecule, which intrigues many scientists worldwide. To explain this effect, two hypotheses have been proposed. The first suggests that parahydrogen is converted into orthohydrogen with a specific arrangement of nuclear spins on the catalyst. The second assumes that in a high magnetic field, orthohydrogen molecules are partially oriented, causing unusual NMR signals. Both hypotheses are based on solid assumptions, but differ in their physicochemical mechanisms. These hypotheses must be verified, which requires further research into the PNL effect.

Therefore, our goal is to definitively understand and explain the nature of the unique PNL effect and resolve any uncertainties about the current state of knowledge on this topic. As part of the project, we will thoroughly investigate how the PNL effect depends on the structure and composition of the catalyst. In particular, we will explain why PNL is more effective with certain catalysts. An integral part of the project is also the study of how experimental conditions affect the observation of this phenomenon. In this case, we will investigate how the PNL effect is modulated by the type of solvent and the strength of the magnetic field in which PNL experiments are conducted. A detailed analysis of the results will allow us to verify the validity of current hypotheses explaining the PNL. We will clarify whether the formation of PNL is due to chemical processes, such as exchange reactions, or physical processes, such as the unique orientation of hydrogen molecules in a magnetic field.

Our research will clarify the current controversies and misunderstandings associated with the PNL phenomenon and satisfy the curiosity and thirst for knowledge on this topic in scientific communities. We hope that it will demonstrate the extent to which the PNL effect can be utilized in the study of important processes and chemical molecules. In particular, understanding PNL may be significant in studies of systems with documented biological properties, such as biocatalysts known as hydrogenases. It seems probable that the occurrence and nature of PNL in such biological systems can provide information about the interaction of hydrogen with the biocatalytic center. Our research may also be significant in the application of PNL in studies of chemical catalysts, including those relevant to the pharmaceutical industry. Our research will also lead to a deeper understanding of the conversion processes between orthohydrogen and parahydrogen. Detailed knowledge of this topic is crucial, for example, in safety procedures during the storage of hydrogen when it is used as fuel.