The main goal of the research project titled: "Research on the reaction mechanism of electrocatalytic oxygen release using an interfacial system of metal and single-wall carbon nanotubes" is to develop and understand new, efficient electrocatalysts that could contribute to a breakthrough in this field. Single-wall carbon nanotubes (SWCNTs) are an excellent candidate as an electrocatalytic material due to their unique properties such as high mechanical strength, large aspect ratio, large surface area, excellent optical properties, high thermal conductivity, and electrical conductivity. The project aims to investigate in detail the role of carbon and its interaction with the metal catalyst located on its external and internal monoatomic surfaces in the OER reaction. The effect of the size of the doped metal on the electroactivity of the SWCNTs-based catalyst will also be investigated. This will allow the development of new carbon-based catalytic materials with improved electrocatalytic parameters.

In the face of growing challenges related to environmental protection and ensuring sustainable development, finding an alternative to fossil fuels has become one of the most important goals of modern science and technology. There are several key reasons why this is essential: fossil fuels such as coal, oil, and natural gas are the main source of emissions of carbon dioxide (CO_2) and other greenhouse gases that contribute to global warming, burning fossil fuels leads to air, water and soil pollution and the fact that they are non-renewable resources mean that their reserves on Earth are limited.

Replacing fossil fuels with renewable energy sources causes scientists around the world to look for new, effective methods of obtaining energy. One promising alternative is electrochemical water splitting, a process in which, under the influence of an applied electric current, water molecules break down, generating hydrogen and oxygen in processes known as the hydrogen evolution reaction (HER) and the oxygen evolution reaction (OER). However, the wide-scale application of this process is limited by the slow kinetics (rate) of the OER reaction, which is a complex process requiring the transfer of four electrons. Even though the electrochemical decomposition of water has been known since the 19th century, the oxygen evolution reaction (OER), i.e. the anode reaction of water electrolyzers, remains a mystery and its mechanism is still not fully understood. A major limitation in the wide-scale application of this process is the currently used electrocatalysts composed of expensive and rare noble metals, compounds that require a lot of energy to initiate reactions and are characterized by low stability in aggressive conditions.

The research will include the design of electrocatalysts based on single-wall carbon nanotubes. This means that we will be dealing with a single layer of carbon with a diameter of approximately 0.8-2.0 nm. We will then decorate both its outer wall (exohedral functionalization) and inner wall (endohedral functionalization) with active metal particles of different sizes to improve their catalytic properties. The obtained materials will be examined using advanced spectroscopic techniques, diffraction, and microscopic methods. The prepared electrocatalysts will be tested in the electrochemical release of oxygen, which will allow them to verify their practical potential, but more importantly, the use of the most advanced characterization techniques will help determine the reaction mechanism and discover the role of carbon.

This project offers innovative and promising results as the endohedral functionalization of SWCNTs leads to a more robust electrocatalytic system as the single-layer cylindrical carbon structure can mitigate the rapid dissolution of metal compounds. The single atomic layer of carbon will increase the conductivity of the system and facilitate charge transfer. In turn, exohedral functionalization of SWCNTs will result in greater stability, faster reaction, and increased dynamics due to the metal-electrolyte interphase. The final result of the project enabled the design of efficient carbon electrocatalysts for the electrochemical decomposition of water, making hydrogen as an energy carrier more available and sustainable.