The era of the ever-growing worldwide energy demand imposes the development of new ways of energy conversion that will allow for replacing fossil fuel-based technologies in the foreseeable future. Consequently, numerous solutions based on electrocatalytic processes have been proposed as a way to achieve more energy-efficient and pollution-free energy conversion, including water electrolysis, fuel cells, and metal-air batteries. Water electrolysis is a type of direct conversion of electric power to chemical energy, leading to the splitting of H_2O molecules into gaseous hydrogen (hydrogen evolution reaction, HER) and oxygen (oxygen evolution reaction, OER), where the former can be stored and utilized as a fuel *e.g.* in fuel cells. Taking into account the ever-growing popularity of hydrogen-based technologies, as well as the fact that as of today nearly 95% of hydrogen necessary for the production of ammonia, steel, and alumina, but also for CO_2 conversion, comes from the reformed fossil fuels, the development of affordable and environmental-friendly methods of hydrogen production has become a matter of crucial importance. Unfortunately, the state-of-the-art catalytic materials utilized as electrodes in the electrolysis systems, are based mainly on platinum, and precious metal-based compounds, which is associated with prohibitively high costs, rendering the technology uneconomical. Among the most promising alternatives are the transition metal chalcogenides, especially the pentlandite- and metal-like pseudo-spinel structures, which combine the affordability and simplicity of materials preparation with good catalytic activity towards both HER and OER. However, bringing their performance to an even higher level, and in the process making them industrially-feasible replacement of the currently applied materials, still remains a challenge. In the current project, one of the possible design strategies capable of addressing this problem will be explored, namely maximizing synergistic effects between elements. The general idea behind it is to utilize several components, enhancing the number of interactions between them, which often leads to the generation of new properties outside of the rule-of-mixtures predictions, as well as tends to improve the stability of the systems.

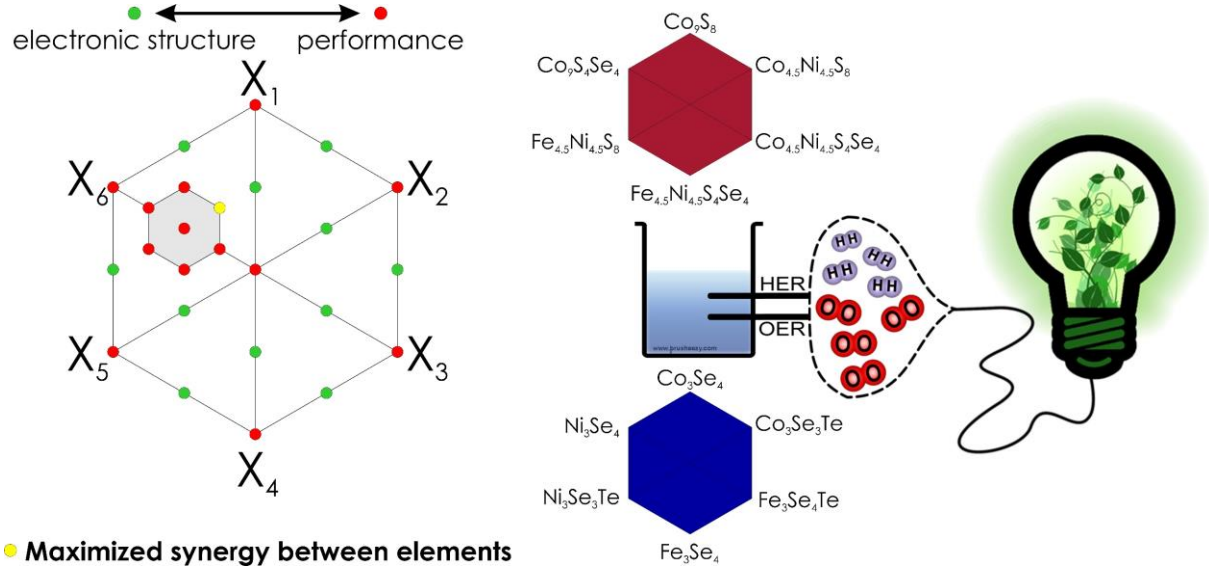

Fig. 1 *Schematic representation of the project's concept.*

In the project, the potential of the multicomponent approach will be maximized by combining the experimental characterization of the materials with extensive use of theoretical calculations, allowing for determining the so-called catalytic activity descriptors – electronic structure-derived parameters, which can be correlated with the electrochemical performance of the material. As a result, a design tool of considerable predictive power will be obtained, allowing for effective screening of the vast compositional space. The identified, best-performing materials will be then thoroughly studied, including industry-relevant conditions, to provide an in-depth understanding of the composition-structure-performance relationship in the chalcogenide systems, at the same time serving as the proof of the proposed concept of effective and affordable, transition metal-based electrocatalysts.