Reg. No: 2025/57/N/ST4/03315; Principal Investigator: mgr Mateusz Szczerba

Understanding the structure-activity relationship in transition metal sulfoselenides as electrocatalytic materials for hydrogen evolution reaction

Mateusz Szczerba

Popular science abstract

Modern science faces a growing demand for knowledge about energy conversion processes. Among many directions of fundamental research, a particularly active area involves the development and understanding of new electrocatalytic materials for the hydrogen evolution reaction (HER), a key step in water electrolysis. Transition metal sulfoselenides – compounds combining sulfur and selenium with metallic elements – are emerging as promising alternatives to noble metals in HER, but many questions remain regarding how their composition, structure, and synthesis history affect their performance.

The aim of this project is to study sulfoselenides of cobalt (Co) and iron (Fe) as model systems for investigating how chemical composition, micro/nanostructure, and synthetic strategy influence electrochemical activity in HER under alkaline conditions. These materials are of particular interest due to their tunable electronic structure, high theoretical activity, and compatibility with low-cost manufacturing methods. By systematically varying the composition and preparation route, the project seeks to identify structural features – such as morphology, crystallinity, or heteroatom distribution – that most strongly influence catalytic behavior. This is a fundamental research project, focused not on producing commercial materials, but on gaining a deeper understanding of structure-activity relationships in a complex class of non-precious-metal catalysts.

In the first stage of the research, cobalt will be electrodeposited onto two different conductive substrates – carbon foam and nickel foam – and subsequently modified via hydrothermal treatment using sulfur and selenium precursors to form sulfoselenide structures. Based on the results, one substrate will be selected for continued studies. In the next phase, iron will be introduced either through hydrothermal doping or direct use of electrodeposited Co/Fe alloys. Comparing these two methods will help determine how the incorporation pathway of Fe affects the material's phase composition, presence of defects, morphology, and electrocatalytic performance.

The project will include extensive materials characterization using scanning and transmission electron microscopies, X-ray diffraction, Raman and XPS spectroscopies, and a variety of electrochemical techniques. The electrocatalytic performance of the synthesized electrodes will be assessed through voltammetric and impedance-based methods, as well as long-term HER testing in alkaline solutions. Selected samples will also undergo re-characterization after testing to assess their structural stability and durability.

The outcomes of this project will provide valuable insights into the physicochemical factors that determine the performance of transition metal sulfoselenides in HER and will contribute to a more rational design of catalytic materials for hydrogen-related energy technologies. In particular, the systematic comparison of two iron incorporation strategies (via hydrothermal doping and alloy deposition) will shed light on the structural roles and chemical environments of Fe in mixed-anion systems. The results will help clarify how different synthetic routes lead to distinct active site distributions, phase compositions, or electronic structures. Moreover, the findings will contribute to the broader field of heteroanionic material design by offering guidelines for controlling composition-structure-activity relationships in complex transition metal compounds. Although the research is fundamental in nature, the knowledge gained could influence how future electrocatalysts are engineered, especially in the context of scalable and cost-effective hydrogen production.