

Surface engineering of anodic WO₃ by modification with Co and Se compounds as a strategy for understanding the mechanism of formation of n-p heterojunctions with enhanced and long-term activity in photoelectrochemical water splitting

Lay Summary of the Project

The production of green hydrogen using solar energy – via a process known as photoelectrochemical (PEC) water splitting – is one of the most promising research directions in the context of energy transformation and combating climate change. A key challenge in this field is gaining a better understanding and control of the physicochemical phenomena occurring in semiconductor materials capable of converting sunlight into chemical energy. Particularly important is the design and investigation of complex, multi-layered materials with different electronic properties – named heterojunctions – where efficient separation and transport of light-induced electrical charge carriers can take place.

One of the well-studied material in PEC context is tungsten trioxide (WO₃), a light-absorbing n-type semiconductor that generates hole-electron pairs when exposed to solar radiation. While many of its properties are well known, several fundamental questions remain unanswered – especially regarding how its performance changes when combined with other functional materials.

The aim of this project is to understand how structures based on WO₃, cobalt and selenium compounds work together to enhance solar-to-chemical energy conversion. The interest will be focused on what happens at the interfaces between different material layers – the so-called heterojunctions – where a p-type semiconductor meets an n-type one, creating a unique region with distinct electronic behavior. In this way structures like n-WO₃/p-CoO_x/p-Se or n-WO₃/p-CoSe_x can be created.

The research will involve synthesizing these multi-layered anodic WO₃-based materials modified with cobalt and selenium compounds (using hydrothermal and/or electrodeposition methods), and thoroughly characterizing them in terms of their physical, chemical, semiconductor, and photoelectrochemical properties. Characterization of the materials will be performed using electron microscopy (SEM/TEM), Raman spectroscopy, X-ray diffraction (XRD), photoelectron spectroscopy (XPS), impedance spectroscopy (EIS, Mott–Schottky), potentiometric/amperometric techniques, and incident photon-to-current conversion efficiency (IPCE) measurements. A key goal will be to link structural–function relationship - in other words, to understand how specific changes in morphology and composition influence the overall performance of the material in photoelectrochemical water splitting.

The project seeks to answer fundamental questions such as: what changes occur in the electronic structure and charge transport mechanism when anodic WO₃ is modified with cobalt oxide layers? Can the addition of selenium – deposited before or after Co-based layer – further enhance charge separation, performance, or stability of the system? And finally, do the observed improvements in photoelectrochemical activity arise solely from contact between different materials, or are they also due to the formation of new phases or energy gradients that lead to more complex effects in designed heterojunctions?

This research is part of fundamental studies at the intersection of materials chemistry, solid-state physics, and electrochemistry/photoelectrochemistry. The knowledge gained may form the basis for future development of practical PEC materials, but most importantly, it will deepen the understanding of how complex semiconductor structures operate in solar energy conversion processes.