Designing Efficient Photoanodes for Solar Water Splitting: Unraveling Structure–Performance Relationships in Nanostructured $WO_3/FeVO_4$ Heterojunctions

In recent decades, rapid population growth, industrialization, and technological advancement have significantly increased global electricity demand and accelerated the depletion of fossil fuel resources such as coal, oil, and natural gas. In addition to being finite, the use of fossil fuels has a devastating impact on the environment - contributing to acid rain, ozone layer depletion, and global warming, which in turn triggers extreme weather events like flash floods, hurricanes, and heatwaves. Moreover, fossil fuels have recently been used as political and economic leverage, further underscoring the need to develop alternative, sustainable energy solutions.

Among the various renewable energy sources, solar energy is the most abundant and environmentally friendly. The Sun delivers more energy to the Earth in one hour than humanity consumes in an entire year. Harnessing this energy efficiently is therefore one of the greatest opportunities of our time. One promising approach involves converting solar energy into chemical energy, which can be stored in clean energy carriers such as hydrogen. This can be achieved through photoelectrochemical (PEC) water splitting, where semiconductor materials, when exposed to sunlight, generate pure hydrogen and oxygen from water.

Common semiconductor photoelectrodes like TiO_2 and WO_3 are non-toxic, cost-effective, and stable. However, their wide band gaps limit their ability to absorb sunlight efficiently, as they primarily utilize ultraviolet (UV) light, which accounts for only 3–5% of sunlight at the Earth's surface. As a result, the efficiency of current PEC systems remains low - typically under 5%. To improve this, materials with a narrower band gap (around 2.0 eV) are needed to harvest more visible light while still providing sufficient energy for water splitting reactions.

A promising solution is to form heterojunctions - composite materials combining two semiconductors with complementary properties. In this project, we aim to enhance the photoactivity of WO_3 by forming heterojunctions with $FeVO_4$, a narrow band gap semiconductor (approximately 2.0 eV) with well-matched energy levels. The goal is to design and optimize a new class of nanostructured photoanodes composed of nanoporous anodic WO_3 decorated with $FeVO_4$ nanoparticles or nanowires. The study will explore various morphologies and compositions of both WO_3 and $FeVO_4$ to understand their effect on photoelectrochemical performance. Nanoporous WO_3 and carbon/nitrogen-doped WO_3 will be fabricated via anodic oxidation of tungsten under optimized conditions. $FeVO_4$ (and its doped variants with Mo or W) will be synthesized through a simple hydrothermal method, yielding either nanoparticles or nanowires. The heterojunctions will be formed by direct growth of $FeVO_4$ on WO_3-based substrates or by coupling separately synthesized components. Special attention will be given to the interface between the two semiconductors, as it plays a critical role in charge separation and transport. Therefore, additional engineering - such as introducing ultra-thin carbon layers or arrays of carbon nanoparticles - will be employed to improve the quality of the junction and, consequently photoactivity of the obtained heterojunctions. Comprehensive characterization of all photoanodes will be conducted, including analyses of their structure, composition, semiconducting properties, and PEC performance. The ultimate objective is to establish clear correlations between material structure and photocatalytic efficiency, contributing to the development of more effective solar-driven water splitting technologies.