VRIJE UNIVERSITEIT BRUSSEL

The faculty of Engineering of the Vrije Universiteit Brussel invites you to attend the public defense leading to the degree of

DOCTOR OF ENGINEERING SCIENCES

of **Beatriz de la Fuente**

The public defense will take place on **Wednesday 21st January 2026 at 5 pm** in room **I.2.01** (Building I, VUB Main Campus)

To join the digital defense, please click here

UNVEILING THE POTENTIAL OF NOVEL PHOTO-ELECTROCATALYTIC SEMICONDUCTORS FOR CARBON CAPTURE AND UTILIZATION: INSIGHTS FROM NANO-SCALED MOLECULAR AND SURFACE CHARACTERIZATION

BOARD OF EXAMINERS

Prof. dr. ir. Francis Berghmans

Prof. dr. ir. Dimitrios Angelis

Dr. Nick Gys

Dr. ir. Juliet Risner-Jamtgaard

Prof. dr. Vera Meynen

Prof. dr. Ing. Tom Breugelmans

PROMOTORS

Prof. dr. ir. Tom Hauffman

Em. Prof. dr. ir. Annick Hubin

Abstract of the PhD research

Fossil fuel-driven industrial growth has caused an unprecedented increase in atmospheric carbon dioxide (CO_2) concentrations, significantly contributing to the greenhouse effect and accelerating global warming. In response, innovative approaches to carbon capture and conversion are gaining momentum. Among these, solar-driven CO_2 conversion holds great promise, with photo electrochemistry (PEC) emerging as a key technology. By directly harnessing the light from the sun to drive chemical reactions, PEC provides a highly efficient and selective method for converting CO_2 into carbon-neutral fuels.

A crucial aspect of advancing PEC technologies lies in the materials used for the conversion process. Earth-abundant, non-toxic metal oxides and chalcogenide-based semiconductors, such as $CuInGaS_2$ (CIGS), $AgCu_2ZnSnS_4$ (ACZTS), Sb_2S_3, and Cu_3BiS_3 (CBS) are gaining attention as sustainable and environmentally-friendly alternatives for PEC technologies. However, their performance is often limited by a lack of understanding of their structure-electronic property relationships, which are crucial for optimizing the materials towards the desired reaction. Specifically, it is essential that the materials conduction band (CB) and valence band (VB) are positioned correctly to facilitate efficient charge transfer and ensure optimal performance in driving reduction reactions, such as hydrogen evolution reaction (HER), carbon dioxide reduction reactions (CO_2RR) or, nitrogen reduction reactions (NRR).

This thesis makes significant contributions to advancing PEC technology by providing a comprehensive analysis of the electronic parameters at the semiconductor/current collector interface. The energy level alignment of several chalcogenide-based materials for different PEC reactions are investigated via cutting-edge techniques, such as Ultraviolet Photoelectron Spectroscopy (UPS) and the less-explored Low-Energy Inverse Photoelectron Spectroscopy (LEIPS). In addition, the introduction of co-catalysts is explored as a strategy to enhance both the performance and durability of the studied materials. Through advanced electrochemical characterization techniques, including voltammetry and impedance spectroscopy, this work uncovers valuable insights into charge transfer resistance and electrochemical stability, critical factors for the long-term efficiency of PEC systems.

Overall, a detailed framework for the design and characterization of advanced PEC semiconductors is developed, facilitating advancements in CO_2 reduction, solar fuel production, and renewable energy technologies, thereby contributing to sustainable strategies for mitigating the global carbon crisis.