

Thesis subject

Laboratory: CINaM (UMR CNRS-AMU 7325), *Surface Nanostructuring for Energy (SuNE)*
www.cinam.univ-mrs.fr/cinam/team/nanomateriaux/sune/

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Thesis title: Synthesis of Ternary Silicides as Efficient Catalysts for Water Photooxidation

Subject:

Hydrogen is now considered a key energy vector because it exhibits a high energy density and its use produces no CO₂. Unfortunately, H₂ is mainly produced from fossil sources. Alternatively, water electrolysis is now envisioned as a large-scale production scheme of H₂ that is sufficiently pure for direct use in fuel cells. In parallel to the various electrolysis approaches, H₂ and O₂ production from H₂O photoelectrolysis appears to be a more straightforward approach. It has opened an attractive, though challenging, field of investigations that ultimately tackles the direct water dissociation using an unbiased photoelectrochemical cell (PEC) under sunlight: solar fuel production. This direct approach is appealing because PEC exhibits a theoretical solar-to-hydrogen (STH) efficiency of 34% while coupling two devices such as a PV tandem cell and an electrolyzer leads to a similar ideal yield of 36% with potentially higher manufacturing and maintenance costs. To reach such challenge, it is possible to optimize the PEC architecture, to find cost-efficient materials (absorbers and co-catalysts), to perform electrode micro- or nanostructuring and, finally, to combine different materials. In previous works, our group has shown the positive impact of the electrode structuring using anodic processes and the interest of combining materials to preserve the efficiency of the electrodes.

Recently, a new class of promising cost-effective co-catalysts for water photooxidation has been evidenced and patented. This project tackles therefore the study and development of an innovative catalyst family, based on those very promising preliminary results. It is therefore intrinsically original. This PhD thesis will consist of synthesizing, characterizing and probing the photoelectrochemical properties of different compositions of this new family of materials. Those catalysts will mainly be grown on Si-based electrodes using atomic layer deposition (ALD). Although the group has a long experience on this deposition process, the synthesis will not be limited to ALD and other approaches as well as other substrates will be investigated. The deposition parameters will be optimized to control the chemical composition, crystalline structure and the morphology. The photoelectrochemical performances of these systems will be assessed and correlated with their physico-chemical properties as well as their electronic structure that will be calculated by DFT with specialists at CINaM. The catalysts will be studied using the various analytical techniques available in the institute. The morphology will be observed by electron microscopies (SEM, TEM), the crystalline structure by electron and x-ray diffractions and the chemical composition by XPS and FTIR. The electrodes performances will be tested using different (photo-)electrochemical setup of the group. Additional investigations will be performed in collaboration with the University of Rennes and possibly with University of Erlangen (Germany).

The Candidates should hold a Master Degree with honours in chemistry, physics or Materials science with a preferential background in thin film deposition, electrochemistry.

Duration: 3 years (01/10/22 – 30/09/2025)

Gross salary: 1770 €/month (additional 210 €/month salary for teaching is possible)