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Laboratoire d'Electrochimie
et de Physico-chimie des Matériaux et des Interfaces
(UMR 5279)

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Saint Martin d'Hères, le 19 février 2025

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Understanding the Structure-Activity-Stability Relationship of Nanostructured Noble Metal-Free Materials for Alkaline Water Electrolysis

Keywords: Electrocatalysis, Hydrogen Production, Materials Science, Nanomaterials, Oxygen Evolution Reaction

Offer description for a PhD thesis (école doctorale I-MEP2):

Hydrogen, as a strategic energy carrier, plays a crucial role in storing and regulating electricity production from renewable energy sources. Proton-exchange membrane water electrolysis (PEMWE) is currently the most advanced technology for producing "green" hydrogen from renewables, but geological resources limit its large-scale deployment (notably the utilization of noble metals such as platinum and iridium). In alkaline devices, 3d transition metals can be used and their (hydro)oxide forms exhibit good stability at high pH. Unlike noble metals, 3d transition metals such as nickel and iron are naturally abundant and therefore cheaper, which explains the lower cost of alkaline devices. Moreover, significant advances have been made with anion-exchange membranes and ionomers, making it possible to envision alkaline water electrolyzers operating with an anion-exchange membrane, combining the best of PEMWE and alkaline devices. In this context, the proposed thesis aims to design advanced electrodes made from non-noble metal nanocatalysts for use in anion-exchange membrane water electrolyzers (AEMWE).

The development of synthetic strategies able to produce 3d transition metal oxides of controlled size and shape, at low cost, using environmentally friendly reagents and capable of being produced on a large scale, is a major lock-in in materials chemistry. The properties of nanoparticles depend on their size, shape and chemical composition. For example, atoms located at the edges and corners of the surface are generally chemically reactive and catalytically active, which contributes to their high potential in electrochemistry. Moreover, particle size not only affects the surface, but also generates new electrochemical properties, due to the electron confinement effect and surface state. To better understand the properties of AEMWE electrodes composed of noble-metal-free nanocatalysts at a fundamental level and unlock their full potential, it is essential to study their behaviour and properties.

In this thesis, nanocatalysts of controlled shape, size and composition will be prepared to form a library of customized materials. These will be characterized using innovative, state-of-the-art analytical tools, both *ex situ* and *in situ*, to establish structure-activity-stability relationships. This involves studying their electrocatalytic performance under conditions that simulate stationary (constant current) operation, as well as start-up and shutdown processes of the AEMWE, and assessing changes before and after accelerated stress testing to identify operational limits. Structural, chemical and phase changes will be analysed to assess surface deactivation and degradation mechanisms.

Location: LEPMI laboratory on Grenoble University campus, FRANCE

Goals:

- Preparing a library of nickel- and nickel-iron-based nanomaterials of different sizes and morphologies.
- Development of relationships between the structural state of shape- and size-controlled nanomaterials and their electrochemical performance and stability in rotating disk and gas diffusion electrodes to improve alkaline hydrogen production systems.

Student profile: Background in chemistry and/or material science, familiar with electrochemistry and/or energy storage thematic.

Duration: 36 months **Starting date:** October 2025

To apply to this thesis, please send your CV and motivation letter to Kavita Kumar (kavita.kumar@grenoble-inp.fr)