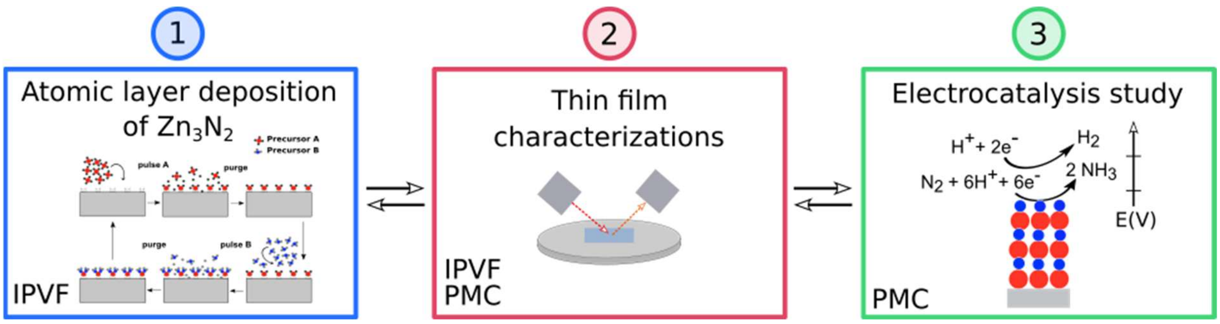
Titre du projet	**Atomic Layer Deposited nitride thin-films for Electrochemical Reduction reactions**
Acronyme	**ALDER**
Nom, prénom, laboratoire du porteur	BADIE, Clémence, clemence.badie@polytechnique.edu Laboratoire de Physique de la Matière Condensée, Ecole Polytechnique
Nom, prénom, laboratoire du partenaire	SCHNEIDER, Nathanaelle, n.schneider@cnrs.fr Institut Photovoltaïque d'Ile-de-France, IPVF, UMR 9006
Action de recherche du stage	RA 1 : Production d'énergie décarbonée RA 2 : Décarbonisation et capture
Stage	Date approximative de début : 31/01/2026 Durée : 25 semaines (6 mois) Type : Master 2 Consommables et utilisation plateforme : 5k euros

Key words: atomic layer deposition, thin films characterisations, electrocatalysis, HER, NRR

Project

In the context of energy transition and the promotion environmental-friendly processes, the carbon-free emission production of green H_2 and NH_3 is in high interest. H_2 and NH_3 are widely consumed in industry (e. g. oil refining and fertilizers production) and their production is manly based on fossil fuels: e. g. steam methane reforming and Haber-Bosch process, respectively. However, they can be produced by alternative approaches to reduced their ecological impact such as electrolysis. H_2 is generated by water splitting from proton reduction (HER) and NH_3 from N_2 reduction reaction (NRR) in aqueous media. To maximize such reactions, electrocatalysts are used at the electrodes. Noble metals such as Pt, Pd, Ir and Ru are state of the art materials thanks to their high catalytic activity, electrical conductivity and stability in time. However, being critical elements, alternative materials are required and already investigated such as transition metals (TMs) in metallic, oxide (TMOs) and lately nitride (TMNs) form[1]. Looking for cheaper and Earth-abundant compounds is one leverage point; another one is to optimize the material mass/efficiency ratio. Therefore, precise thin-film deposition techniques are required to finely control the thickness and the composition of the electrocatalyst layer. Chemical vapour deposition (CVD) techniques such as Atomic layer deposition (ALD) fulfil these requirements thanks to the self-limited growth of the deposited layer on the substrate[2]. Conformal (dense and uniform) coating is achieved even on 3D substrates: this allows the preparation of systems with large specific area and makes it even more suitable for application as electrocatalyst.

The project will be composed of three steps:



1/ Development of a novel TMN process: Zn_3N_2 using an ALD reactor equipped with a plasma assistance at IPVF, first on planar substrates then on 3D ones.
2/ Thin film characterizations of the obtained layers in terms of morphology, crystallinity, chemical composition, electrical resistivity at both IPVF and PMC.
3/ Assessment of their performance as electrocatalyst for hydrogen evolution reaction (HER) and further with nitrogen reduction reaction (NRR) in aqueous media at PMC.

Implementation and risk management:
1/ Although, ZnO deposition has been extensively explored and is long-established at IPVF[3], Zn_3N_2 is much less investigated by ALD with only a couple of publications reported using diethyl zinc (DEZ) and NH_3 gas[4,5]. The objective is to develop an ALD process using: diethyl zinc (DEZ) and either NH_3 or NH_3 plasma as Zn and N sources, respectively. Such strategy has been already employed for another nitride layer by the project coordinator[6].
2/ Both laboratories are well equipped for thin film characterizations: morphology and microstructure (SEM, TEM, AFM), crystallinity (GIXRD), thickness measurement (SE and XRR).
3/ The electrochemical study is exploratory since few publications are assessing this compound[7]. However, TMNs are actually in high interest because of their chemical stability, and their metallic-like properties in terms of electrical conductivity, higher then corresponding oxides[8,9] which is the case of Zn_3N_2[10].

In addition, this internship is an opportunity for both lab: IPVF and PMC, and each supervisor to collaborate and to initiate further projects. It will also support C. Badie, new tenure-track assistant professor at Chemical Depart., M4S (01/09/2025), to start her activities faster.

References

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