

2026 Doctoral Contracts

Thesis project title: Selectivity and kinetics of gas hydrate formation for the purification of biogenic hydrogen

Thesis supervisor(s): Bertrand Chazallon

Thesis project abstract (maximum 20 lines):

In the context of renewable hydrogen production, this thesis aims to explore purification strategies for biogenic hydrogen derived from biomass gasification. The project focuses on the separation of complex mixtures containing H₂, CO₂, CH₄ and potentially CO, representative of industrial synthesis gases. Two approaches will be investigated: (i) a fractional separation incorporating carbon monoxide, and (ii) a prior conversion of CO via the Water-Gas Shift reaction, leading to a simplified H₂/CO₂/CH₄ mixture. In this framework, biogenic methane, although a minor component, could act as a thermodynamic promoter by facilitating hydrate formation.

The objective is to assess to what extent the co-encapsulation of CO₂ and CH₄ in structure I hydrates can lower the formation conditions while promoting the exclusion of hydrogen into the gas phase, thereby opening the way for selective separation. A central focus of the project concerns the study of hydrate formation kinetics, in connection with intensification strategies (kinetic additives, porous media). Performance will be analysed in terms of storage capacity, formation rate and selectivity, under various initial conditions (ice, liquid water, aqueous solutions). Characterisation will rely primarily on spectroscopic techniques, in particular in situ Raman spectroscopy, enabling real-time monitoring of phase equilibria, formation kinetics and cage occupancy in complex gas mixtures. These approaches will be complemented by volumetric measurements and, occasionally, by X-ray diffraction for structural analysis.

Beyond the application to hydrogen purification, this work is part of a broader perspective on the study of gas-water interactions under extended thermodynamic conditions, such as the extreme environments of the icy moons of the solar system.

Planned recruitment date: 09/01/2026

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Additional remarks/comments: