



DN-MSCA-Horizon Europe  
Grant n°101119277

In the frame of the Doctoral Network MSCA Horizon Europe "ChimSep" dedicated to the integration of membrane separations (Organic solvent nanofiltration and membrane distillation) in fine chemistry, 13 PhD projects are funded for 36 months: 8 dealing with membrane science and 5 dealing with homogeneous catalysis.

See all the 13 projects at <https://theses.doctorat-bretagne.fr/dn-chimsep>

**Title- ChimSep-PhD#3: Atomistic modelling and molecular simulations of Organic Solvent Nanofiltration (OSN)**

**Joint doctorate**

## Offer description

At University of Rennes (22 months), PhD#3 of DN ChimSep will acquire skills in molecular simulations and will apply them to OSN for which the limited understanding of transport phenomena is currently one of the main hurdles to development despite its many potential applications.

He/she will develop molecular models of OSN membranes, considering polymer (Polyimide, PDMS...) membranes and polymer/MOF (HKUST-1, ZIF-8, MIL-53...) mixed matrix membranes.

He/she will further use molecular dynamic simulations to gain insight into solvent/membrane interactions at the molecular scale and to rationalize transport phenomena in OSN with pure solvents and solvent mixtures.

His/her work will allow for a better understanding of transfer inside complex membrane structures and of the solute/membrane and solvent/membrane affinities as well as preferential solvation of solutes in solvent mixtures. In order to complete his/her theoretical training on the fundamental aspects of OSN and to be able to apprehend the specific problems of OSN applications,

He/she will spend 12 months at K.U. Leuven (Belgium) to implement OSN experiments involving solvent mixtures. He/she will further compare the predictions from the simulations he/she will have performed at University of Rennes with the experimental results obtained at K.U. Leuven also using feedback from other experimental results of the DN ChimSep.

PhD#3 will spend 2 months at the TIA company (France) for training on process design at industrial scale and industrial requirements.

## Keywords:

Membrane separation, organic solvent nanofiltration, Modelling, molecular simulation

**PhD starting date:** 01/11/2023

**Application deadline:** 31/08/2023 (23:59:00, Paris)

<https://theses.doctorat-bretagne.fr/dn-chimsep>

**Work location:** Rennes, France (two years) & KU Leuven, Belgium (one year)

The Doctoral Candidate will be enrolled in a joint doctorate between two partners of the network. He/she will spend 22 months with the hosting partner (University of Rennes, France) of the present application and a mobility of 12 months at KU Leuven, Belgium

During the doctoral period, the PhD will also spend 2 months at TIA, Bollène-France working on membrane pilot design for industrial applications.

## Contacts

Thesis main supervisors (France)

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Thesis second supervisor (Belgium)

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**Required Education Level :** Master degree or equivalent

## Skills/Qualifications

The candidate will hold a Master degree or equivalent in chemical engineering or in chemistry with competencies in processes and/or membrane processes or in process modelling or molecular physics modelling

A previous experience in molecular simulation will be appreciated as well as in handling membrane processes will be appreciated

Enthusiasm, autonomy, scientific curiosity and ability to communicate are required qualities.

**Required Language:** English, level: Good

## Required research experience

An internship of several months in a research laboratory involved in modelling and/or membrane separation will be appreciated

## Website for additional job details;

See application platform: <https://theses.doctorat-bretagne.fr/dn-chimsep> section "Présentation de l'école doctorale » (doctoral network presentation)

## Salary

The EU provides support for each recruited researcher in the form of

- Gross salary per month: 2 764 € (net should be around 2 200 €) , an additional annual premium could be paid
- + 600 € of mobility allowance. All eligible researchers recruited within a DN are entitled to receive this allowance. It contributes to the private mobility related expenses of the researcher.

- + 495 € of family allowance per month (if eligible to the conditions: be married or equivalent and/or have a child; family, long-term leave and special needs allowances. The family status of a researcher will be determined at the date of their (first) recruitment in the action and will not evolve during the action lifetime.