PhD Position in Computational Simulation of Hydrogels for Water Purification Processes

The *Innovation in Materials and Molecular Engineering (IMEM)* research groups is looking for a PhD researcher to develop his/her PhD thesis project on the simulation and understanding of multifunctional, conductive polymer hydrogels that are responsive to thermal or electrochemical stimuli, with the goal of applying them to water purification processes. The ideal candidate should hold a degree in Chemistry, Physics, Chemical Engineering, Physical Engineering, or related disciplines, with a strong computational profile. Additional training through a Master's degree in Computational Simulation will be highly valued, and prior laboratory experience will be considered an additional merit.

The project will be developed primarily from a theoretical and computational perspective, although it may include an experimental component in collaboration with other members of the research team, depending on the specific needs of the project.

Project description: NEXT-GENERATION HYDROGELS FOR FUTURE WATER DESALINATION PROCESSES (HYDRO4F, PID2024-157005OB-I00)

The Hydro4F project seeks to develop sustainable water purification technologies by combining advanced hydrogel systems with solar and electrochemical desalination methods. It focuses on designing hybrid synthetic–biopolymer hydrogels integrated with photothermal materials (PTMs) to create efficient, reusable solar-driven evaporators (SDEs) for freshwater production from brackish sources, optimizing hydrophobic–hydrophilic balance and minimizing energy losses. In parallel, the project advances capacitive deionization (CDI) through the development of charged superabsorbent hydrogels that act as ion-exchange membranes in customized modular CDI cells to improve ion separation and filtration efficiency. Complementary theoretical simulations will support experimental work by elucidating hydrogel–water–salt interactions, guiding the molecular design of materials.

Activities to be carried out by the candidate: The selected candidate will undertake a doctoral thesis that provides original and scientifically significant results in the field of materials chemistry. The main objective of the thesis will be the simulation and understanding of multifunctional, conductive polymer hydrogels that are responsive to thermal or electrochemical stimuli, with the goal of applying them to water purification processes.

To achieve these objectives, theoretical and computational simulation methodologies will be employed, including Molecular Dynamics (MD), Coarse Graining (CG), Quantum Mechanics (QM), and hybrid QM/MM approaches, among others. Complementary experimental techniques may be applied for the preparation and characterization of hydrogels with optimized properties for the intended applications.

The PhD work will require the publication of research results in high-impact scientific journals, presentations at relevant conferences, participation in specific and transversal training courses, and the writing and defense of the doctoral thesis.

Duration of the Contract: The maximum duration of the contract will be **4 years**, in accordance with Section 3 of the call's terms and conditions.

Remuneration: 24,468.22 €/year as established in Royal Decree 203/2019. The corresponding amount will be paid in 12 monthly installments. The salary may not be less than 75% of the wage set for equivalent categories in the applicable collective agreements during any year of the contract.

Project Funding:

- Ministry of Science, Innovation and Universities (State Research Agency)
- Co-financed by European Social Fund Plus (ESF+)

Working Hours: 37.5 hours per week (full-time position)

Workplace: Escola d'Enginyeria de Barcelona Est (EEBE), Campus Diagonal-Besòs, Barcelona

Department: Chemical Engineering

Specific Requirements for Candidates: The selected individual must meet the requirements set out in Article 21(a) of Law 14/2011, of June 1, to be eligible for a predoctoral contract, or be in a position to meet these requirements at the time of the contract's formalization.

How to apply?

More information about this call can be found at:

https://talenthub.upc.edu/en/jobs/r1/ajuts-formacio-de-doctors-2025/ajuts-formacio-de-doctors-2025

Application **registrations period will be open from 30/10/2025 up to 24/11/2025**, and it will be done through the UPC electronic portal:

https://seuelectronica.upc.edu/ca/tots-els-tramits/Convocatoria_ajuts_contractes_predoctorals_formacio_doctors

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Application Deadline: November 24th, 2025

Candidate incorporation: March 1st – May 1st, 2026

Information about the research groups can be found at:

IMEM: https://imem.upc.edu/en

https://futur.upc.edu/IMEM-BRT

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