



INSTITUTO DE
TECNOLOGÍA
QUÍMICA



EXCELENCIA
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2023-2026



CSIC
CONSEJO SUPERIOR DE INVESTIGACIONES CIENTÍFICAS



UNIVERSITAT
POLITÈCNICA
DE VALÈNCIA

PHD POSITION IN COMPUTATIONAL CATALYSIS AND MACHINE LEARNING

The Advanced Materials for Novel Transformations Group of the Institute of Chemical Technology ITQ (UPV-CSIC) in Valencia offers a PhD position linked to the project entitled **"AI-Enabled Defect Engineering and Mechanistic Discovery in MFI Zeolites"**, funded by the "la Caixa" Foundation within the Junior Leader Postdoctoral Fellowships Program.

Structural defects in zeolites, such as silanol nests associated with framework vacancies, critically influence their catalytic performance, yet their atomic-scale origin and role in reactivity remain poorly understood. The project addresses this open problem by integrating high-throughput Density Functional Theory, machine-learning interatomic potentials, and automated transition-state search pipelines with advanced experimental characterization. The research is organized around three aims: (i) systematic characterization of silanol defects and their topological impact on zeolite pores, (ii) mechanistic understanding of why defect-containing zeolite samples can outperform defect-free analogues, and (iii) development of an AI-driven agent for automated validation and mechanistic interpretation of large simulation datasets. The project is led by Dr. Pau Ferri Vicedo within the group of Dr. Mercedes Boronat, and benefits from a unique environment at ITQ, where computational work is developed in direct collaboration with experimental researchers covering zeolite synthesis, advanced characterization, and catalytic testing. The candidate will develop a versatile computational profile acquiring expertise in periodic DFT calculations, neural network potentials, automated reaction-network exploration, and scientific large language model agents, all applied to chemically and industrially relevant problems at the frontier of zeolite science.

Candidate requirements:

Bachelor's degree in Chemistry

Holding a Master's Degree in Theoretical Chemistry or related topics by the contract-signing date. Background or strong interest in at least one of the following: DFT/molecular simulation, machine learning for chemistry, or zeolite/heterogeneous catalysis.

Contract details:

Three-year pre-doctoral contract, renewable for a fourth year, with competitive salary in accordance with CSIC regulations.

Contract-signing date: October 2026.

Doctoral Thesis in the Sustainable Chemistry Program of the Universitat Politècnica de València.

Interested candidates should send a motivation letter and CV to Dr. Pau Ferri-Vicedo; pafervi2@itq.upv.es and Dr. Mercedes Boronat; boronat@itq.upv.es.

Deadline for applications: June 15th, 2026