

Project title: **Optimizing Catalyst Design through Computational Chemistry and Machine Learning**

Job Offer

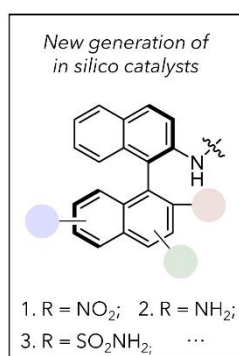
One 4-year funded PhD position is available at the ISQCH-University of Zaragoza, provided by the Spanish State Research Agency (AEI). The project offers a unique opportunity to work on catalyst discovery using computational chemistry, cheminformatics, and machine learning.

Requirements: A) a 240 ECTS BSc with a 60 ECTS MSc degrees, or B) a 300 ECTS BSc degree.

Job description and prospective applicant's profile

We are a dynamic research group that employs state-of-the-art techniques in computational chemistry and machine learning to explore different types of catalysis using automated protocols. Given the multidisciplinary nature of the project, applicants are expected to engage in collaborations with other computational and experimental groups. This entails a willingness to participate in international research stays, present their work at national and international conferences, and maintain a strong motivation to learn and effectively communicate with researchers working in different fields of chemistry.

Related references: *WIREs Comput. Mol. Sci.* **2023**, 10.1002/wcms.1663; *Chem. Eng. J.* **2023**, 466, 143346.



1. Computational screening



2. Machine learning predict.

- Yield
- Conditions
- Enantioselectivity

3. Experimental validation

- Collaborations with experim.

Gross salary and starting date

Starting date: January - February 2024

Deadline: September 30, 2023

Benefits

- One funded international research stay (3 months - 6,000 EUR provided)
- Funded attendance to national and international conferences (encouraged, 1,500 EUR/year)
- Final bonus (approx. 3,000 EUR)
- Optional remote working for 20-40% of the time (upon approval and after initial training)

Recommended skills

- Prior experience in computational chemistry, cheminformatics and/or Python programming
- Understanding basic concepts of physical organic chemistry
- Good written and oral English (an interview in English will be part of the selection process)
- A 3-month international research stay and attendance to one conference/year will be expected

Applications

Applications will be addressed to Dr. Juan V. Alegre Requena via email (jv.alegre@csic.es) including:

1. Motivation letter expressing interest in the research topic and computational research
2. CV detailing previous experience in computational chemistry and/or Python programming
3. At least one letter of support