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

Job Offer

One 3- or 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.
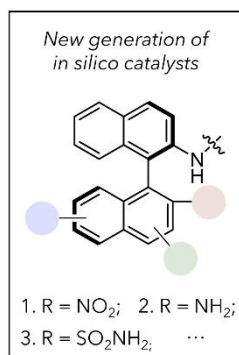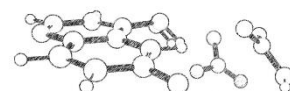
Gross salary, starting date and deadline

FPI 3- or 4-year PhD contract: year 1: 17,200 EUR, 2: 18,500 EUR, 3 and 4: 23,000 EUR pre-taxes. The total amount of money that the student obtains per year is significantly increased with bonuses (see below).

Starting date: March 2024   **Deadline for applications:** January 26, 2023

Bonuses and benefits

- One funded international research stay (3 months, 6,800 EUR after-taxes provided)
- Optional second international research stay (1 month, 6,000 EUR after-taxes provided)
- Funded attendance to national and international conferences (encouraged, 1,500 EUR/year)
- Final bonus (approx. 2,700 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
- *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