

PhD Position in Materials Simulations

Duration: 4 years

Gross salary: approximately 20k€/year

Location: Institute of Molecular Science, University of Valencia (Spain)

Funding: PhD Scholarship (FPI) within the research project “Computational Modelling of Complex Systems for Energy and Sustainability (CompPlex)”, reference PID2024-162840NB-I00, funded by the Spanish Ministry of Science, Innovation, and Universities (MICIU).

We offer a **4-year PhD position** in the MolMatTC group, under the supervision of Profs. [Juan Aragón](#) and [Joaquín Calbo](#) at the University of Valencia, to work in the field of solid-state theoretical simulations. The group’s research interests cover a wide range of topics, including charge transport, electroactivation strategies, and host–guest noncovalent interactions, from a computational perspective.

The research plan focuses on applying state-of-the-art theoretical methods within a multilevel approach to model and predict the structural and electronic properties of novel porous frameworks relevant to energy storage and conversion. Special emphasis will be placed on disentangling structure–property relationships to identify the most promising compositions for efficient charge transport. The theoretical work will be carried out in close collaboration with leading experimental groups, including Profs. Manuel Souto (CiQUS, USC) and Guillermo Mínguez Espallargas (ICMol, UV), experts in the synthesis and characterization of porous frameworks.

Eligibility: Applicants must hold a BSc degree in Physics, Chemistry, or Materials Science, and an MSc degree in a related field. A strong background in theoretical chemistry and/or physics is required. Solid computational and/or programming skills will be highly valued, as well as prior experience in computational modelling. Excellent written and oral communication skills in English are essential.

Start date: Tentatively late 2025 / early 2026. The selected candidate will join the Institute of Molecular Science (ICMol) at the University of Valencia, an interdisciplinary research center recognized as a “*María de Maeztu Unit of Excellence*” by the Spanish Research Agency.

Application: Interested candidates should contact Profs. [Juan Aragón](#) (juan.arago@uv.es) and [Joaquín Calbo](#) (joaquin.calbo@uv.es) by 20 October 2025. Applications should include a motivation letter, a short CV, and the contact details of two references. Please use the subject line: “*FPI 2025 application MolMatTC*”.