Call reference number	(2025-03)
Call name	Predoctoral position: Computational Nanochemistry
Application Deadline	2025/03/31

Introduction and main description

BCMaterials, Basque Center on Materials, Applications and Nanostructures, Leioa, Spain (www.bcmaterials.net), is an autonomous research center, belonging to Ikerbasque, the Basque Foundation for Science and the University of the Basque Country (UPV/EHU).

We seek a pre-doctoral student in Computational Materials Chemistry within the Horizon Europe MSCA Doctoral Network Track The Twin project. We offer a full-time position as a doctoral fellow for three years.
Quantum dots (QDs) exemplify the successful transfer of innovative nanomaterials from a lab-scale invention to a technology that offers better and more power-efficient electronic devices, or makes buildings generate renewable energy. Such implementations, however, keep QDs under permanent loading, such as constant illumination, elevated temperature or exposure to environmental agents. Efforts to make QDs resilient against loading induced ageing and loss of performance are time-consuming and costly.

The EU Doctoral Network Track The Twin addresses this problem through a research and training program aimed at creating and using QD digital twins (QDDTs). Focused on the case of QDs under illumination, this goal creates an exceptionally rich environment for research training of doctoral candidates (DCs) in nanomaterials. Research topics range from the latest methods of synthesis, structure analysis and time-resolved spectroscopy – from infrared to x-ray – to computational materials science. DCs will join forces to reach the common goal of demonstrating loading-resilient QDs synthesized according to best QD structures as predicted by the QDDTs.

To facilitate such a collaborative endeavour, all DCs will be trained to use and co-develop a common data platform and they will be permanently exposed to the diversity of environments needed to implement together a QDDT. Moreover, thanks to the deep collaboration between word-leading academic beneficiaries and start-up companies in nanomaterials and computational chemistry, scientific training is complemented by extensive transferrable skills.

Skills and Requirements

The candidate must have a Master in Materials Science, Chemistry, Physics or related areas.
Strong background in quantum chemistry (DFT) and/or molecular simulation. Familiarity with machine learning force-fields, Python-based computational chemistry workflows, or reaction network exploration tools is a plus.
Proficiency in speaking and writing in English.
Self-motivated and ability to work in a team and willing to coordinate the research in a particular topic.
A high level of motivation and independent thinking abilities.
Ability and eagerness to learn new skills outside own discipline
Presentation skills and able to meet the deadline are also required.

Work Program / Duties / Responsibilities

Main responsibilities include:

Applying multi-timescale simulation strategies (e.g., accelerated molecular dynamics, metadynamics) in the AMS by package by the Software Company and Modelling (SCM) to study QD reactivity pathways and photoexcitation-induced changes.
Integrating the ML force-fields into large-scale simulations, ensuring robust and accurate modeling of bond-breaking, surface reconstructions, and degradation mechanisms.
Benchmarking simulation outcomes against experimental data provided by experimental collaborators, and refining the simulation protocols to match observed trends in QD stability.
Developing custom data management strategies to efficiently handle and standardize large simulation datasets, in collaboration with project partner MZ.
Participating in project-wide discussions to provide feedback on QD surface reactivity and contributing to publications, presentations, and outreach activities.

The candidate will also:

Contribute to the use of QDs by improving understanding of their long-term stability and processes-of-failure under illumination.
Explore reversible and irreversible reactivity pathways on QD surfaces, using ML-driven reaction exploration tools combined with quantum chemical methods.
Assess the influence of environmental conditions (temperature, ligand coverage, gas atmosphere) on degradation mechanisms through multi-timescale modeling.
Demonstrate illumination resilience of optimized QDs by benchmarking computational results against experimental spectroscopic data (e.g., lifetime measurements, PL spectra).

Finally:
The PhD student will be incorporated at BCMaterials at the Computational Materials Science transverse lines under the supervision of Ivan Infante, Ikerbasque Research Professors.
The candidate will be in close contact with several renown international groups in the field of QDs, in Europe and the rest of the world.

Application Procedure

Apply by submitting a motivation letter and a CV (in English) using the "Contact" button at the corresponding offer, at the "Join Us" area on BCMaterials' portal (https://www.bcmaterials.net/join-us).
Your name and email address will be required for furher contact too.

Other Relevant Information

Include contact details for 2 referees.
Interviews will be conducted soon after the deadline.
The preferred starting date to join is June 2025.

For full details, visit: https://euraxess.ec.europa.eu/jobs/320915