Call reference number	(Track-MSCA-DN-1)
Call name	Pre-doctoral position EU Doctoral Network Track-the-Twin: Computational Nanochemistry
Application Deadline	2024/08/31

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 training.

Skills and Requirements

The candidate must have a PhD in Materials Science, Chemistry, Physics or related areas.
A background in computational chemistry is desirable but not compulsory. Knowledge in the modelling of QDs is also required.
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 his/her own discipline.
Presentation skills and being able to meet the deadline are also required.

Work Program / Duties / Responsibilities
The Pre-doctoral candidate's primary focus will be to use density functional theory to perform static and dynamic electronic structure calculations of QD models in their ground and excited states. These will be used to develop machine-learning force fields of QDs. The Predoc will be incorporated at the Computational Materials Science transverse research line of BCMaterials, under the supervision of Ivan Infante, Ikerbasque Research Professor. 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
Only applications entered through EURAXXES will be considered. **For full details, please visit: https://euraxess.ec.europa.eu/jobs/251120**

Other Relevant Information
After a first assessment of the quality of the CV and the motivation letter, best-ranked candidates will be invited for an interview during September 2024. The final selection will be based on the CV, the motivation letter and the interview. Contracts will start on December 1st, 2024 at the earliest. We do not accept late applications.