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| **Call reference number** | (2026-02) |
| **Call name** | Predoctoral position: Computational Nanochemistry |
| **Application Deadline** | 2026/02/06 |

## 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 are seeking a predoctoral researcher to join our research team to design in-silico using Density Functional Theory an array of novel colloidal Quantum Dots (QDs) for high performance radiation detectors, with particular emphasis on double beta decay. This rare nuclear process if proceeds without neutrino emission can establish neutrinos as Majorana particles and explain the asymmetry of the universe.

The work will be carried out at BCMaterials in Ivan Infante's computational group. This project has been funded by the European Commission within the EIC-Pathfinder Open with title: "Hybrid Nanocomposite Scintillators for Transformational Breakthroughs in Radiation Detection and Neutrino Research" (UNICORN).

This is a full-time position and the successful candidate will be enrolled for one year. If you are interested in this opportunity, please submit a CV and cover letter outlining your relevant experience and research interests.

## Skills and Requirements

The candidate must have a Master in Materials Science, Chemistry, Physics or related areas.
A background in computational chemistry and machine learning is desirable but not compulsory.
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

The PhD candidate's primary focus will be on studying the electronic structure and optical behavior of semiconductor quantum dots (QDs), along with how these properties interact with ligands. This will involve a detailed analysis of the electronic structure, investigating how doping alters these properties, the impact of surface termination, and the role of surface traps. To achieve this, the candidate will use density functional theory (DFT) and classical molecular dynamics calculations. These calculations are crucial for predicting the strength of optical transitions in new compounds and determining the exact energy level of dopants in quantum dots. This information is vital for advancing our quantum dot engineering projects

| **Work Program / Duties / Responsibilities** |
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| The PhD student will be incorporated at BCMaterials at the Computational Materials Science transverse lines under the supervision of Ivan Infante, Ikerbasque Research Professors.<br><br>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** |
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| 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).<br>Your name and email address will be required for furher contact too. |

| **Other Relevant Information** |
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| Include contact details for 2 referees.<br>Interviews will be conducted soon after the deadline.<br>The preferred starting date to join is March 2026. |