PhD Position in Theoretical Chemistry and Computational Modelling

Applications are invited for a 4-years predoctoral contract in computational chemistry, available from May 2026, to work under the supervision of Dr Daniel Reta in the Faculty of Chemistry at the University of the Basque Country, Donostia, Spain. The candidate will be enrolled in the Doctoral Programme in Theoretical Chemistry and Computational Modelling (TCMM).

This position will focus on the computational description of intramolecular charge-to-spin conversion in organic molecules, in the context of the ERC Starting Grant "*RadicalProtON*". The project aims at establishing new ways of introducing radical properties in organic molecules and gain mechanistic insights into their chemical reactivity and biological function.

Position Details:

- **Title:** Computational Design of Organic Molecules for Charge-to-Spin Conversion.
- **Duration**: 4 years.
- **Start Date**: Flexible, between May and August 2026.
- **Gross Annual Salary**: Approx. €21.000
- **Location**: Faculty of Chemistry, University of the Basque Country EHU, Donostia, Spain.

About the Project:

Organic radicals –metal-free molecules with unpaired electrons– offer unique magnetic and reactivity properties, allowing access to, for instance, novel qubit implementations and valuable chemical transformations. However, due to the reactive nature of radicals and the non-trivial chemistry required for their preparation, strict structural and electronic limitations are imposed on the available systems, limiting their potential applications.

In our group, we approach this problem from a multidisciplinary perspective that integrates computational modelling, advanced spectroscopic techniques and organic synthesis. The overall aim of our research is to develop mechanisms that enable facile radical formation in simple reaction conditions, employing available and inexpensive reactants, and applicable to a broad range of molecules, to fully harness the extraordinary properties of organic radicals.

Building on ongoing studies at the group, you will contribute to our goal using a range of computational chemistry methods. In particular, you will be involved in the following tasks:

- Design purely organic molecular architectures capable of undergoing charge-to-spin separation.
- Study the formation process and electronic structure of the resulting radicals. For this you will employ density functional theory and multireference-based methods.
- Investigate the reactivity of radicals to characterise reaction profiles and gain mechanistic insight into novel chemical transformations and biological functions. This work will employ molecular dynamics approaches, using both classical and *ab initio* formalisms.
- Data processing, following internal procedures to comply with FAIR practises, and report writing.
- Participate in group meetings and present periodically your research progress.
- Attend conferences and congresses to present the results obtained.

You will be joining a young, highly motivated, and dynamic group, where you will work in close contact with group members specialising in the synthesis and characterisation of the molecules under study. As a result, you will be in an environment that will allow you to validate your work, engage in a continuous and

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constructive exchange of ideas with your experimental colleagues, and maximise the impact of your research. Overall, you will be contributing towards advancing a highly ambitious and multidisciplinary project, with the potential to reveal new, radical-based reaction mechanisms and establish fundamentally novel design strategies in the field of organic magnetism.

Alongside computational work, you will be trained in critical data analysis, experimental design, and interpretation of mechanistic results, developing strong problem-solving and reasoning skills. You will also receive guidance in scientific writing, oral communication, and presentation skills, as well as project management, time management, and research planning. Opportunities for networking and interdisciplinary collaboration will further enhance career readiness. This integrated approach ensures that you will graduate with a broad skill set encompassing computational, analytical, mechanistic, and professional competencies, preparing you for diverse careers in academia, industry, or sustainable chemistry leadership.

More information can be found in the group's website.

Qualifications:

We seek a highly motivated candidate with the following qualifications:

- **Required**
  - MSc in Chemistry, Physics, or a closely related field. Applicants finishing their MsC in Summer 2026 will also be considered.
  - Good oral and written communication skills in English.
- **Preferred**
  - Experience with wavefunction-based methods.
  - Experience modelling open-shell systems.
  - Experience with molecular dynamics calculations.

Benefits:

- Opportunity to work in a state-of-the-art laboratory with access to advanced research facilities and international collaborators.
- The possibility to undertake research secondments in world-leading institutions to broaden your skillset.
- A highly stimulating research environment and unique career development opportunities.

About the Team:

Our research group deals with different aspects of molecular magnetism and our interest ranges from purely organic systems to metal-containing compounds, spanning almost every magnetic element of the periodic table. Current efforts in our group focus on establishing a general approach to obtain diradicals in π-conjugated donor-acceptor molecules, by exploiting the interplay between charge transfer and open-shell states. For this, we direct a concerted experimental and computational effort to synthesise targeted molecules, characterise their magnetic and optical properties, and model their electronic structure. For the former, we count with a newly refurbished laboratory, hosting a recently installed Bruker *EMX-Plus* X-band electron paramagnetic resonance spectrometer – for the latter, we count with *Hyperion*, a new, free to access, state-of-the-art supercomputer at the Donostia International Physics Centre (DIPC), ensuring access to the required computational infrastructure.

Additionally, we are part of the *Theoretical Chemistry* group at the EHU, a broader research environment with established expertise in diverse computational chemistry methodologies, ranging from formal

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development of electronic structure methods to applied bioinorganic chemistry. This rich and supportive environment offers a depth of expertise that is difficult to match and provides an ideal setting for scientific development.

Selection process:

Shortlisted candidates will be notified of the interview date **w/c 20 April 2026**. Interviews will be held online between the 27th - 30th April 2026. As part of the interview process, candidates who have been shortlisted will be required to make a brief presentation: 3 slides and no more than 5 minutes. This will be about a research project you have undertaken/is undertaking (e.g. final year undergraduate project). Adjustments for interviews will be made to ensure equality for the candidates, e.g., questions in advance for individuals with neurodiversity; flexible interview timings for individuals with caring responsibilities, socioeconomic status, etc.; extra time if necessary for individuals with disabilities.

How to apply:

Applications, in a single PDF file, should be emailed to Dr. Daniel Reta with the subject "RadicalProtON – Computational PhD Application", to daniel.reta@ehu.eus before April 17th 2026, containing:

1. Curriculum vitae.
2. A short description of previous research (0.5 pages).
3. Contact information for two academic references (optional).

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