



PhD Position in Spectroscopic Studies of Charge-to-Spin Conversion in Organic Molecules

The group of Daniel Reta, located at the Faculty of Chemistry of the UPV/EHU in San Sebastian, Basque Country, Spain, is looking to appoint a motivated and talented PhD student. This position will focus on the magnetic and optical characterisation of charge-to-spin conversion in organic molecules, within the framework of the ERC Starting Grant project “*RadicalProtON*”. The project aims to establish new ways of introducing unpaired electrons in organic molecules, and as such, radical and magnetic properties, and exploit them to develop novel chromophores and drugs. The candidate will be co-supervised by Dr. Virginia Martinez (Faculty of Science and Technology, EHU/UPV, Leioa, Vizcaya).

Position Details:

- **Duration:** 4 years.
- **Start Date:** Flexible, but November 2024 would be preferred.
- **Location:** Faculty of Chemistry, UPV/EHU, San Sebastian, Basque Country, Spain.

Research Focus:

Organic molecular magnetism is a rapidly evolving field that offers exciting applications in diverse areas, ranging from qubits to chemical synthesis. However, the currently available molecular architectures use only a fraction of the available chemical space, inadvertently limiting the full potential this field has to offer. Current efforts in our group aim at remedying this – we employ a concerted experimental and computational approach to establish and exploit general strategies that introduce magnetic properties in broader families of organic molecules.

Building on ongoing studies at the group, you will apply a range of spectroscopic techniques to study the electronic structure of organic diradicals that can convert charge into spin. In particular, you will:

- Characterise the magnetic properties of the proposed molecules by means of electron paramagnetic resonance and magnetometry (San Sebastian).
- Investigate the optical properties of the targeted molecules by means of absorption, emission and time-resolved, transient spectroscopy (Leioa).
- Assistance in synthesising the targeted molecules (San Sebastian).

You will be joining a young, highly motivated, and dynamic group, where you will work in close contact with group members who focus on the computational description of the molecules you will study. As such, you will be in an environment that will allow you to validate your work, engage in a continuous and constructive exchange of feedback with your theoretical 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 chromophores and covalent inhibitors.

The candidate will be based at the Faculty of Chemistry of the UPV/EHU, in San Sebastian, Spain, but will undertake short visits to Dr Martinez’s lab. The position is funded by the European Union within the program “Horizon Europe” under the ERC-2023-StG, [RadicalProtON](#), 101116089.



**Qualifications:**

We seek a highly motivated candidate with the following qualifications:

- **Required**
 - Master's degree in Chemistry, Physics, or a closely related field.
 - Good oral and written communication skills in English.
- **Preferred**
 - Experience with spectroscopic techniques (NMR, IR, UV-Vis, etc).
 - Experience in programming to analyse data.

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 is based at the Faculty of Chemistry of the University of the Basque Country, located in the beautiful city of Donostia. We work in the field of molecular magnetism and our interest ranges from purely organic systems to metal-containing compounds, spanning almost every magnetic element of the periodic table. Among others, and related to this project, 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. To tackle this ambitious project, we count with a newly refurbished laboratory that hosts a recently installed *EMX-Plus* X-band electron paramagnetic resonance spectrometer, that will be used to carry out the magnetic characterisation. For the optical studies, Dr Virginia Martinez, who will be the candidate's PhD co-supervisor, will provide the necessary expertise and instrumentation, ranging from standard photophysical characterisation to time-resolved spectroscopy. Dr Martinez is based at the Faculty of Science and Technology of the EHU/UPV, in Leioa, a short 50-minute drive from San Sebastian.

More information can be found in the group's [website](#).

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How to apply:

Applications should be emailed to Dr. Daniel Reta and Dr Virginia Martinez-Martinez with the subject “RadicalProtON – Spectroscopy PhD Application”, to daniel.reta@ehu.eus and virginia.martinez@ehu.eus before October 18th 2024, 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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