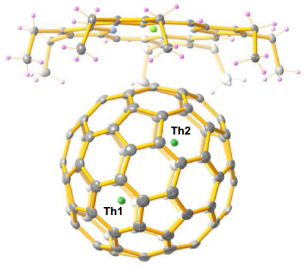
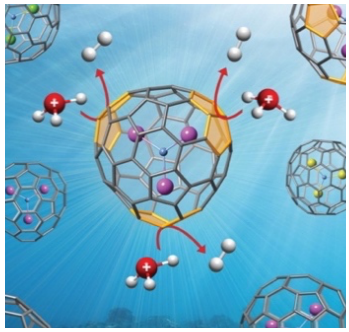
PhD Position in the Quantum Chemistry Group at the URV (Tarragona)

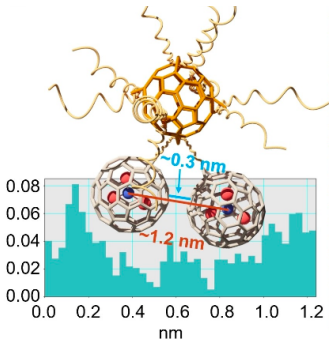
The Quantum Chemistry Group (QCG) of the Universitat Rovira i Virgili (URV) has a long research tradition that goes back to the end of the 1970s. Ever since, the primary goal of the QGC has been to contribute to the understanding of the electronic structure and the properties of complex systems. The present research lines of the QCG involve the analysis and modeling of (photo-)catalytic reaction mechanisms, both homogeneous and heterogeneous; the physico-chemical properties of carbon nanostructures and molecular metal oxides; and the development of the GronOR code for non-orthogonal configuration interaction.

The QCG is now accepting applications for a 4-year PhD position within the call 2026PMF-PIPF of the *Martí i Franquès Program*, financed by the Universitat Rovira i Virgili (code 2026PMF-PIPF-22) to work in the thesis project "Computational study of the metal-metal bond, reactivity and electrocatalytic properties of carbon nanostructures" under the supervision of Prof. A. Rodríguez-Fortea. During the PhD period, presentation of the results in international conferences and a 3-month stay abroad are expected.
[call: *https://seuelectronica.urv.cat/treballar-a-la-urv/2026pmfpipfenglish.htm*]

Research lines to develop during the PhD
(i) Characterization of the structure and the physico-chemical properties, metal-metal bond as well as the reactivity, of new carbon materials, focusing on new lanthanide and actinide-based endohedral metallofullerenes.
(ii) Modeling of electrocatalytically activated environmental-benign and high value-added processes, such as HER, ORR and OER, using carbon nanostructures.







Methodology
State-of-the-art computational methods: Quantum methods, Classical Molecular Dynamics (MD), *Ab initio* Molecular Dynamics (AIMD).

Requirements of the candidates
We are looking for an enthusiastic person with strong motivation for scientific research recently graduated in a MSc degree in Theoretical or Computational Chemistry or related disciplines as Chemistry, Physics, or Material Sciences. High English level (oral and written) is mandatory. Good communication skills and the ability to work well, both individually and as team member, are also required. Practical experience in the use of high-performance computers, Linux environments, quantum chemistry codes (electronic structure calculations, molecular dynamics, solid state) and machine learning techniques will be positively assessed.

Submission of online applications
From May 11th 2026 to June 12th 2026.

Conditions
Contract length: 1+1+1+1 years
Estimated incorporation date: October 2026.

Interested candidates please send to Prof. Rodriguez-Fortea (antonio.rodriguezf@urv.cat) a motivation letter, a full CV (with academic records), a recommendation letter and the name and email addresses of two senior scholars that have worked with the candidate.