PhD fellowships 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 derived properties of large and complex systems. The present research lines involve the analysis and modeling of homogeneous and heterogeneous catalytic reaction mechanisms; the study of photochemical reactions; the interpretation of spectroscopic, red-ox and magnetic properties of molecules, nanoclusters and solids.

The QCG is now accepting applications of graduate students to join one of the two following projects:

1) "Computational Study of Low-Valent Actinides Interacting with Carbon Nanoforms" led by Dr. Antonio Rodríguez-Fortea.

2) "Electron and energy transfer in organic solar cell materials: Method development in GronOR, a massively parallel code for nonorthogonal configuration interaction" led by Dr. Coen De Graaf.

Project #1: Computational Study of Low-Valent Actinides Interacting with Carbon Nanoforms, supervised by Dr. Antonio Rodríguez-Fortea.

Description

Our group has so far significantly contributed to the understanding of the electronic structure and reactivity of endohedral metallofullerenes (EMFs, carbon cages that encapsulate metal atoms or clusters) [*Angew. Chem. Int. Ed.* **2005**, 44, 7230; *Nature Chem.* **2010**, 2, 955]. EMFs that contain actinides have been synthesized and characterized very recently, as for example, the thorium-containing metallofullerene $Th@C_{82}$, in the group of Ning Chen in Soochow (China), which shows very interesting luminescence properties. Echegoyen at UTEP (USA) and Chen have detected in mass spectrometry experiments new cages encapsulating U atoms, as $U@C_{2n}$ (2n = 74, 76, 80-88), $U_2@C_{2n}$ (2n=78, 80) or clusters $U_2C@C_{72}$, $U_2N@C_{72}$, $U_2O@C_{72}$, $U_2O@C_{74}$, $U_2N@C_{78}$. Our group has already analyzed some of these systems and seen that the interaction between the actinide and the fullerene cage is more covalent than for lanthanides [*JACS* **2018**, 140, 18039]. Following the collaboration with the groups of Chen and Echegoyen, in the present project we plan to analyze the uranoclusterfullerenes observed so far by these groups and those actinidofullerenes eventually to come focusing on the actinide-fullerene interaction and the actinide-actinide bond in $An_2@C_{2n}$. Recent work in our group has shown that the U dimer can be formed with a rather strong U-U bond inside a fullerene or on a 2D graphene sheet [article submitted for publication]. These carbon nanoforms are able to stabilize uranium ions with low oxidation states (3+ or 2+) that can share their electrons to form dimers with strong triple or quadruple bonds. It is our goal in this project to go beyond uranium and study the bond in other actinide dimers as for example Th_2, Pa_2, Np_2, etc. when supported on graphene. We will also plan to dope the graphene layer with boron and evaluate the increase in the interaction energy of the actinides with graphene so that these B-doped layers could be potentially used as extracting agents of uranium and plutonium from spent fuel in nuclear power plants. In collaboration with the experimental groups in UTEP and Soochow, functionalization of

these carbon nanoforms with external groups (donor or acceptors) will be also considered, to analyze the intramolecular charge transfer processes.

Requirements of the candidates

The applicant should have (by the incorporation date) a master degree in fields related to chemistry, physics, material sciences or chemical engineering. High English level (written and oral) is mandatory, and the ability to work well, both individually and as team member, is also required. Practical experience in the use of high-performance computers, Linux environments, quantum chemistry codes (electronic structure calculations, molecular dynamics, solid state) will be positively valued.

Conditions

Contract length: 1+1+1 years
Estimated incorporation date: The candidate is expected to begin in October 2019.

Candidates please send a CV and a motivation letter to antonio.rodriguezf@urv.cat with the subject "PhD fellowship at the QCG".

Project #2: Electron and energy transfer in organic solar cell materials: Method development in GronOR, a massively parallel code for nonorthogonal configuration interaction, supervised by Dr. Coen de Graaf.

Traditional silicon-based solar cells have become quite efficient both in production costs and conversion, but organic photovoltaics have several potential advantages such as lower production costs, portability, flexibility and their light weight. Although efficiency is steadily increasing, the solar cells based on organic materials still need further development to become serious additions to the silicon based cells. Inter- and intramolecular transfer of energy and electrons play a key role in these materials. These concepts, rather elusive from the experimental point of view, can be studied in great detail with theoretical approaches. Many theoretical studies rely on simple phenomenological models or TD-DFT approaches, ignoring essential factors such as orbital relaxation or electron correlation. The nonorthogonal configuration interaction (NOCI) implemented in GronOR as open-source code offers a thorough and reliable way to evaluate energy and electron transfer without loosing the beauty of the intuitive interpretation of the results inherent to the phenomenological models. The NOCI approach starts with the generation of a set of monomer many-electron wave functions that include full orbital relaxation, static and dynamic electron correlation, and environmental effects. These monomer wave functions are then used to construct spin-adapted diabatic states of the whole system, followed by a NOCI between these many-electron basis functions to calculate the energies and wave functions of the relevant electronic states, together with the electronic coupling between the diabatic states. In this way the final wave function expansion remains short, facilitating the interpretation of the physics of the system.
GronOR is a joint initiative of the University of Groningen (Netherlands), the Universitat Rovira i Virgili (Tarragona, Spain) and the US National Laboratory at Oak Ridge, Tennessee. It is massively parallelised and runs very efficiently on CPU/GPU machines, but the code needs to be further optimised and additional features have to be implemented to unleash the full power of the NOCI. In addition to the implementation of a properties section, Cholesky decomposition of the integrals, gradients and non-adiabatic couplings are some of the items on the to-do list. Combining code development with applications

of the method in the field of organic solar energy has the potential to make important contributions to the development of efficient and clean alternatives to traditional fuel sources.
We are looking for an enthusiastic person with experience in coding and/or method development, recently graduated in a Master related to alternative energy sources, Theoretical Chemistry or Physics. Note that the grant implies some teaching duties in the bachelor degree in Chemistry of the Universitat Rovira i Virgili. Teaching can be done in English, Spanish or Catalan.

For further information please contact Coen de Graaf (coen.degraaf@urv.cat).