

Spin-Crossover Systems in Carbon Nanostructures

We offer a four-year PhD position (FPI) at the Theoretical and Computational Chemistry Institute (IQTC-UB) at the University of Barcelona, in the field of computational modelling of spin-crossover (SCO) devices inserted in carbon nanostructures.

The successful candidate will study by means of computational and theoretical tools the interplay between the spin-state of a transition metal complex and the electronic properties of several carbon nanostructures, including carbon nanohoops, nanoribbons, graphene layers and nanotubes, among others. Due to the nature of the project, interaction with experimental groups is anticipated.

We are looking for a student with a Master's degree in Chemistry, Theoretical Chemistry, Nanoscience or related field, with a strong background in inorganic/coordination chemistry and good written and oral communication in English. Good programming skills and expertise with Python, bash scripting, computational modelling or Linux/Unix management will be valued.

IQTC-UB is located at the University of Barcelona, and has renewed its accreditation as Center of Excellence by the Spanish Agency for Research. Find more information about the institute at <https://www.iqtc.ub.edu/>.

Interested candidates must send a motivation letter and Curriculum Vitae to Dr. Jordi Cirera (jordi.cirera@qi.ub.es) with the email subject "SCO-nanoC". Application period will be 12th to 26th of January 2023. The successful candidate is expected to start on September 2023.