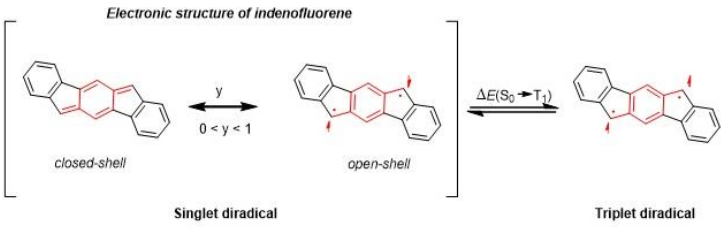
Single-Molecule Electrical Conductance Measurements of Novel Organic Biradicals

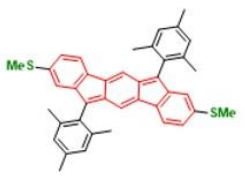
❖ About the project

This PhD project aims to investigate novel organic biradical molecules based on the indenofluorene moiety and to assess their conductance, spintronic and thermoelectric performance in single molecule junctions. The candidate will participate in the project BIINTEL (PID2021-127964NB-C21) which combines the synthetic group of Alba Millán (University of Granada, Spain) and the molecular electronics group led by Edmund Leary (IMDEA Nanociencia). The synthesis of new organic biradicals will be undertaken at UGR whilst the transport measurements will be performed at IMDEA Nanociencia.

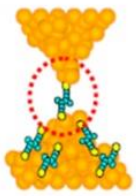
Biradicals have an even number of electrons, but with two existing in an unpaired state. This open-shell electronic structure makes biradicals interesting candidates for applications in key areas of molecular electronics and materials science, such as molecular magnets, and as efficient conductors of electrical charge. Furthermore, such compounds show great promise for thermoelectric devices thanks to their typically sharp transport resonances in energy spectra. This is expected to generate large Seebeck coefficients, essential for making highly efficient devices. The aim is to improve on current technology which relies on materials with toxic elements like bismuth telluride.

Indenofluorenes are relatively stable, synthetically flexible, organic compounds which exist in the ground state as a mixture of open and closed shell electronic configurations. Interestingly, the singlet-triplet energy gap can be rather small, meaning interconversion can occur simply by changing the temperature. This opens up the possibility of making temperature sensitive devices, if the conductance can be shown to depend on the electronic configuration. Further testing will also look at bias voltage control over the switching.





Indenofluorene incorporating binding groups



Schematic of a molecular junction

The candidate will be tasked with characterizing each compound using the scanning tunneling microscopy break-junction technique. This forms single molecule junctions which will then be subjected to further characterization using current-voltage (I-V) spectroscopy and thermopower measurements. Initially, gold electrodes will be used, which are robust and stable to oxidation. Gold is, however, non-magnetic and other metals will be explored to probe spin transport phenomena. The candidate will develop the methodology necessary to work with these metals, including nickel, cobalt or iron, which are highly sensitive to surface oxidation. Protocols will be

developed to use these metals as electrodes, leaving their surfaces free from oxide and thus able to bind directly to individual molecules. Electrochemical techniques as well as environmental chambers will be explored. As part of the PhD, a secondment of 3-6 months at IBM Europe is envisaged to undertake complementary characterization of the compounds.

For further information about the project please contact the project lead Dr. Edmund Leary (edmund.leary@imdea.org) and visit https://idealcofund-project.eu/phd/phd-projects/single-molecule-electrical-conductance-measurements-of-novel-organic-biradicals/.

❖ Applicant´s requirements

An ideal candidate would have a degree in Chemistry, Physics or Engineering. Previous knowledge in electrochemistry, nanoelectronics or spintronics will be valued. They will also have completed (or be about to complete) a Master's degree.

Prior knowledge of scientific acquisition/analysis programs (such as Labview or Matlab) will be valued, as will demonstration of programming skills with these or other programs.

It is expected that the successful candidate will be independent, creative, curiosity-driven, motivated to explore solutions to difficult scientific problems, and have a strong work ethic.
A good knowledge of English is required.

❖ How to apply

Application deadline: 10 April 2023 (17:00 CET)

This project is part of the IDEAL PhD Fellowship Programme led by Fundación IMDEA Nanociencia and co-funded by the **Marie Skłodowska-Curie Actions (MSCA) COFUND programmes.** IDEAL PhD will offer 12 fellowships in two open calls to outstanding doctoral candidates to undertake a PhD research project in any of the programmes at the Institute. More information at IDEAL PhD Fellowship programme.

Applicants must submit their applications through the IDEAL PhD Fellowship Programme website. Before submitting your application, please download and check the Guide for Applicants and templates.

❖ About IMDEA Nanociencia

The IMDEA Nanoscience Institute, created in 2006 at the initiative of the Community of Madrid, is an interdisciplinary research centre dedicated to the exploration of basic Nanoscience and the development of nanotechnology applications in connection with innovative industries. IMDEA Nanociencia has been a "Severo Ochoa" Centre of Excellence since 2017, this is the highest national recognition for scientific excellence granted by the Ministry of Economy, Industry and Competitiveness. The Institute is located and forms part of the UAM-CSIC Cantoblanco Campus of International Excellence, a highly competitive research environment worldwide.