ESR 10 position

Project title: Dynamic covalent capsules based on calix[4]pyrrole scaffolds

Location: ICIQ, Spain

Supervisor: Prof. Pablo Ballester

Objectives of the individual project:

- 1) Acquisition of expertise in synthetic and characterization procedures of calix[4]pyrrole capsules based on dynamic imine covalent bonds (WP1).
- 2) Evaluate and study the self-assembly of the capsules in the presence/absence of a templating guest and their self-assembly reversibility.
- 3) Characterize the prepared dynamic covalent capsules and their encapsulation processes by different techniques (NMR, HRMS, X-ray diffraction).
- 3) Gain experience in mass spectrometry techniques for quantitative thermodynamic measurements of his/her already prepared molecular capsules (Academic Secondment) (WP4).
- 4) Discover the power of computational methods in supramolecular chemistry.
- 5) Find out the importance of the industrial sector in research development (Industrial Secondment)



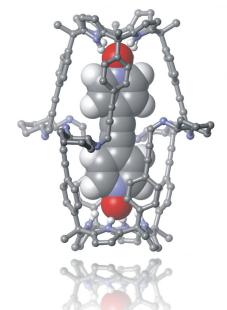
The ESR is expected to develop a series of molecular assemblies based on dynamic covalent bonds able to operate in water or in organic solvents recognizing revenant guest (either biologically relevant or catalysts and initiators for adhesive formulation). In addition, she/he will demonstrate the switchable ability of some of the molecular capsules by an external stimulus (i.e. moisture, light incidence). Moreover, a complete characterization of the assemblies is expected: solid-state structures, thermodynamic, kinetic and photophysical characterization in solution, and gas-phase characterization.

Planned secondment(s):

Academic secondment: During his/her 3 months of secondment at FUB ESR10 will investigate the potential of mass spectrometry techniques for quantitative thermodynamic measurements on systems that show the most promise or most difficulty using other techniques.

Industrial Secondment: Six-months secondment at Covestro facilities in ChemPark in order to gain experience in industrial applications of capsules in coating materials (stability studies of the capsules in polyurethane matrices, determination of the new coating properties such as transparency, scratch resistance, adhesion tests, curing...).







Eligibility requirements

EU eligibility criteria for candidates: Candidates of any nationality, but in order to be eligible for the positions the following criteria applies to all applicants:

- The applicant shall at the time of recruitment be in the first four years of his/her research career and have not been awarded a doctoral degree.
- The applicant must not have resided or carried out his/her main activity in Spain for more than
 12 months in the 3 years immediately prior to the recruitment.

Candidates profile: candidates must hold a Master's degree in Chemistry with excellent academic transcripts. We are looking for highly motivated students with good communication skills

All candidates must **prove full proficiency in spoken and written English** (B2 certificate, TOEFL, or equivalent).

Questions regarding the recruitment can be sent to: noah@noah-itn.eu.

Questions regarding the project can be sent to: pballester@iciq.es or garagay@iciq.es



