FINAL MASTER PROJECT PROPOSAL

Title

Elaboration and study of covalent organic frameworks

Supervisor(s)

Dr. Ignacio Gascón Sabaté
Dr. Olivier Roubeau

Summary of the project

The fabrication of covalent organic frameworks (COFs) two-dimensional (2D) nanofilms with large lateral size and homogeneous morphology is a great challenge for the development of nanotechnological devices.

The aim of this proposal is to study the formation and structure of COFs at an air-liquid or liquid-liquid interface, thereby favoring 2D thin films that can then be easily transferred to many substrates for their study. Metalloporphyrin molecules bearing 4 amine substituents and simpler aromatic building units with various amine groups will be used in combination with adequate aldehyde reagents to form ordered 2D and porous 3D polyimine networks, respectively.

The used metalloporphyrin nodes can embody molecular spin-based quantum bits. The studies planned in this master project are of great interest for their implementation into solid-state devices proposed as architecture to develop quantum computation. On the other hand, porous 3D COFs can adsorb specific gases depending on their pore size and chemical composition, thereby arousing interest in gas separation applications. Through this master project, thin membranes of the selected 3D porous COFs will be accessed, and their ability to adsorb CO_2 and volatile organics studied.

The films structure, crystallinity and domain size will be determined (techniques: X-Ray diffraction, Scanning and Transmission Electron Microscopy, Scanning Probe Microscopy) and the conditions of their formation optimized accordingly. Spectroscopic and magnetic characterization will be used to ensure the metalloporphyrins 2D COF films maintain the properties of interest of the isolated nodes. (techniques: UV-Vis absorption spectroscopy, magnetic susceptibility, Electron Paramagnetic Resonance). Preliminary assessment of the CO_2 adsorption/desorption of the porous COFs films will be done using quartz crystal microbalance.

This is an interdisciplinary work that requires two supervisors: Dr. Gascón for the optimization of the film interfacial formation and studies of gas adsorption and Dr. Roubeau for the synthesis of different building units for the films, and for the study of their magnetic properties.