



Post-doctoral position

Study of the interaction between model molecules and carbonaceous surfaces in porous biochars for the determination of an optimum compatibility between adsorbent and contaminants

Contact : Diane Rébiscoul, phone : +33 4 66 33 93 30, e-mail : diane.rebiscoul@cea.fr

Location: Institut de Chimie Séparative de Marcoule (ICSM) CEA Marcoule BP 17171 - 30207 Bagnols sur Cèze, FRANCE

Duration: 12 months from the 1st december 2024 to the 30rd november 2025

Salary: 2700 euros/month

Topic

Biomass can be used to prepare Porous Carbon Materials (PCM) such as hydrochars and biochars. Despite the energy costs involved in their fabrication, these materials have a negative net carbon balance by storing 20% of the carbon in a stable form. Generally, these materials present a large pore size distribution, from the macro to the microscale. They are used as fertilizers, but can also be used as adsorbent materials for organic molecules present in liquids and gases (volatile organic compounds, condensable hydrocarbons). Moreover, their addition to the soils allows a sequestration of contaminants during their degradation limiting their bioavailability. Their efficiency depends on their preparation methods and is related to the surface properties of the carbon matrix which interacts with organics (hydrogen bonds, electrostatic, hydrophobic/hydrophilic and π - π interactions) and its accessibility (open and closed porosity, pore sizes and connectivity). Although these interactions are well identified today, there is a lack of data about the **interactions between confined carbonaceous surfaces and organic molecules in the PCM** (Figure 1). These data are fundamental since they give access to the ability of PCM to immobilize organic contaminants.

The innovative approach of this study proposed by several laboratories (ICSM, LLB, MADIREL and COVACHIM) aims to determine the location of model molecules of varying size, polarity, flexibility and charge distribution, confined in PCM using adsorption measurements, infrared and Raman spectroscopies, small angle X-ray and Neutron scattering. In addition, the model molecule dynamics will be characterized from the picosecond to the microsecond timescale using Quasi-elastic neutron scattering and NMR analysis. To this end, hydrochars and biochars derived from biomass such as *Arundo Donax* (Canne de Provence) and *Sargassum* (seaweed) will be prepared and used as PCM.

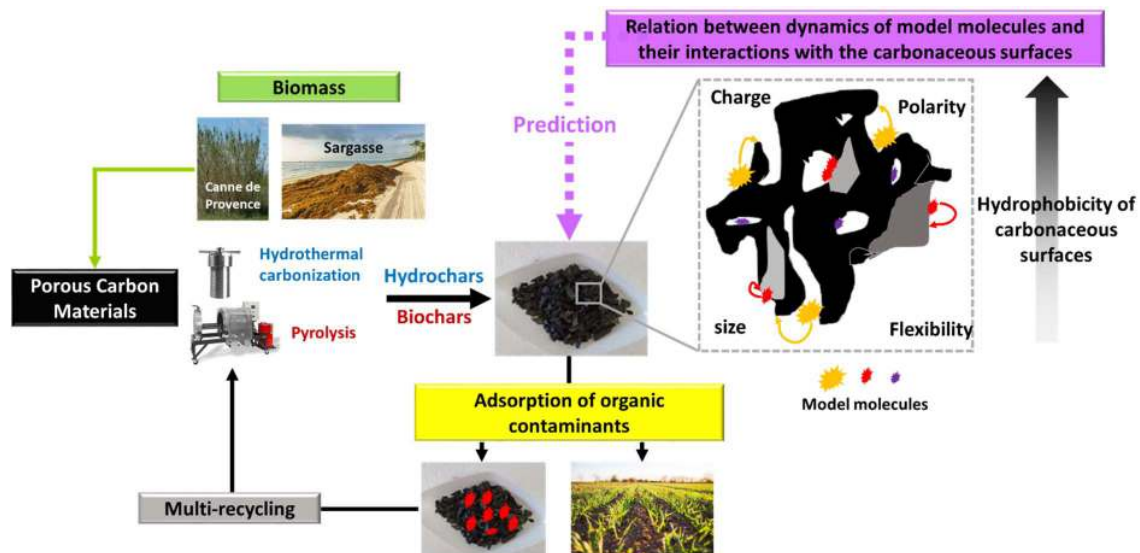


Figure 1 : Synopsis of the study context.

Candidate

Ph.D in physical-chemistry or in material science.

Good knowledge of the use of neutrons and scattering techniques.

Good communication and writing skills.

Interest of the candidate

The ICSM is a dynamic institute, where the young researcher will be able to work with world-renowned specialists in their scientific field and/or certain techniques, as well as within a multidisciplinary team with the various members of the project. As well as acquiring new scientific skills or improving existing ones, the young researcher will also be able to develop his/her contacts via the project itself, participation in seminars (internal and external) and conferences (national and international), and training courses.

<https://www.youtube.com/watch?v=yWImA3LFthg>