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ÉCOLE DOCTORALE DE CHIMIE

Bourse doctorale du ministère

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SUJET : Functionalization of elastomeric structured catalytic supports for the intensification of catalytic processes

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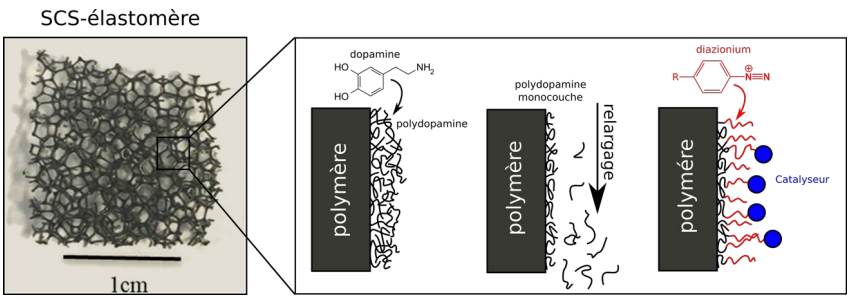
Research teams : PolyCatMat (former-C2P2) and MMAGIC (former-LGPC)

Ecole doctorale : Ecole Doctorale de Chimie de Lyon - ED 206

Langue de travail : Anglais/Français

Overview of the research: Fixed bed reactors under continuous flow are frequently used in the chemical industry for multiphase reactions. They provide a better control of reaction conditions in order to optimize conversions and yields. Moreover the separation steps between the catalyst and the products can be avoid [1]. These processes make use of Structured Catalytic Supports (SCS) having a high specific surface and low pressure drops. Among SCS, open-cell polymer foams (*e.g.*: PU foam, melamine, etc.) are serious candidates [2]. In addition, thanks to their elastic properties, these foams enable *in-situ* controlled deformation of their morphology within the reactor itself. These periodic deformations allow an intensification of mass transfer with low energy cost.



In this context, the objective of this PhD is: (i) to functionalize/activate in a green and robust way these SCS-elastomers without modifying their elastic properties and, (ii) to implement them in an innovative reactor for the intensification of catalytic reactions of major

interest. To meet these two challenges, the the catalyst deposition onto these new SCS-elastomers will be achieved through two versatile and complementary techniques: (i) using polydopamine, a bio-inspired polymer with remarkable adhesion and reduction properties and (ii) using diazonium salts which lead to the formation of a covalently grafted polymers film. Polydopamine coating exhibits a very good adhesion to any type of support [3] but leaching can occur, whereas grafting with diazonium salts allow to covalently bound various functional groups but must be adapted for each type of support [4]. The first objective is therefore to combine these two methods, hence benefiting from both their advantages. The PDA monolayer is very adherent and can serve as an intermediate layer to graft diazonium salts, the latter allowing many functionalities to be introduced at the surface of these SCS. This method can thus be adapted to the different nature or morphology of SCS elastomers available and then used for multiphase catalysis reactions (hydrogenation / oxidation). Thanks to the approach proposed in this PhD, the catalyst can be either in the form of nanoparticles (Ag, Au) or organic (metal complexes) and covalently grafted onto the film. This part will be supervised by the PolyCatMat team and supervised by Fabrice Brunel and Elodie Bourgeat-Lami. The second objective is to make use of the elastic properties of these functionalized SCS-elastomers in a new type of innovative reactor currently developed within the MMAGIC team (the piston-to-crankshaft reactor) [5]. A detailed characterization of the processes involved in this type of reactor will be carried out and the prepared SCSs will be tested for targeted applications. This part will be under the supervision of Pascal Fongarland and David Edouard (MMAGIC team). The objective of this PhD, namely, **the development of an intensification reactor at low energy cost and based on an innovative bio-inspired structured catalytic support, is a scientific challenge, which is fully in line with the societal challenges of tomorrow : greener and more ecofriendly.**
The combination of complementary skills from the two teams (PolyCatMat and MMAGIC) of the CP2M Laboratory will facilitate the success of this ambitious project.

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[2] (a) E. Pardieu *et al. Chem. Commun.* 2016, *52*, 4691. (b) L. Lefebvre *et al. Environ. Chem. Eng*. 2017, *5*, 79. (c) A. Ait Khouya *et al. Chem. Commun*. 2019, *55*, 11960.
[3] Lee *et al.* (2007) *Science*, 318, 426-430
[4] Mohamed *et al.* (2015). *Adv. Colloid Interface Sci.*, *225*, 16-36.
[5] Thèse de Laura Birba (ANR POLYCATPUF)

Keywords: supported catalysis, polymer / elastomer, functionalization / grafting, reactor / process engineering, green chemistry / ecofriendly