PhD Université de Rennes
Start: 1er October 2023 Duration: 3 years Salary: 2 135 € Brut
Keywords: Energy, supercapacitor, electrochemistry, surface functionalization.

Title: Controlled grafting of capacitive materials.

Currently, electrical energy storage devices range from electrochemical capacitors (or supercapacitors), which can deliver high power, to batteries, which suffer from moderate power but can deliver high energy density. For many years, researchers have been confronted with the difficulty of obtaining electrical energy storage devices combining both high power and high energy density. New storage systems, combining carbon materials (capacitive) and redox molecules (faradaic), have appeared where additional charges can be stored. Unfortunately, when redox molecules are immobilized on capacitive materials, their faradaic activity makes a fragile contribution to charge storage, i.e. it disappears in the first thousands of cycles. This fragile contribution is probably due to desorption phenomenon and/or (electro) reactivity of the grafted molecules which become inactive. Thus, in order to satisfy our future energy needs, new strategies for integrating electro-active molecules within electrode materials must be studied so that the grafted molecules are no longer an obstacle to the stability of these new energy storage devices.

The objective of this research project is the covalent functionalization of capacitive porous carbonaceous materials by monolayers of electro-active molecules. Monolayer functionalization is required here to preserve the integrity of the porous structure of the material to be functionalized, but also to maximize the quantity of electro-active molecules covalently bound to the carbonaceous material and their stability during cycling. The grafting of electro-active molecules on carbonaceous materials is one of the expertise of the host laboratory. Two surface functionalization methods developed by the host laboratory will be studied during the PhD for the functionalization of porous carbonaceous materials: the so-called protection-deprotection method [1] and a new technique based on a catalyzed Diels-Alder reaction on the surface. [2]

The recruited PhD candidate will be hosted at the Institut des Sciences Chimiques de Rennes (ISCR). The candidate will have access to an organic laboratory in order to synthesize the molecules necessary for the surface functionalization (aryl diazonium salts, electro-active molecules bearing azido or alkyne groups). He/she will also have access to an electrochemical laboratory with dedicated potentiostats to surface functionalization and supercapacitor characterization. Additional characterization equipment necessary for the project is available on the campus site (NMR, XPS, BET measurement, Raman, etc.) and will be used by the candidate. He/she will also carry out electrochemical analyzes (cycling and stability) of the supercapacitor materials in button cell and pouch cell format in partnership with the IMN laboratory in Nantes, and will therefore have to carry out a part of his/her contract over there.

Skills: The candidate must have good knowledge in at least one of the following disciplines: electrochemistry, physical chemistry, organic chemistry and hold a Master 2 or equivalent. The B2 level in English is highly recommended.

Interested candidates can send a CV + cover letter to:
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Corinne Lagrost corinne.lagrost@univ-rennes1.fr, 02 23 23 59 40

References:
[1] Efficient Covalent Modification of a Carbon Surface: Use of a Silyl Protecting Group To Form an Active Monolayer. J. Am. Chem. Soc. (2010) 132(40), 14039-14041.
[2] Functionalization of carbon surfaces using copper-catalyzed Diels-Alder Reaction. Submitted.