

## 'Physique et Chimie des Matériaux' – ED 397 – année 2020

### PhD project for funding (max 1p), to send to

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Research unit (full name + acronym) : Laboratoire de Chimie de la Matière Condensée de Paris (LCMCP)

Team if applicable : Nano and RMES

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Supervisor name (HDR) : Sophie Carencó

Position : Researcher CNRS

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Number of PhD under supervision : 3

Participation to supervisor training? yes      Year 2018

Co-supervisor name : Natacha Krins

HDR ? no

Research unit : LCMCP

International co-supervision ? No

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Keyword 1 : Nanoparticles

Keyword 2 : Electronic Properties

Keyword 3 : Operando Spectroscopy

Keyword 4 : New compositions

Select co-funding programme if applicable : select

Project title : Design of Nanoparticles with Novel Compositions and Monitoring of their Electronic Properties

Project Description (~4000 characters, font 11 min):

Nanoparticles with novel compositions, i.e. far removed from the oxides or metals that are often studied, are at the heart of a lively research activity. On the one hand, much remains to be discovered about the compositions and structures accessible at the nanoscale. On the other hand, a very large number of applications (lithium batteries, photovoltaic cells, catalysts, fuel cells, therapeutic vectors, etc.) benefit from the contribution of these new nanostructures. In this project, we are interested in the synthesis and surface reactivity of new nanoparticles based on abundant transition metals (e.g. iron, cobalt, nickel), into which we will insert light elements: carbon, phosphorus and sulfur. These will allow us to modulate the electronic properties of the nanoparticles, which are mostly semiconductors. To explore these compositions, we will use : (1) a well-established know-how: the use of reactive molecular precursors in colloidal air-free synthesis, (2) a variety of chemical bonding modes with three families of compounds: from the most covalent (metal phosphides of composition M-P, carbides M-C) to more ionic-covalent ones: oxysulfides M-O-S (the nanoparticles crystallinity will be characterized by powder X-ray diffraction and their morphology by transmission electron microscopy), (3) an expertise in operando synchrotron techniques with gas and liquids.

We will then start exploring their reactivity, starting with a description of the chemical surface state: (1) exposed to model gas (O<sub>2</sub>, CO<sub>2</sub>), and (2) at the interface with an organic electrolyte in open circuit conditions. We will monitor their electronic properties (surface oxidation state, band position) using X-ray absorption spectroscopy, ex situ and in situ under model reactive conditions (with gas, in solution without/with an applied current, etc.).

Expected results: (i) the preparation of novel nanoparticles for a few compositions and their structural characterization; (ii) the description of their surface state; (iii) selected analyses by synchrotron spectroscopies, in order to better understand their electronic properties as well as the mechanism of formation (nucleation, growth crystallization); (iv) preliminary test in reactivity toward common electrolytes as well as O<sub>2</sub> and CO<sub>2</sub> gas. The PhD student will have the opportunity to evolve in a dynamic environment, within a leading and generously equipped laboratory. He/she will be able to develop rare and sought-after skills, both in terms of experimental manipulation (Schlenk and glovebox techniques, synthesis in various reaction media) and in terms of characterization (electron microscopies, X-ray powder diffraction, NMR, UV and IR spectroscopies, X-ray absorption spectroscopy, electrochemical impedance spectroscopy, etc.). It will favor the development of autonomy, project management, teamwork and communication in French and English.