# Master internship/PhD

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| **Internship/job title** | **Realization of MOF passivating layer on Si anodes for Li ion Battery** |
| **Location :** | Laboratoire PMC – Ecole Polytechnique – Route de Saclay – 91128 Palaiseau |
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| **Date of publication** | 01 / XII / 2020 |
| **Observations** | Starting date to be defined with the candidate |

## Context

Silicon is one of the best anode material for Li ion battery due to its high storage capacity which is theoretically 10 times higher than that of carbon. However, in practice, the performances of Silicon anodes remain limited because of two main phenomena: i) huge volume variations during Li charge and discharge leading to severe damaging of the Si electrodes and ii) charge losses during cycling due to the continuous electrochemical formation of an instable passivation layer (SEI: Solid-Electrolyte Interphase).

## Scientific Project

Within this context, the purpose of the internship is to explore the possibility of fabricating an artificial electronic insulating but ion conductive layer onto the silicon electrodes to prevent or reduce the formation of the SEI and to improve the electrode cyclability.

The idea is to use Metal Organic Framework (MOF) as a passivating interfacial layer (**Fig.1**). MOFs are a class of crystalline porous materials obtained by self-assembly of metal ions and organic linkers in solution [1]. They are generally non electron conductive and their porosity (size and pore shape) can be tuned by the choice of the precursors. These materials are anticipated to be good candidates to form ion conductive membranes allowing for the transfer of Li ions between the electrolyte and the silicon but preventing the electron transfer to the solution, which is responsible for the formation of the SEI through electrochemical reactions with the electrolyte.

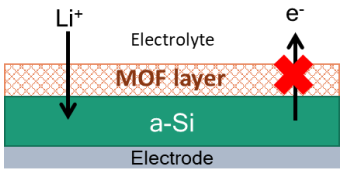
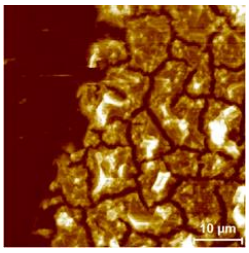



**Figure 1**: ***(left)*** *Scheme of Si-MOF hybrid electrode allowing for $Li^+$ charge and discharge through an insulating MOF layer.* ***(right)*** *Example of a Fe-based MOF layer grown onto crystalline Silicon (Atomic Force Microscopy).*




The main working axes will be: i) the development of a new synthesis method based on microwave heating to promote/favor the growth onto the silicon surfaces, ii) the structural and physico-chemical characterizations of the MOF layers and iii) the investigation of the electrochemical behavior of the Si-MOF electrodes.

The growth of MOF layers will be investigated first onto crystalline silicon which will allow for the implementation of highly sensitive characterization techniques. Once established the procedures will be adapted for the growth onto the amorphous silicon anodes in order to study the electrochemical properties of the hybrid Si-MOF systems.

The preparation of the Si-MOF electrodes will be carried out according to experimental protocols developed at PMC lab. Their structural and physico-chemical properties will be investigated by different surface characterization technics accessible at PMC lab (Electron and Atomic Force Microscopies (SEM, AFM), XRay technics (XRD/XRR)). Optical characterizations by spectro ellipsometry will be implemented in collaboration with the PICM lab. The electrochemical behavior of the Si-MOF electrodes will be studied using usual electrochemical methods (galvanostatic cycling, voltammetry, impedance spectroscopy).

[1] Ivo Stassen et al., Chem. Soc. Rev., 2017, 46, 3185-3241.

**Profile:** The internship will involve experimental work and data processing. The candidate will conduct a research, starting from sample preparation up to advanced characterizations. A strong background in physical chemistry and surface science is required. Self-motivation and very good organization are also mandatory.