## M2 Internship available 1st Semester 2021

**Interfacial Chemistry of Novel 2D materials in solvent water with ab initio methods.**


**Abstract**

The 2D materials like their prototypical examples graphene and hexagonal boron nitride have recently displayed an unexpected chemical reactivity in contact with water leading to their large surface charging and to potential applications in blue energy – harvesting energy from salinity gradients-(Siria2013, Secchi2016). These findings arose from subtle conducting measurements in nanotubes and their quantitative interpretation required to consider the quantum nature of all components of the interface : the materials and the water solvent via extensive ab initio molecular dynamics (AIMD) (Grosjean2019).

There are a plethora of novel 2D materials emerging. Borophene, a synthetic two-dimensional (2D) material composed of elemental boron arranged in a planar structure, is a relatively young member of the 2D material family. However borophene comprises many allotropes due to the structural flexibility of the electron-deficient B atom.

Recently one novel borophene phase has been grown epitaxially on atomically flat surface like Ir and then decoupled via Au intercalation (Vinogradov2019). Hence this boron allotrope could produce a defect-free borophene sheet. In this context it becomes very interesting to gain novel insight in the interfacial chemistry of borophene in water.



**References:**

[Siria2013 : Nature 494, 455–458 (2013).]
[Secchi2016 : Phys. Rev. Lett. 116, 154501 (2016).]
[Grosjean2019 : Nat. Comm. 10 (2019).]
[Vinogradov2019 : ACS Nano. 13 (2019).]


**Working context**

The project will be realized inside the theory team of PASTEUR laboratory, UMR8640 at the Ecole Normale Supérieure within PSL University.

The project will focus on the modelling of the interface between the borophene and water at the quantum atomistic scale via Ab Initio Molecular Dynamics. The master student will learn how to construct an interface cell with a liquid and perform dynamic runs. If time allows one self-ion of water (hydronium or hydroxide) can be introduced in order to see whether the pH conditions play any role on the surface reactivity of borophene.

**Profile and requested skills**

Theoretical work with numerical simulations and advanced competences and taste in software advanced uses will be highly appreciated. The supercalculations will be performed in the national supercomputer center GENCI via selective computer grant proposals.

**Allowance: Internship allowance will be provided**
**Subject could be continued with a PhD thesis: potentially in related topics**


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