'Physique et Chimie des Matériaux' – ED 397 – année 2022

PhD project for funding, to send by 28/02/2022 to

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Research unit (full name + acronym) : Institut des NanoSciences de Paris INSP UMR 7588

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Project leader (PI): Michel Goldmann HDR? yes Position : Other

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Nber of phD under supervision 1.5 Participation to supervisor training? select Year

Co-supervisor : Sylvie Spagnoli HDR? no Position : Lecturer SU

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Research unit : Institut des NanoSciences de Paris INSP UMR 7588

International co-supervision ? No

Keyword 1 : Graphene monolayer Keyword 2 : polydiacetylenes layer

Keyword 3 : Langmuir Films Keyword 4 : Structural studies

Select co-funding programme if applicable : select

Project title : Interaction between polydiacetylene monolayers and graphene oxide sheets.

Project Description :

Graphene-based ultrathin films are promising nanomaterials through their unique combination of electrical, optical and mechanical properties. Reduced graphene oxyde (rGO) exhibits semiconducting properties and optical transparency. Its interaction with organic film enhances the conductivity and produce synergistic effects on light-induced charge/energy transfer. These systems thus appear as a potential alternative for conventional metallic and ITO electrodes or Grätzel solar cells. We are developing a method based on the Langmuir film procedure to obtain and study a molecular layer/rGO interface.

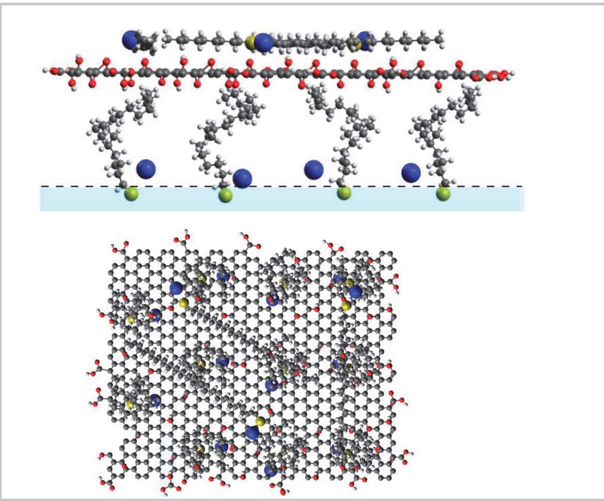
Langmuir monolayers are formed by amphiphilic objects adsorbed at the water/air interface. On can easily adjust the physico-chemical conditions of these films (surface density, surface pressure, temperature etc.) by using a “Langmuir trough”. These films present the great advantage of being able to be probed at different scales, macroscopic by thermodynamic measurements, mesoscopic by optical microscopy at the Brewster angle (BAM) and microscopic by x-ray reflectivity (XRR) and surface diffraction (GIXD) completed by AFM and KPFM measurements.

Polydiacetylenes (PDA): =(RC-C≡C-CR’)n= are conjugated polymers obtained from the photopolymerization of diacetylenes (DA). This project consists in obtaining and studying PDA/rGO interfaces by the Langmuir procedure. The first step will consist in mastering the formation of PDA/GO interfaces. For this, we will explore several strategies derived from the Langmuir's films procedure.

The first one consists in depositing simultaneously the two species on the water surface. One then forms a mixed monolayer which can be compressed until one of the species "climbs" over the other one. We will thus obtain the desired interface whose structure will be studied. This procedure is quite sur but has the drawback that one cannot define which specie remains in contact with the water subphase which interaction can

influence the final structure and then properties.
An alternative allowing to choose the species interacting with water consists in depositing it in a first step, compressing the film until obtaining a homogeneous monolayer and then depositing the second species on top of it. The drawback of this approach is that it is not possible to vary the physico-chemical conditions of the film after the second deposition. Obtaining a homogeneous "bilayer" will therefore require a longer study.
The next step will consist in observing in-situ the transition between monolayers and multilayer (forming the interface) by BAM. This will allow to identify the nature of the domains remaining on the water surface. At the same time, the films will be characterized after transfer onto a solid substrate by AFM and KPFM.
Then, we will study the microscopic structure of these interfaces by surface x-rays scattering. Two types of measures will be performed:
1) XRR measurements to measure the electron density profile perpendicular to the film. We can then determine/verify the stacking order of the species and estimate the 2D density of the layers.
2) GIXD to determine the structure of the layers if they are crystallized. If so, the commensurability or incommensurability of the 2D network formed by the diacetylenes with the one of rGO will provide a valuable assessment of the interaction between these components.
Due to the weakness of the scattered signal resulting from the very small thickness of the sample associated with the low scattering power of the atoms, these experiments will be implemented on synchrotron sources.
Additionally, the photopolymerization will be tempted before and after the deposition on the rGO sheets followed by a spectroscopy study (UV-Vis absorption and Raman). Indeed, the initial blue polymer turn red when stressed. We will study the influence of the coupling with the rGO sheets on the PCDA electronic structure

Although the proposed research program is mainly experimental, numerical simulations using molecular dynamics (MDS) with our colleagues from the Instituto Superior Tecnico of the University of Lisbon (Portugal) can be considered.



Schematic representation of organic monolayer coupled with a graphene plane