

3D-molecular building blocks for functional 2D-supramolecular self-assemblies

Surface functionalisation needs the rational design of molecular systems to produce optimized materials in their properties (electronic, optical, or magnetic) and requires the development of nanoscale architectures, more and more elaborated^{1,2}. The formation of ordered networks of molecules via self-assembly is a simple and scalable route towards the fabrication of functional, integrated nanostructures based on functional surface-confined 2D-assemblies³. The fabrication of such functional materials relies on the design of a molecular building block that is capable of forming long-range, well-ordered self-assemblies and that possesses a functionality that does not interact with the surface once assembled⁴. A series of 3D-building blocks based on phthalocyanine⁵ and porphyrin derivatives⁶ with varied design features will be studied to investigate and understand several factors (self-assembling properties with different substrates such as HOPG, graphene and gold, intra and intermolecular interactions in the self-assembled 2D-systems, functional properties of the 2D-self assemblies).

In this PhD project, the approach, still unexplored in a systematic way, must make it possible to understand the influence of various parameters on the physical properties of supramolecular edifices formed on a surface either by trapping in a nanoporous organic monolayer, or by direct self-assembly of the functionalised molecular entities on a substrate. The objectives identified are therefore related to:

- The judicious and rational choice of molecules, to the fabrication of supramolecular edifices (drop-casting or evaporation)
- The characterization of both self-assembling properties (structural properties) of the 3D-molecular building blocks (on graphenoid and metallic substrates) and functionalities at the molecular and supramolecular level (electronic properties) by means of a wide variety of techniques available in our laboratory such as scanning probe microscopies (STM/STS at solid/liquid interface, solid/air interface and in ultrahigh vacuum and also AFM)
- The study of the influence of intra and intermolecular interactions on the optical properties of the 2D assemblies by Raman, IR, fluorescence...

All these investigations should lead to the fabrication of optoelectronic devices such as OFETs.

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6. M. J Cook, A. N. Cammidge, D. L. Hughes, M. Rahman, L. Sosa Vargas, **Phthalocyanine analogues: unexpectedly facile access to non-peripherally substituted octa-alkyl tetrabenzotriazaporphyrins, tetrabenzodiazaporphyrins, tetrabenzomonoazaporphyrins and tetrabenzoporphyrins**. *Chem. Eur. J.* 2010, 17, 3136-3146.

This PhD work will be carried in the NARCOS team (NANomatériaux et matériaux nanostructurés : Réactivité, Caractérisation et spectrOscopies) of the laboratory MONARIS (de la Molécule aux Nano-objets : Réactivité, Interactions et Spectroscopies - UMR 8233) at Sorbonne University (Paris). Highly motivated candidates (expecting a master degree or equivalent with excellent academic records) with a background in physical chemistry and material science are strongly encouraged to apply. Knowledge of the candidate in scanning probe microscopy, Raman spectroscopy and/or IR spectroscopy will also be appreciated. Previous laboratory experience in surface functionalization, nanomaterials, supramolecular architectures or any other field that could benefit the project would be valuable but is not mandatory.

Applications should include a CV, motivation letter, diploma with transcripts and contact details for at least two professional referees, and send to Imad Arfaoui (imad.arfaoui@sorbonne-universite.fr).