Grenoble Alliance for Integrated Structural & Cell Biology

# INTERNSHIP PROPOSAL

**Institute and Group: Institut de Biologie Structurale - Groupe MEM**

**Supervisor: JL PELLEQUER** **Email**: jean-luc.pellequer@ibs.fr

**Phone: 045742 8756**

**Research project title: Supramolecular assembly of functionalized nanostructures**

**5 Keywords to describe the project: Atomic force microscopy, computational modelling, photochromes**

**Description of the project (aims, experimental techniques, recommended background):**
This study is part of the realization of functionalized nanostructures based on supramolecular assemblies, such as intelligent surfaces. Intelligent surfaces are based on the assembly of functionalized molecules on a substrate that respond collectively, reversibly and stable (in time and temperature) to an external stimulus. Photochrome molecules are capable of photoisomerizing even in 3D single crystals. Most studies on diarylethenes study them in devices (thin layers, nano-particles, crystals, etc.) but very little in monolayer on a surface. The self-assembly and photoisomerization properties of a specifically synthesized diarylperfluorocyclopentene molecule was studied on HOPG by near-field microscopy (STM) at the liquid-solid interface at the IS2M, our partner in Mulhouse. The aim of the project is to pursue the development of methods that enable the laboratory to reconstruct large biological molecular complexes using high-resolution topographic surfaces from atomic force microscopy or scanning tunneling microscopy. Our hypothesis is that it is possible to build large structures using their individual components with the aid of topographical surfaces obtained with AFM/STM. The reconstruction protocol is based on a six-dimensional docking of individual components. The core of the project is the testing of different scoring methods from docking orientations. The candidate will work in a Linux-based computer environment and should be familiar with some level of programming as well as some basic knowledge in structural biology.

**Justification that the internship's subject fits with the general theme of GRAL:**

This project aims at using novel structural information obtained by atomic force microscopy and STM which are additional techniques toward integrating knowledge on the structure and dynamics of molecules and their function. Therefore, it expands the goal of the GRAL Labex.

**Relevant publications of the team:**

Nair M.N., Mattioli C., Cranney M., Malval J.-P., Vonau F., Aubel D., Bubendorff J.-L., Gourdon A. and Simon L. (2015) STM Studies of Self-Assembled Tetrathiafulvalene (TTF) Derivatives on Graphene: Influence of the Mode of Deposition. J. Phys. Chem. C 119: 9334–9341.

Chaves R.C., Dahmane S., Odorico M., Nicolaes G.A.F. and Pellequer J.-L. (2014) Factor Va alternative conformation reconstruction using Atomic Force Microscopy. Thromb. Haemost. 112: 1167-1173.

Trinh M.-H., Odorico M., Pique M.E., Teulon J.-M., Roberts V.A., Ten Eyck L.F., Getzoff E.D., Parot P., Chen S.-w.W. and Pellequer J.-L. (2012) Computational reconstruction of multidomain proteins using atomic force microscopy data. Structure 20: 113-120.