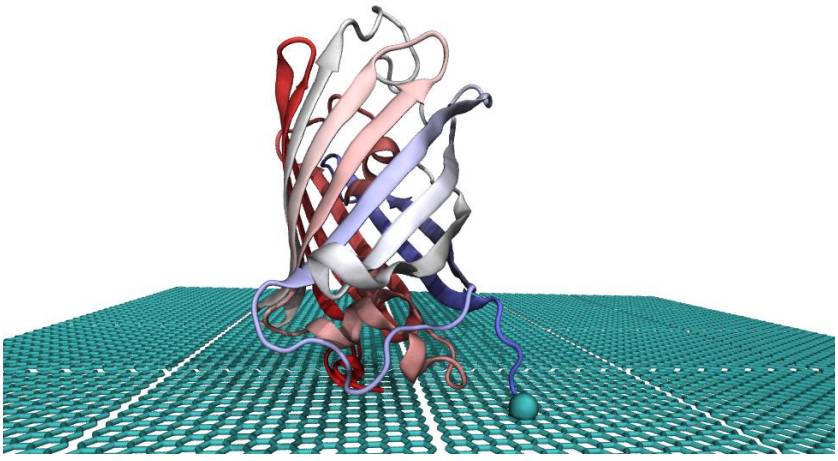
SUMMER INTERNSHIPS 2016

TITLE: Effects of protein and enzyme immobilization in stability and function

DESCRIPTION (Objectives, tasks, materials, equipment…):

The immobilization of biomolecules on inert surfaces is widely used in biotechnological applications. In particular, supported enzymes are extensively used as heterogeneous biocatalysts to carry out modern chemical processes. They are highly active and selective and they enable the separation and recycling of the catalyst, thus increasing both the efficiency and sustainability of the process. Also, many electrochemical DNA sensors rely on the prior tethering of biomolecules to a surface. A myriad of biomolecules have been stabilized by attaching them to solid supports through different immobilization chemistries ranging from single to multi-point attachments. However, it is difficult to know in advance the effects of the immobilization in the stability of the biomolecule, which critically affects its function.

In this project we will use computational methods to study the effects of different immobilization chemistries on protein stability. In particular we will focus in the case of the green fluorescent protein (GFP), a widely used model system for which abundant experimental data is available. We will use molecular dynamics simulations to study the stability and dynamics of the system in bulk, and how these are modified when the protein is tethered to a surface. This will allow for us to identify optimal ways for surface tethering of proteins, which will be testable by our experimental collaborators at CIC biomaGUNE.



The work in this project will be purely computational, although the candidate will be trained to think with reference to experimental results. During the internship, the candidate will be equipped with a skillset that is currently in high demand both in academia and in industry, including some basic knowledge of UNIX systems,

programming in the Python scripting language, computing in parallel architectures, and using analytics methods akin to those used in Big Data industries. No prior knowledge of computer programming is required.

SUPERVISOR: David De Sancho

SUITABLE FOR: chemists, physicists, computer science scientists