The goal of this project is to expand our knowledge of hybrid, protein-graphene systems by assembling a multidisciplinary team of computational chemists and physicist. The research project focuses on the computational study of new hybrid protein-graphene interfaces, linked together with organic linkers, as a possible candidate for bio-electronic devices, such as bio-sensors, bio-fuel cells, solar-to-fuel devices and biomolecular nanoelectronics. The protein under investigation are small light harvesting proteins (SLHP), responsible for absorption of light and its conversion into energy in bacteria and plants, while for the material component we chose graphene for its extremely interesting electronic properties. Graphene is a monolayer of carbon atoms bonded together in a two dimensional honeycomb structure. This peculiar structure is responsible of the extremely high transfer of charges measured in graphene. The study will focus on the interaction of SLHP with linkers and a graphene layer as conducting material and charge carrier. The main question which will be investigated is how to suppress the recombination of charges that is observed at the protein/graphene interface of working devices.

The way these components (protein, linkers and graphene) interact is crucial to ensure a working device and thus the investigation of the nature of the interface is essential. Through the use of atomistic simulation methods, we will investigate the binding energy that determines the strength of the interaction between SLHP and graphene. A more complex interface presents the addition of a monolayer of molecules forming a Self-Assembled Monolayer (SAM), such as pyrene and azobenzene derivatives, in between the protein and graphene, which might improve the charge transport as well as the stability of the system.

In this project, we will resort to a multiscale computational approach for the description of chemical and physical properties of the systems of interest. First we will model the time-evolution of SLHP, linkers and graphene with a classical molecular dynamic method, which consist of considering the atoms bonded together in a spring-like way, without considering the electronic attractive forces explicitly. This allows us to consider realistic model systems (thousands of atoms) and physically meaningful time-scales (hundreds of nanoseconds), for the investigation of the time-evolution of the interaction between SLHP, linkers and graphene, with and without environment (the final device is an all-solid state device). The energy analysis of these systems will allow us to quantify the interaction energy and the stability of the hybrid system.

Next, we will focus on smaller parts of the system (i.e. the only the few interacting aminoacids of SLHP with SAM/graphene) using more sophisticated and accurate methods, that account explicitly for the electrons, to describe and understand the electron transfer mechanism occurring at the interface. To accomplish this goal, we will divide the system in three blocks, each presenting a different interface: SLHP/SAM, SAM/graphene as well as SLHP/graphene. From this quantum-mechanical approach we will analyse the electronic wavefunction and the consequent change in electronic properties of graphene, by mean of energy level alignment (for the charge transport mechanism), band-gap opening (for electronic properties), absorption abilities (for the optical properties) and electron and energy transfer mechanisms. Moreover, the designed interface will be build and experimentally characterize to assess the predictive power of computation.

Our project offers a rational design of novel complex systems composed of proteins and organic surfaces, with the possible use of such interface in the future as bio-organic photovoltaic cells and transistors, which may solve the problem of rapidly growing World energy consumption. The proposed project will contribute to a better understanding of the impact of graphene on the stability and physical and chemical properties of the photosystem's reaction center and *vice versa*. The comprehensive theoretical approach proposed provides us with an accurate characterization of new systems and leads to the development of a rational design of new complex bio-organic interfaces.