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The goal of this project is to expand the 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 a new hybrid protein-graphene system, as a possible candidate for bio-electronic devices, such as biosensors, bio-organic photovoltaic cells (bio-OPV) and bio-organic transistors (bio-OFET). The protein under investigation is the widely studied reaction center (RC) of the photosystem II protein, responsible of absorption of light and conversion into energy in bacteria, while graphene is a monolayer of carbon atoms bonded together in a two dimensional honeycomb structure. The study will focus on the interaction of RC with a graphene layer as conducting material and charge carrier.

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

In this project, we 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 RC of the photosystem II system and graphene with a classical molecular dynamic method, which consist in considering the atoms bonded together in a spring-like way, without considering the electronic attractive forces explicitly. This allows 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 RC and graphene, with and without SAM. The energy analysis of these two systems will allow us to quantify the interaction energy and the stability of the hybrid system.

In the second step of the project we will focus on a smaller portion of the system (i.e. the only the few interacting aminoacids of RC with graphene or RC/SAM/graphene) using more sophisticated and accurate methods, that account explicitly the electrons, to describe and understand the electron transfer mechanism occurring in between the RC and graphene layer. 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) and band-gap opening (for electronic properties).

Our project offers a rational design of novel complex systems composed of proteins and organic surfaces, with the possible use of such systems 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 systems.