Academic Year 2017/2018

Department of Biotechnology, Chemistry and Pharmacy, Università di SIena, ITALY

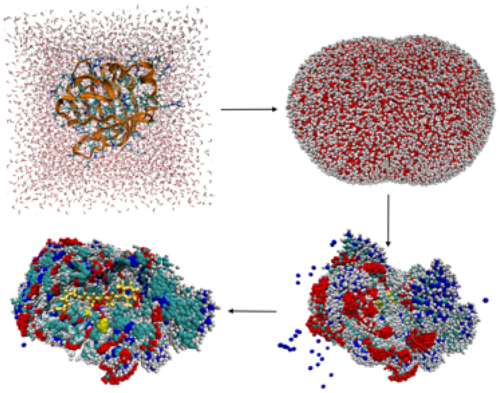
A **grant covering the entire doctoral studiy period (3 years)** is available within the **Graduate Program in Chemistry**. The position has the following features:

Area: Computational Photochemistry and Photobiology

Engineering of genetically encodable light-powered molecular motors

Supervisor: Prof. Massimo Olivucci; Co-Supervisor: Dr. Luca De Vico

Description and Requirements



The proposed research activity is focused on the computational design of proteins hosting synthetic photochemical switches. The targeted proteins would feature a protein environment capable to transform the switch into an effective molecular motor. The graduate student will learn how to realistically model/design such systems in solution and use them to simulate, using non-adiabatic and adiabatic molecular dynamics, the protein response to light.

The reasearch will provide the opportunity to execute a part of the thesis in an international environment and vist other institutions in the United States and France. The student will also have the opportunity to interact with the supervisor experimental coworkers in a synergistic approach where the computational work would provide information useful for the lab prepararion (e.g. organic synthesis, protein espression) and characterization (e.g. x-ray crystallography and time-resolved spectroscopy) of the designed system.

The suitable candidate should be interested in acquiring a deep knowledge of computational quantum chemistry with an emphasis on photochemsitry and photobiology and on innovative QM/MM technologies. An MSc in Chemistry or Physics with experience in quantum chemistry is highly desirable. A knowledge of linux shell scrpting or, even better, programming (e.g. phyton, C or fortran) will constitute a preferential title.

Bibliography

1) Paolino, M. et al. Design, Synthesis and Dynamics of a GFP Fluorophore Mimic with an Ultrafast Switching Function *J. Am. Chem. Soc.* **2016***, 138,* 9807-9825.

2) Luk, H. L. et al. Molecular bases for the selection of the chromophore of animal rhodopsins. *Proc. Natl. Acad. Sci. U. S. A.* **2015***, 112,* 15297-15302.

3) Gozem, S. et al. *Chem. Soc. Rev.* **2014***, 43,* 4019-4036.

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