

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

Area: Computational Photochemistry and Photobiology

Title: **Engineering of genetically encodable, light-powered molecular motors**

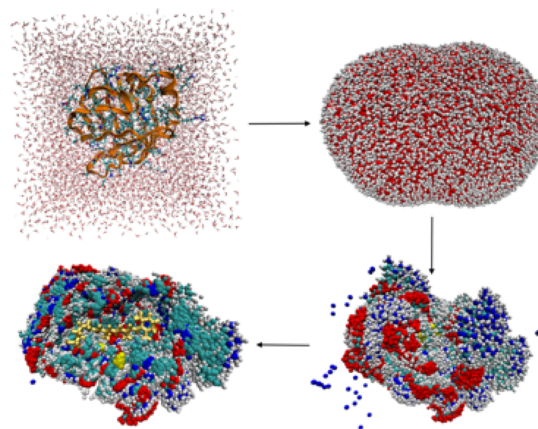
Supervisor: Prof. Massimo Olivucci; Co-Supervisor: Dr. Luca De Vico

<http://ccmao11.chim.unisi.it>

Description and Requirements:

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

The research will provide the opportunity to execute a part of the thesis work in an international environment and visit other institutions in the United States and France. The student will also interact with the supervisor's experimentalist co-workers in a synergistic framework, where the computational work will provide useful information for lab preparation (e.g. organic synthesis, protein expression) and characterization (e.g. x-ray crystallography and time-resolved spectroscopy) of the designed systems.



From top to bottom: Different components of the multiscale QM/MM protocol developed and applied in the supervisor lab to a protein mimic of the eye photoreceptor.

The suitable candidate should be strongly interested in acquiring a deep knowledge of computational quantum chemistry, with an emphasis on photochemistry, photobiology and innovative QM/MM technologies. An MSc in Chemistry or Physics (or related disciplines) with experience in quantum chemistry is desirable. Knowledge of Linux shell scripting or, even better, programming (e.g. Python, 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.

Recruitment will follow rules and requirements as set by the graduate school of the Università di Siena. Information can be found at <https://en.unisi.it/research/doctoral-research-schools>; ufficiodottorato@unisi.it.

For further information write to Prof. Massimo Olivucci (olivucci@unisi.it or molivuc@bgsu.edu)