USC Dornsife
Dana and David Dornsife
College of Letters, Arts and Sciences

DEPARTMENT OF CHEMISTRY
Arieh Warshel
Nobel Laureate
Dana and David Dornsife Chair in Chemistry
Distinguished Professor

Towards Systematic (High Throughput) Quantum Chemical Studies of Natural and Artificial Rhodopsins

Massimo Olivucci
Research Professor, Bowling Green State University &
Professor of Organic Chemistry, University of Siena

Monday, April 10, 2017
2:00 p.m., SGM: Mudd Room (460); 4th floor

Abstract: Biologists are intensively using computational methods for investigating molecular-level diversity within protein families. However, these studies are often limited to the alignment of protein sequences, which do not provide direct information on structural or functional similarities. When focusing on the rhodopsin family, this has the consequence that the mechanistic diversity of certain processes, such as those regulating the absorption wavelength or the photoisomerization timescale, remains unexplored. Here, we report on a prototype protocol (a computer software) for the fast construction and automation of relatively simple but congruous sets of quantum chemistry-based models of rhodopsins, suitable for the computational investigation of trends in spectroscopic and photochemical properties. We also show that the same basic methodology can be used to design rhodopsin mutants and rhodopsin mimics bringing about the possibility of achieving a tool useful for driving the engineering of light-responsive proteins in general.

Background:

Massimo Olivucci is a full professor of Organiz Chemistry at the Univcersity of Siena and a Reseach professor and Director of the Laboratory of Computational Photochemistry and Photobiology at Bowling Green State University, Bowling Green, Ohio.

Research Interests: We use conventional and novel computational tools to investigate the reactivity of organic and biological molecules in their electronically excited states. One major target of our work is the mapping of the photon-induced "force field" which sets an equilibrium molecular structure into motion in realistic molecular environments (e.g., in solution or in a protein cavity). We also investigate the reactive motion itself up to time scales beyond 10-12 seconds. This force field can be calculated and represented in terms of photochemical reaction paths: i.e., paths that start on an excited state potential energy surface and end on the ground state energy surface. Photochemical reaction paths comprise mechanistic elements that are not involved in the description of thermal reactions. These correspond to real crossings of different potential energy surfaces. For photochemical reactions prompted by direct irradiation these crossings often correspond to conical intersections that are regarded as the photochemical analogues of transition states. Given the central role of photochemical reaction paths, excited state trajectories and conical intersections (as well as singlet/triplet surface crossings) in the investigation of the excited state reactivity of proteins (e.g., biological photoreceptors) or solvated molecules (e.g., dyes in solution), we also develop computational strategies based on a combination of ab-initio quantum chemical methods and molecular mechanics methods that allow to study the effects of light irradiation on complex molecular systems.

- Hosted by Distinguished Professor, Arieh Warshel and The Warshel Lab -