

**Joint Seminar Series of the
CENTRE FOR RESEARCH IN MOLECULAR MODELING
and the DEPARTMENT OF CHEMISTRY AND BIOCHEMISTRY**

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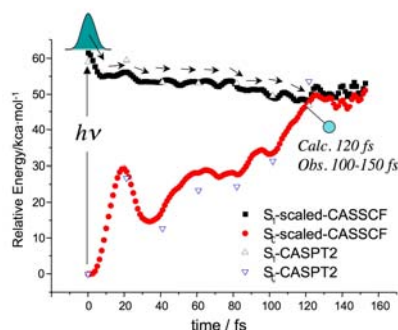
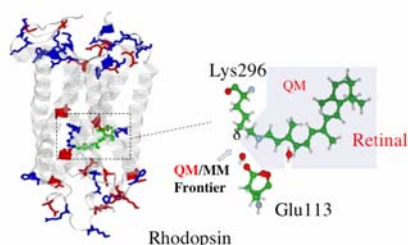
Towards Computational Photobiology

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In this lecture, we show how the development of a hybrid quantum mechanics/molecular mechanics computational strategy (see Figure below) based on multiconfigurational perturbation theory and complete-active-space-self-consistent-field geometry optimization has recently allowed for the correct evaluation of the excited-state properties of *chemically different* chromophores *embedded in different protein environments and in solution*.

In particular, we show how it has been possible to investigate the static and dynamics factors responsible for the color and ultrashort excited state lifetime (see Figure below) observed for *rhodopsin proteins* (such as rhodopsin and sensory rhodopsins) featuring a cationic retinal chromophore. The same progress in the field of the computational design of artificial bio-mimetic switches will be revised.



[1] Structure, Initial Excited-State Relaxation and Energy Storage of Rhodopsin "Resolved" at the CASPT2//CASSCF/AMBER Level of Theory Andruniów, T.; Ferré N. and Olivucci M. *Proc. Nat. Acad. Sci.* **2004**, 101, 17908-17913. [2] Excited State Properties of the Green Fluorescent Protein resolved at the CASPT2//CASSCF/CHARMM Level A. Sinicropi, T. Andruniow, N. Ferré, R. Basosi and M. Olivucci *J. Am. Chem. Soc.* **2005**, 127, 11534-11535. [3] Coto, P.B.; Strambi, A.; Ferré, N.; Olivucci, M.; "The Color of Rhodopsins at the *ab initio* Multiconfigurational Perturbation Theory Resolution"; *Proc. Nat. Acad. Sci.* **2006**, 103, 17154-17159. [4] The Fluorescence of Tryptophane in Monellin and Parvalbumin Resolved at the *ab initio* Multiconfigurational Perturbation Theory Level Sinicropi[§], A.; Pistolesi[§], S.; Pogni, R.; Basosi, R.; Ferré, N. and Olivucci, M. *in preparation*. [5] Tracking the Excited State Time Evolution of the Visual Pigment with Multiconfigurational Quantum Chemistry Luis Manuel Frutos, Tadeusz Andruniów, Fabrizio Santoro, Nicolas Ferré and Massimo Olivucci *Proc. Nat. Acad. Sci.* **2007**, 104, 7764-7769.



Massimo Olivucci graduated in 1984 and took the Ph. D. in Chemistry in 1988 at the Dipartimento Chimico "G. Ciamician" of the University of Bologna working with Prof. Fernando Bernardi. From 1989-1991 he carried out research work with Prof. Michael Robb at King's College London. In 1991 he was appointed Lecturer at the University of Bologna. In 1998 he moved to the University of Siena where he was appointed Associate Professor in 1998 and Full Professor of Organic Chemistry in 2001. In 2006 he was appointed Research Professor at the Department of Chemistry and Center for Photochemical Sciences at the Bowling Green State University, OH and created the Laboratory for Computational Photochemistry and Photobiology (LCPP) with joined activities in the United States and Italy. Massimo Olivucci is author of over 190 research papers in international journals. In 1999 Massimo Olivucci was awarded the Premio Nazionale "FEDERCHIMICA". He is one of the finalists of the 2001 "René Descartes" European Prize. Further information on the research group can be found at <http://ccmaol1.chim.unisi.it/>.