UNIVERSITÀ
DEGLI STUDI DI TRIESTE

AVVISO DI CONFERENZA

Il giorno **VENERDI' 1 DICEMBRE 2017,**
alle ore **11:15**, nella **SALA DEL CONSIGLIO (I piano)**
del DIPARTIMENTO DI SCIENZE CHIMICHE
E FARMACEUTICHE,
Università di Trieste, Edificio C11, Via Giorgieri 1

il Prof. MARCO GARAVELLI

del Dipartimento di Chimica Industriale "Toso Montanari" Università di Bologna
terrà una conferenza dal titolo:

Towards an accurate computational photochemistry and photobiology: the paradigmatic case of vision.

L'evento potrà essere seguito tramite videoconferenza anche dall'Università Ca' Foscari (Venezia), presso la Sala Conferenze.
Tutti gli interessati sono cordialmente invitati

Il Direttore del Dipartimento di Scienze Chimiche e Farmaceutiche

Prof. Silvano Geremia

Towards an accurate computational photochemistry and photobiology: the paradigmatic case of vision.

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The use of the computer to simulate light induced events in photoactive molecular materials has given access to a detailed description of the molecular motions and mechanisms underlying the reactivity of organic and bio-organic chromophores. Thus, different computational strategies and tools can now be operated like a "virtual spectrometer" to characterize and understand the photoinduced molecular deformation and reactivity of a given dye, allowing for an accurate description of photochemical/photobiological processes and a rational of the corresponding photophysical properties including time-resolved spectroscopy.
This contribution reviews recent advances in this field, by presenting methodological developments and applications in modeling the photophysical/photochemical properties of organic chromophores and complex photoactive molecular architectures. Retinal systems and visual proteins will be presented as a paradigmatic case [1-2]. Hybrid QM/MM calculations will be shown to be an elective tool for modeling photoinduced events and dynamics, including tuning/controlling effects of the environment. For this purpose, our new implementation of a general hybrid QM/MM approach, that is able to integrate some specialized softwares and acts as a flexible computational environment, eventually allowing for so far inaccessible calculations (e.g., non-adiabatic molecular dynamics of unprecedented accuracy on large molecular materials) will be illustrated. The information collected by these studies can be exploited for the design of novel photoactive molecular and soft materials, including a novel paradigm of electrochromism for applications in a new generation of color tunable displays and e-ink devices. Finally, our latest achievements in developing (and modeling) non-linear bi-dimensional electronic spectroscopy as a novel diagnostic tools for tracking structural/dynamical problems in complex environments (e.g., biologically relevant systems such as proteins and DNA) will be presented [3-4].

[1] D. Polli, et al. Nature 467 (2010) 440.
[2] O. Weingart, et al. PCCP 13 (2011) 3645.
[3] I. Rivalta, et al. PCCP 16 (2014) 16865.
[4] I. Rivalta, et al. JPCB 118 (2014) 8396.