LECTURE NOTICE

On **MONDAY SEPTEMBER 29TH 2025** at **15:00**, in the Aula Magna of the C11 building of Trieste University

Prof. Benedetta Mennucci

from the Department of Chemistry of **Pisa University**

will give a lecture entitled:

Multiscale modeling of light-driven processes in biological systems

All interested people are warmly invited!

The Director of the Dipartimento di Scienze Chimiche e Farmaceutiche

Prof. Paolo Tecilla

Multiscale modeling of light-driven processes in biological systems

Benedetta Mennucci

Department of Chemistry, University of Pisa, via G. Moruzzi 13, 56126 Pisa, Italy

E-mail: benedetta.mennucci@unipi.it

Web: molecolab.dcci.unipi.it

Living organisms across diverse domains of life have evolved specialized light-sensitive proteins that enable them to detect, harness, and respond to light. Despite employing distinct molecular strategies, these systems share a common initial event: the electronic excitation of a chromophoric unit embedded within the protein scaffold. This excitation propagates through space, undergoing transformations into various forms of energy, and ultimately drives the biological function of the organism. The full sequence of events spans a wide range of spatial and temporal scales, from ultrafast electronic processes occurring within subnanometer regions of the chromophore to large-scale conformational rearrangements of the protein on the microsecond-to-millisecond timescale.

Capturing this complex cascade at an atomistic level poses a real challenge for theory and simulation, as it requires models and computational approaches capable of describing dynamics across multiple scales. A particularly effective strategy couples quantum chemical and classical descriptions, embedding them within dynamics simulations to achieve a multiscale framework.

In this seminar, I will present an overview of this computational strategy, discuss its application to representative light-driven biological processes, and highlight current challenges and perspectives for improving its efficiency and scalability.