ICFO



INSIGHT SEMINAR: The multiscale modeling of light-driven processes in biology

BENEDETTA MENNUCCI

May 23, 2024
10:00 to 11:00
Elements Room

BIO:
Benedetta Mennucci is full professor of physical chemistry at the University of Pisa and since 2022 she is the Vice-Rector for the Promotion of Research of the same University.
Mennucci's research primarily focuses on the development and application of computational models to study how the environment affects the behavior of molecular systems, particularly in the context of photochemical and photophysical processes. Her work involves the integration of quantum mechanical methods and multiscale models to explore the interactions between light and matter in complex systems, such as biological systems, and nanostructured materials.
The international impact of this scientific activity is reflected in her list of more than 300

publications. Mennucci is the recipient of numerous awards, including the i¿½Premio el Ministro della Culturai¿½ assigned by the Italian Accademia dei Lincei (2022), the i¿? Cesare Pisani Medali¿½ of the Italian Chemical Society (2020), an ERC Starting Grant (201) and an ERC Advanced Gran

ABSTRACT:

Organisms of very different life domains possess the capability to sense, harness, and respond to light via photosensitive proteins. While the molecular strategies employed are varied, the most common initiating event is an electronic excitation occurring within a chromophoric unit that is embedded into the protein matrix. This initial excitation propagates through space, transforming into different energy forms, and ultimately contributes to the organism's biological function. The entire process encompasses a broad spectrum of spatial and temporal scales: starting from the ultrafast electronic processes within the chromophoric unit, extending through protein conformational changes that occur over microseconds to milliseconds and involve extensive portions of the protein, and culminating in the initiation of new protein-protein interactions that may take several seconds or longer. The theoretical investigation of this cascade of processes necessitates the development of models and computational approaches capable of capturing dynamics across these diverse scales. Achieving this is a formidable challenge, as the interactions and dynamics at each scale are governed by distinct principles, ranging from quantum laws at the smallest scales to classical mechanics at larger scales. An effective strategy is to couple quantum chemistry and classical models and integrate the resulting multiscale approach into adiabatic and nonadiabatic dynamics.

Here, we present an overview of the main theoretical and computational breakthroughs attained so far and discuss the challenges that we still must overcome.

Hosted by: Prof. Dr. Nicoletta Liguori