Computational photochemistry and photophysics

Logo

UNIVERSITÀ DI SIENA 1240

RESEARCHER

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DIPARTIMENTO

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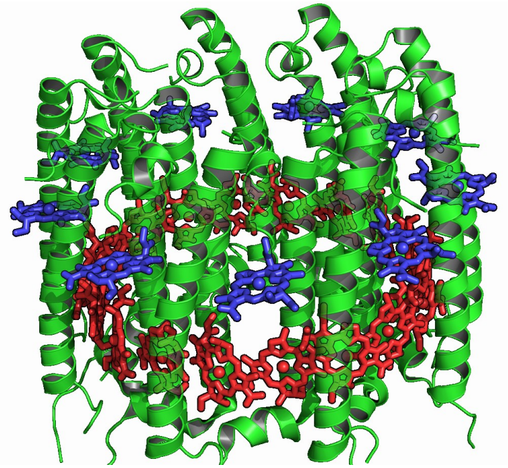
LAB

Research activity

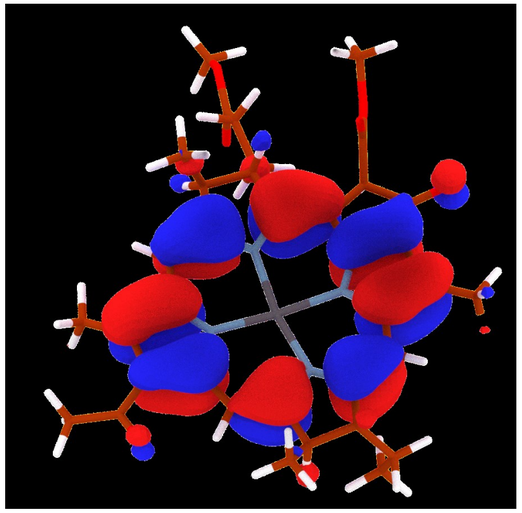
Brief description of the research activities

The research activity focuses on the simulation of the chemical and physical properties of molecules when they interact with light: these molecules are called chromophores. We are interested in absorption processes (the color of a substance), emission (fluorescence and phosphorescence), and photo-production of new chemical species. Additionally, we also simulate chemiluminescence processes, such as the light of fireflies.
The strength of the research group lies in the ability to use extremely accurate computational methods, often considered too complex for such molecules.
Finally, we have recently developed the capability to apply these methods to aggregates of molecules as well. In this way, we can evaluate and predict how different geometries and relative arrangements can modify chromophore aggregates' properties.

Images

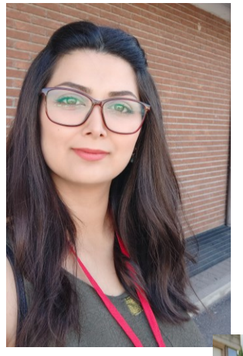


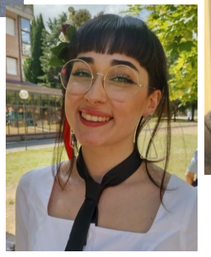
LH2 (light-harvstingcomplex 2): an example of a complex system of protein-chromophores studied in our group.



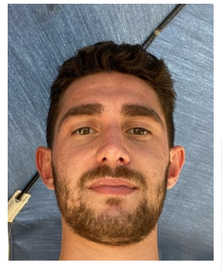
Representation of a chromophore (a bacteriochlorophyll) and its quantum mechanical nature

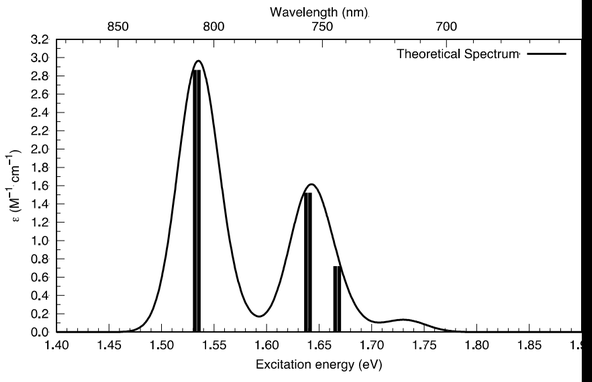
Prof. Luca De Vico. Read the QR code to reach my OrcID page

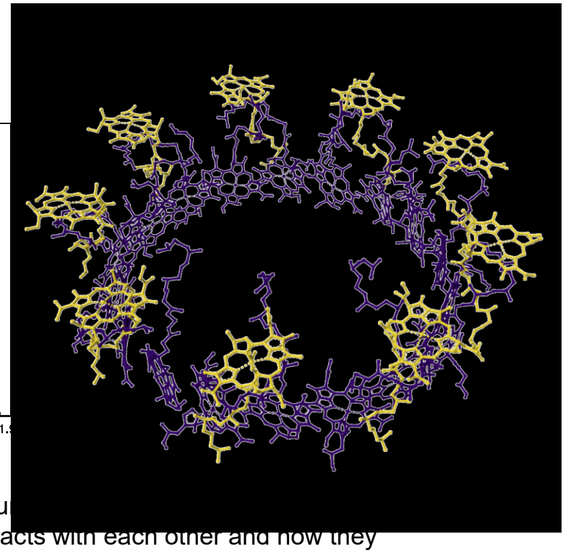




The group







Simulation of the LH2 absorption spectru
which of the various chromophores interacts with each other and how they contribute to the overall spectrum.

Technologies and services

We utilize the resources of High-Performance Computing (HPC) available within the department. Additionally, we have access to resources from the CINECA computing center, which we access based on competitive projects.

We are part of the international development group of the OpenMolcas computational program (www.openmolcas.org), which provides state-of-the-art tools for the quantum mechanical study of the photochemical and photophysical properties of molecules. We have both the capability to utilize all the tools available in OpenMolcas and the possibility to introduce new methods if necessary to study new properties.

Applications and collaborations

Currently, we have an ongoing research collaboration with Aligned Bio AS (alignedbio.com) in Lund, Sweden. We provide a platform for studying their products, but we cannot disclose further details at this time.

For more information

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