A quantum chemical view of the light-harvesting function in photosynthetic organisms

Benedetta Mennucci

Department of Chemistry, University of Pisa, via G. Moruzzi 13, 56124 Pisa, Italy

E-mail: benedetta.mennucci@unipi.it

The sun light is the main source of energy for most of the living organisms on earth, and the capability of converting it in a useful chemical form has allowed the first photosynthetic bacteria to survive and evolve into more complex organisms such as algae and plants.{1} In the course of this long evolutionary development, different apparatus for photosynthesis have been adopted by nature. In all of them the photosynthetic process is initiated by light-harvesting (LH) pigment-protein complexes. These LH antennae are special proteins carrying a large number of light-absorbing pigments aimed at capturing sunlight and transferring the energy toward the reaction centers in the optimal way according to the environmental conditions. A key role in the fulfillment of this function is played by formation and evolution of excitonic states resulting from the interactions among the pigments. To investigate such a role, multiscale models based on quantum chemistry represent a very effective strategy.[2} In this talk examples of application of this strategy to different LH antennae will be presented with the aim of revealing the delicate interplay between structural, dynamical and environmental effects in determining the LH function.

References:

[1] R.E. Blankenship, *Molecular Mechanisms of Photosynthesis*; John Wiley & Sons, 2014
[2] C. Curutchet, B. Mennucci, *Chem. Rev.* **2017**, *117*, 294.