Investigating the environment effects in natural light-harvesting systems: a multiscale quantum chemical strategy

Benedetta Mennucci

Department of Chemistry, University of Pisa,
via Risorgimento 35, 56126 Pisa, Italy

E-mail: benedetta.mennucci@unipi.it
Web: http://dcci.unipi.it/molecolab

Photon absorption and energy transfer (EET) represent the first processes in both natural and artificial light-harvesting systems. In the pursuit of mimicking the optimal design of natural light-harvesting antennae it is of fundamental importance to achieve a molecular-level explanation of these processes and the way they are affected by the environment [1]. Such a goal is a formidable challenge due to the large network of interactions that couple all the parts of the system in a dynamic way and the different time and length scales involved. However, a possible strategy exists and it is represented by the coupling of quantum chemical methods to classical approaches that account for the environment response in all the steps of the process [2,3]. Applications of this strategy to natural LH complexes are here presented and discussed.

[1] B. Mennucci, C. Curutchet, Phys. Chem. Chem. Phys., 13 (2011) 11538.
[2] C. Curutchet, A. Munoz-Losa, S. Monti, J. Kongsted, G. D. Scholes, B. Mennucci, J. Chem. Theory Comput., 5, (2009) 1838.
[3] S. Caprasecca, C. Curutchet, B. Mennucci, J. Chem. Theor. Comput., 8 (2012) 4462.