

#ICMolTalks

Prof. Antonio Monari**Université Paris Cité & CNRS – ITODYS**June 26th - 11:30h

📍 Seminario SS6



Abstract

Don't Help Them to Bury the Light. Multiscale Methods to Simulate Photo-Biological Phenomena

The interaction of biological systems with external stimuli, such as light, is responsible for crucial phenomena related to signaling as well as energy conversion, and storage. Furthermore, while external perturbations, and thus light, may induce harmful effects related most notably to skin cancer development, they can be exploited for therapeutic purposes, for instances in Photodynamic or Light Assisted Therapy approaches.

In this talk, we will illustrate the crucial role played by molecular modeling and simulation in elucidating these complex processes and their interaction patterns in biological systems. We will stress the necessity of describing multiscale phenomena taking into account at the same time complex electronic structure rearrangements and its interplay with dynamic sampling and time evolution in biological macrostructures.

By using appropriate and high-level molecular modeling and simulation strategies we will prove that the scientific field is nowadays ready to provide answers to, and hence rationalize, biological questions related most notably to mutation, DNA replication, cell resistance to stress, cell signaling, and viral infections. We will also see how molecular modeling can assist in developing original photoimmunotherapy approaches. Thus, we will show how molecular modeling can rationalize photobiological phenomena from the light matter interaction up to the biological outcome. Hence, we will prove that we are clearly leaving the age of the simulation of model systems to enter into the age of a veritable in silico photo-biology.



References

1. Francés-Monerris et al. (2018) Chem. Sci. 9, 7885.
2. Dehez et al. (2017) Nucleic Acids Res. 45 3654-3662
3. Bignon et al. (2016) Nucleic Acids Res. 44, 8588
4. Francés-Monerris et al. (2018) Phys. Chem. Chem. Phys. 20, 25666
5. Francés-Monerris et al. (2019) J. Phys. Chem. Lett. 10, 6750
6. Hognon C. et al. (2019) J. Phys. Chem. Lett. 10, 72000
7. Marazzi et al. (2019) J. Phys. Chem. Lett. 10, 7133
8. Bignon et al. (2022) Chem. Sci. 13, 6098
9. Bignon et al. (2022) Chem. Commun. 58, 2176
10. Delova et al. (2023) J. Comp. Inf. Model. 63, 299
11. D'Anna et al. (2023) Chem. Sciences doi: 10.1039/D3SC04004F
12. Delova et al. (2023) Phys. Chem. Chem. Phys. 25 20567
13. Singer et al. (2023) J. Phys. Chem. Lett. 14, 1033
14. Delova A., et al. (2024) Chem. Eur. J. Doi: 10.1002/chem.202304318