



CHEMISTRY & CHEMICAL BIOLOGY COLLOQUIUM:

Proteins & Light: Which Modeling?

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Date:

11/20/2020

Time:

1:30 PM-2:50 PM

Link:

Please email
snsgradstaff@ucmerced.edu
for Zoom link and passcode

About The Speaker:

Benedetta Mennucci is Professor in Physical Chemistry at the University of Pisa in Italy. In the period 2014-2016, she acted as President of the Theoretical and Computational Chemistry Division of the Italian Chemical Society. Starting from 2014 she is Senior Editor for the Journal of Physical Chemistry Letter of the American Chemical Society. Her research interests mainly lie in the development and the application of hybrid QM/classical models to describe molecular properties and processes in environments of increasing complexity such as excitation energy transfers in natural and artificial light-harvesting systems. More recently, her research has been focused on the simulation of photoresponsive proteins, for which, in 2018, she obtained an European Research Council Advanced Grant with a project entitled "LIFETimeS: Light-Induced Function: from Excitation to Signal through Time and Space".

Abstract:

Organisms of all domains of life are capable of sensing, using and responding to light. The molecular mechanisms used are diverse, but most commonly the starting event is an electronic excitation localized on a (multi)chromophoric unit bound to the protein matrix. The initial excitation rapidly "travels" across space and time to be finally used to complete the biological function. The whole machinery is largely determined by the coupling between the electronic process, the nuclear motions of the chromophores and the dynamics of the protein. Here we discuss the main theoretical and methodological challenges of the modeling of such a complexity of interactions and dynamics, and we present possible strategies based on the integration of quantum chemistry and molecular dynamics.

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