

"THE MODELING OF LIGHT-INDUCED PROCESSES IN PROTEINS THROUGH MULTISCALE APPROACHES"

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ORGANIZATION:

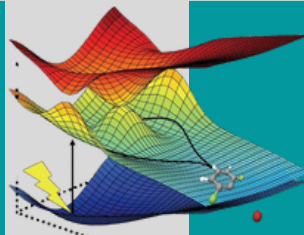
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with the words "Benedetta Mennucci – Virtual" on the "subject"
Deadline: June 09, 2021 (Wednesday), 06pm (BRT time)



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ABSTRACT

The modeling of light-induced processes in proteins through multiscale approaches

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Photoresponsive proteins use light to activate different biological functions. The molecular mechanisms are diverse, but most commonly the starting event is an electronic excitation localized on a (multi)chromophoric unit embedded in the protein. Computational approaches are powerful techniques to investigate these complex systems but only if they can properly describe the interactions between the chromophore(s) and the protein and couple their dynamics. A possible strategy is to combine quantum chemistry and classical models and integrate the resulting multiscale approach into molecular dynamics, but many theoretical and numerical critical issues have to be faced. In this talk, these issues will be discussed, and possible solutions will be presented together with some applications.