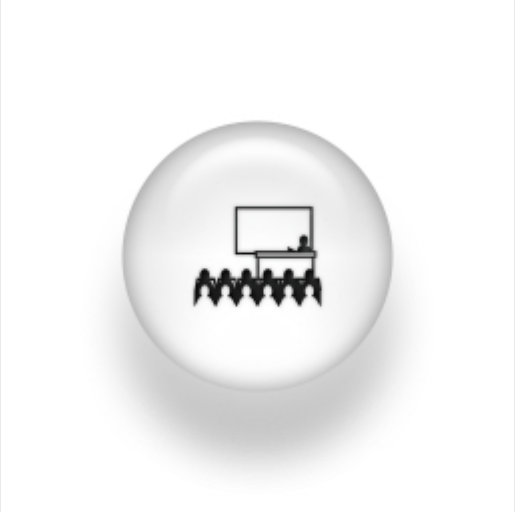
QM/MM Methods: Towards an Efficient and Accurate Description of Biological Photoreceptors and their Rractivity: Rhodopsin-Like Systems as an Example

Wednesday, 24 February 2010, 16:15-17.15

Dr. Pedro B. Coto



Interdisziplinäres Zentrum für Molekulare Materialien (ICMM)
Friedrich-Alexander-Universität Erlangen-Nürnberg

ABSTRACT:
The description of biological processes induced by light absorption is a challenge for state of the art electronic structure methods. Not only the size of the systems but also the need for an appropriate treatment of different electronic excited states make of the theoretical description of these systems a complex task. In this talk, some of the photo-physicochemical processes carried out by prototypical photoreceptors are characterized by using the QM/MM [1] CASPT2//CASSCF/Forcefield protocol, which is able to offer a balanced description of the different electronic states involved in the reaction by including both static and dynamic correlation effects. In particular, the different factors controlling the wavelength of absorption [2-3] and the molecular mechanism underlying the chemical process [4] are analyzed.

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3) P. B. Coto, S. Martí, M. Oliva, M. Olivucci, M. Merchán, and J. Andrés, J. Phys. Chem. B, 112, 7153 (2008).
4) A. Strambi, P. B. Coto, L. M. Frutos, N. Ferré, and M. Olivucci, J. Am. Chem. Soc., 130, 3382 (2008).