



VABILO NA PREDAVANJE / INVITATION TO THE LECTURE

Prof. Dr. Nadja Došlić

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Petek / Friday, 1. 3. 2013, ob / at 13:00

Fegeševa soba na Kemijskem inštitutu / Fegeš Room at the
National Institute of Chemistry; Hajdrihova 19, Ljubljana

Nonadiabatic molecular dynamics: exploring excited state deactivation pathways in biomolecular systems

Abstract:

We present a study of nonadiabatic dynamical processes occurring in biomolecular systems in the gas phase and in solution.

The computation of the pathways of nonradiative relaxation and the corresponding lifetimes typically requires a long time propagation during which the system explores vast regions of the configurational space and hence the approximation of reduced dimensionality becomes inadequate. In this lecture various aspects of full-dimensional nonadiabatic dynamics simulations based on time-dependent density functional theory will be discussed.

On the specific example of the model dipeptide Ac-Phe-NH₂ (NAPA) we will show how nonadiabatic dynamics has been used to provide an insight into the conformers dependent excited state deactivation mechanisms.

Next, the focus will be on the nonadiabatic dynamics in solution.

It will be shown that in combination with quantum mechanics/molecular mechanics (QM/MM) approach, the method is capable of unraveling the relaxation pathways of systems of significant complexity such as the protonated Schiff base of retinal in solution.

Finally, if time permits, the issue of photostability to hydrogen bonded biomolecules will be touched. Previous studies have shown that single and double proton transfer are energetically feasible mechanisms of excited state deactivation.

By comparing the excited state dynamics of the formic acid monomer, and the singly and doubly hydrogen bonded dimer, we show how the competing mechanism, i.e., dissociation of the dimer on the excited electronic state surface that may eventually lead to fragmentation, is effectively suppressed in the doubly hydrogen bonded formic acid dimer.

Vljudno vabljeni! / Kindly invited!

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