Kemijski inštitut
Ljubljana
Slovenija

National
Institute of Chemistry
Slovenia

http://www.ki.si

VABILO NA PREGLOV KOLOKVIJ / INVITATION TO THE PREGL COLLOQUIUM

Prof. Dr. Ursula Röthlisberger

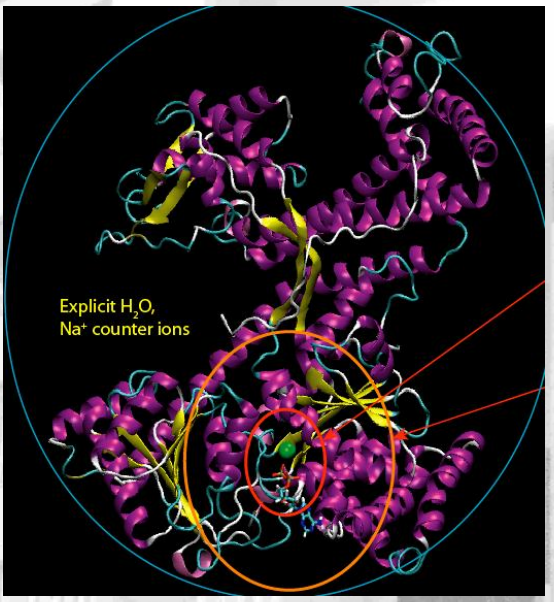
Laboratory of Computational Chemistry and Biochemistry
Federal Institute of Technology, EPFL, 1015 Lausanne, Switzerland

Četrtek/ Thursday 23. 05. 2013, ob / at 13:00

Velika predavalnica Kemijskega inštituta / Lecture Hall
at the National Institute of Chemistry, Hajdrihova 19, Ljubljana

From Anticancer Drugs to Photoactive Proteins:

Dynamics of Complex Systems by Mixed Quantum Mechanical/Molecular Mechanical (QM/MM) Car-Parrinello Simulations



One of the main goals of our research is the description of quantum mechanical phenomena in extended, heterogeneous systems, in particular biological systems. To this end, we have developed a combination of density functional based Car-Parrinello simulations and classical molecular dynamics simulations based on empirical force fields [1]. With such mixed quantum mechanical/ molecular mechanical (QM/MM) simulations complex systems can be described in an hierarchical approach, in which part of the system (the electronically active component) is described at the level of a first-principles electronic structure method whereas the effects of the environment are taken into account within the framework of a classical force field. In this way the mechanism of chemical reactions that occur in extended systems can be studied *in situ* [2].

We have also extended this type of QM/MM ground state simulations to adiabatic and nonadiabatic dynamics [3] in electronically excited states. This extension enables the study of optical and photochemical properties of complex systems, such as e.g. the characterization of photoactive proteins [4].

[1] A. Laio, J. VandeVondele, and U. Rothlisberger, *A Hamiltonian Electrostatic Coupling Scheme for Hybrid Car-Parrinello Simulations*, J. Chem. Phys. 116, 6941-6948 (2002)

[2] C. Gossens, I. Tavernelli, and U. Rothlisberger, *DNA structural distorsions induced by rutheniumarene anticancer compounds,* J. Am. Chem. Soc. 130, 10921-10928 (2008)

[3] E. Tapavicza, I. Tavernelli, and U. Rothlisberger, *Trajectory surface hopping within linear response time-dependent density functional theory, Phys. Rev. Lett. 98, Art. No. 023001 (2007)*

[4] U. Röhrig, L. Guidoni, A. Laio, I. Frank and U. Rothlisberger, *A Molecular Spring for Vision,* J. Am. Chem. Soc 126, 15328-15329 (2004)

Vljudno vabljeni! / Kindly invited!

Info: Janez Mavri; janez.mavri@ki.si