REGIONAL CENTRE OF ADVANCED TECHNOLOGIES AND MATERIALS
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REGIONAL CENTRE OF ADVANCED TECHNOLOGIES AND MATERIALS LECTURES

Tuesday, June 7, 11:00 am
Seminar room of Department of Physical Chemistry (room No. 3.002),
17. listopadu 12, Olomouc

Ondřej Maršálek, Ph.D.

(Stanford University)

„Accurate structure and dynamics of water and concentrated aqueous proton defects: the interplay of nuclear and electronic quantum effects"

Ondřej Maršálek (born in 1984) is a postdoctoral scholar at Stanford University (since 2014) within group of prof. Thomas Markland. He previously worked as Assistant Research Scientist at New York University (2012-2014). His Ph.D. studies were supervised by prof. Pavel Jungwirth at Institute of Organic Chemistry and Biochemistry Academy of Sciences of the Czech Republic in Prague and Charles University in Prague. For his doctoral thesis about "molecular simulations of the effect of ionizing radiation on water and hydrated electron" he was awarded Česká hlava award in 2013. He has published 29 papers in peer-reviewed journals, which were cited 300+ times. His H-index is 10.

Abstract: Describing the structure and dynamics of water and aqueous proton defects requires the accurate treatment of their electronic structure and nuclear quantum effects, such as zero-point energy and tunneling. Path integral simulations, combined with an ab initio evaluation of interactions using electronic structure theory, incorporate the quantum mechanical nature of both the electrons and nuclei. However, for aqueous systems, even at ambient temperatures, the computational cost of these ab initio path integral simulations has traditionally been at least two orders of magnitude greater than treating the nuclei classically, making them prohibitively costly for most applications. In this talk, I will show how our recent work that has extended the ring polymer contraction method to ab initio molecular dynamics simulations and combines it with a multiple time step scheme allows us to now include nuclear quantum effects at a cost below that of a typical classical ab initio molecular dynamics simulation. I will demonstrate how this approach has allowed us to elucidate the interplay of nuclear and electronic quantum effects that give rise to the structure, dynamics and spectroscopy of liquid water and reactive aqueous defects, such as highly concentrated acids, and provides near quantitative agreement with experiment.