Oddělení spektroskopie,
Oddělení chemie iontů a klastrů
a Oddělení teoretické chemie
ÚFCH JH AV ČR

srdečně zvou všechny zájemce na mimořádný společný seminář, na kterém promluví:

Ondřej Maršálek

(Ústav organické chemie a biochemie AV ČR, Praha)

na téma:

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

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 to 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.

Seminář se koná ve **středu, 1. 6. 2016 ve 14:00** v místnosti č. 108 Ústavu fyzikální chemie Jaroslava Heyrovského AV ČR, Dolejškova 3, Praha 8 – Kobylisy.

Jiří Pittner **Ondřej Votava**