Title: Structure and dynamics of electronic defects in liquid water

Author: Ondřej Maršálek
Institute: Institute of Organic Chemistry and Biochemistry, Academy of Sciences of the Czech Republic
Supervisor: prof. Mgr. Pavel Jungwirth, DSc.
Supervisor's e-mail address: pavel.jungwirth@uochb.cas.cz

Abstract: In this thesis we present ab inito molecular dynamics simulations of two different electronic defects in water. Photoionization of liquid water produces a cationic hole, which undergoes ultrafast dynamics and forms the hydrated proton and the hydroxyl radical as its products. We study both the dynamics and spectroscopy of this process. The hydrated electron is a key intermediate in radiation chemistry of aqueous systems. We simulate its equilibrium properties in anionic water clusters as well as the dynamics of vertical electron attachment to cold and warm clusters. The hydrated electron reacts with a hydrated proton to form a hydrogen atom. We examine this reaction at a finite temperature in a larger cluster as well as in more detail in a smaller cluster. Because both of the electronic defects studied here are challenging open-shell species, we put emphasis on benchmarking and testing our computational setup. Six published articles are attached to the thesis.

Keywords: density functional theory, self-interaction correction, ab inito molecular dynamics, hydrated electron, cationic hole, water ionization, photoionization, vertical electron attachment