Seminář odd. 26
Tenkých vrstev a nanostruktur

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TÉMA

Chemistry and Physics Triggered by Light: Molecular Simulations in UV and X-ray domains

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Radiation can be recently sensitively controlled both in time and energy. Chemistry can benefit from the advancement in physics and use light to control matter. In my talk, I will focus on molecular simulations of the chemical processes initiated by the interaction of photons with molecules. Photochemical processes are usually associated with photons in the UV, visible and sometimes also in the IR range. Photochemical simulations describing the processes in this range have significantly advanced in the last decade. I will briefly describe the techniques typically used in the field, emphasizing particularly the role of solvent environment. The field of X-ray initiated photodynamics is much more complicated and much less developed. In fact, dynamical processes initiated by X-ray photons are so far not typically considered as part of photochemistry as the amount of energy deposited into the system is way too large for defined chemical changes. On the other hand, X-ray photons allow us to excite/ionize specific atoms. Here, I will present our recent findings on new processes which we have identified in solvated systems upon X-ray exposure. In this context, I will also discuss new liquid state spectroscopies using tunable X-radiation and allowing us to investigate X-ray initiated processes.

odborný garant: *Ing. Pavel Jelínek, PhD.*