Ultrafast non-adiabatic dynamics in water clusters - hydronium radical as an intermediate in the formation of hydrated electron

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The ultrafast processes taking place in water clusters upon irradiation, and subsequent dissociation pathways following excitation have not yet been elucidated completely. The OH• radical along with the hydrated electron are the key species forming on femtosecond time-scales. Seemingly, when the photon energy is high enough the hydronium moiety forms and plays a significant role in these processes. [1] The results are complying with an experimental study performed along this theoretical study and a cooperative paper is in preparation.

We have performed a series of non-adiabatic *ab initio* molecular dynamics calculations on various-size water clusters and observed the reactivity on a femtosecond time scale. We observe two main dissociative pathways leading to either hydronium formation along with a solvated electron or to a hydrogen atom formation, which is a terminate step. We present an extensive study describing the reactivity of excited water clusters depending on the initial excitation energy and on the size of the water cluster.

The extensive study is supported with description of various-size hydronium-water clusters, their structure, their electron binding energies and the localization of an extra electron.

References:

1. A. L. Sobolewski and W. Domcke, *Phys. Chem. Chem. Phys.* **4** (2001), 4-10.