



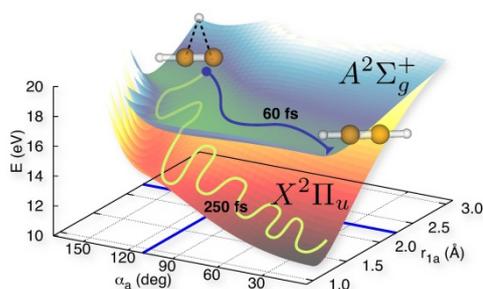
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Building 49, Seminar Room (108)

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Ultrafast dynamics of ionized molecules under XUV light

Recent experiments conducted at FLASH [1,2] explore the ultrafast dynamics of small molecules and clusters upon single photoionization by XUV light. Here, we report on our efforts to understand the processes that unfold after ionization based on molecular dynamics simulations [3]. The photoionized molecules and clusters are produced in excited electronic states of the corresponding ion with outer or inner valence character.



In the case of acetylene (HCCH), our simulations agree with the experimental finding that ionization is followed by ultrafast isomerization to vinylidene (CCHH). We find that close to vinylidene configurations, the system decays from the $A^2\Sigma_g^+$ electronic state to the ground state of the ion $X^2\Pi_u$ through a conical intersection, and both isomerization and electronic decay occur in a time-scale of about 100 fs after ionization. The electronic decay leaves the ion in a vibrationally

hot state. We predict that the excess vibrational energy can be efficiently redistributed among vibrational modes in about 300 to 400 fs, bringing the system back to a quasi-equilibrium state.

In the case of the protonated water dimer $H^+(H_2O)_2$ the system undergoes a Coulomb explosion immediately after photoionization. Our initial results indicate that various conical intersections between excited electronic states of the ionized system are involved in the explosion process.

[1] Jiang YH, Rudenko A, Herrwerth O, Foucar L, Kurka M, Kühnel KU, et al. Ultrafast Extreme Ultraviolet Induced Isomerization of Acetylene Cations. *Phys. Rev. Lett.* 105, 263002 (2010); [2] Lammich L, Domesle C, Jordon-Thaden B, Förstel M, Arion T, Lischke T, et al. Fragmentation Pathways of $H^+(H_2O)_2$ after Extreme Ultraviolet Photoionization. *Phys. Rev. Lett.* 105, 263002 (2010); [3] Madjet M.E., Vendrell O., Santra, R., Ultrafast dynamics of photoionized acetylene. Submitted.