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Ultrafast nonadiabatic processes in photoionized molecular systems probed by time-resolved core-level spectroscopy

ORIOL VENDRELL, Center for Free-Electron Laser Science, DESY, Notkestrasse 85, 22607 Hamburg, Germany

There is a fundamental interest in understanding the coupled nuclear and electronic dynamics associated to charge transfer processes in complex molecules and materials, which is often mediated by electron, electron hole or proton motion. For example, the response of the light hydrogen atoms to a newly created electron hole in a water cluster can be as fast as sub 5 fs [PRL **110**, 038302 (2013)] and involve strong nuclear-electronic couplings. With dramatic improvements in the techniques to generate extreme ultraviolet (XUV) and x-ray femtosecond pulses, it becomes now possible to trigger and probe these kinds of processes in real time. Here, we study the dynamics of an electron hole created by photoionization in the valence shell of protonated water clusters $H^+(H_2O)_n$ and its correlated motion with protons in the hydrogen bond network due to electrostatic interactions. We will discuss from a theory perspective how key aspects of the electron hole dynamics can be mapped out to core-level transient x-ray absorption spectra with femtosecond resolution.