Abstract Submitted
for the DAMOP20 Meeting of
The American Physical Society

Towards Observing Site Selective Chemistry in Real Time[1]

GILLES DOUMY, DIMITRIOS KOULENTIANOS, STEPHEN SOUTHWORTH, LINDA YOUNG, Argonne Natl Lab, XUECHEN ZHENG, JUNZI LIU, LAN CHENG, Johns Hopkins University — The possibility of site-selective photochemistry, where element and site selective excitation or ionization using x-ray photons guides the outcome of the dissociation has been an intriguing problem since the advent of high average flux sources at synchrotrons. So far, only limited selectivity has been observed, hinting at efficient charge redistribution before decay processes happen. The ability to probe this process as it happens is now becoming a reality at x-ray free electron lasers, with the ability to produce two pulses commensurate with the core-hole lifetimes, with very different photon energies, and soon high repetition rates. By initiating an inner shell process at one molecular site and probing at another place in the molecule, one will be able to observe the evolution of the electronic properties, starting from the ionization energies of the core excited states. Making sense of the data will require comparison with high accuracy computational predictions, such as using our newly developed scalar-relativistic delta-coupled-cluster method. We will present calculations for a class of fluoro-alkane molecules that will be the focus of a demonstration experiment at LCLS this year.

[1] This work was supported by the US Department of Energy, Office of Science, Basic Energy Sciences, Chemical Sciences, Geosciences, and Biosciences Division

Gilles Doumy
Argonne Natl Lab

Date submitted: 02 Feb 2020

Electronic form version 1.4