CFEL SCIENCE

# SEMINAR

***11th November 2020 - 2:00 p.m.***

Virtual meeting room in ZOOM (ID: 995 3143 1322 / PW: 849038)

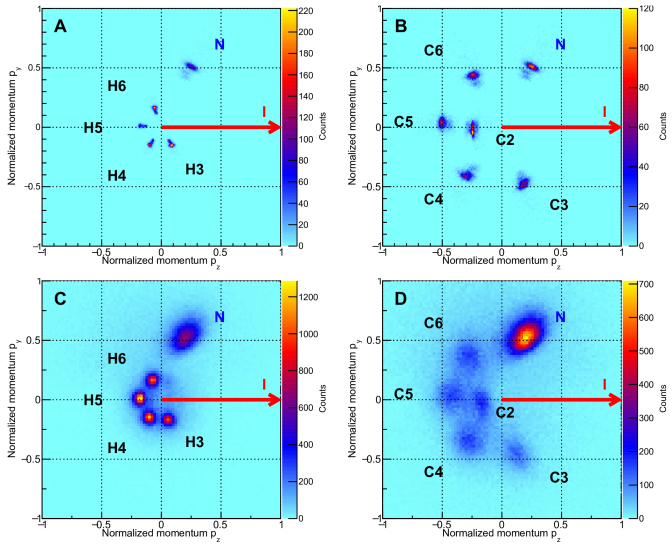

## Julia M. Schäfer

Center for Free-Electron Laser Science, DESY, Germany


# Molecular Modeling of X-ray Induced Coulomb Explosion Imaging with XMDYN

Imaging the structure of single molecules has been the subject of research for decades. Coulomb explosion imaging (CEI) is an approach that involves a rapid charge-up of all atoms, inducing an explosion-like fragmentation due to Coulomb repulsion. The 3D momentum of each fragment ion is recorded, and can be used to deduce the molecular structure.

In an experiment at European XFEL our collaboration could identify all eleven atoms of 2-iodopyridine unambiguously with CEI, by using intense, femtosecond soft x-ray pulses. The Newton plots calculated with our XMDYN toolkit for a coincident detection of $I^+$, $N^+$ and $H^+$ ions (A), as well as $I^+$, $N^+$ and $C^+$ ions (B) agree very well with the experimental equivalents (C, D). This allows us to add time-resolved information to the study, which was experimentally not accessible.




Newton plots of $I^+$+$N^+$+$H^+$ (A,C) and $I^+$+$N^+$+$C^+$ (B,D) of 2-iodopyridine, in theory (A,B) and experiment (C,D).

XMDYN combines atomic *ab initio* x-ray physics with molecular dynamics in a Monte Carlo scheme. In my talk I will present developments and current limitations of our state-of-the-art model, as well as show results of our joint theoretical and experimental study. This XMDYN version represents a benchmark for future CEI investigations with even larger molecules.

Host: Robin Santra – CFEL-DESY Theory Division