Illuminating Biomolecular Complexity: X-ray Free Electron Lasers and Vibrational Spectroscopies for Protein, Aggregates, and Cellular Architectures

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FEL Coulomb Explosion Imaging: Simulation of Coulomb explosion of highly charged 2-Iodopyridine and comparison to experimental data

X-ray Single Particle Imaging has the aim of imaging biomolecules without the need of crystallization. The invention of X-ray Free Electron Lasers (XFELs) provided the instruments for this imaging process, however the technique is still suffering from low signal to noise ratio. Retrieval of the orientation of the sample in the moment of photon-sample interaction would greatly improve the signal and interpretability of experimental data. During the interaction, the intense radiation of the XFEL leads to high ionization of the sample and to a Coulomb explosion, in which positively charged ions repel each other and fly out of the interaction zone. It was found in recent simulations that a record of the Coulomb explosion doesn't only just retrieve the original orientation of the imaged sample, but also bears structural information itself about the molecule. Hence, it was proposed to explore the relationship between structure and Coulomb explosion, a process called Coulomb Explosion Imaging. The biophysics research group of Uppsala University has developed a Molecular Dynamics/Monte Carlo code called MolDStruct4, which is based on GROMACS. MolDStruct replicates the radiation-induced Coulomb explosion of biomolecules and enables the tracking of ion-trajectories. The code is currently benchmarked against the QM/DFT code SIESTA as well as experimental data to ensure that the simulations of the Coulomb explosions are as realistic as possible. In this process, we investigate the biomolecule 2-Iodopyridine, ionize it up to an average ionization of one per atom and record the Coulomb explosion in simulations with MolDStruct. Then, we compare the results with data from a recent XFEL experiment in which highly ionized 2-Iodopyridine was exploded and the ejected ions were measured using a reaction microscope. Additionally, we execute QM/DFT simulations with the code SIESTA and also record the Coulomb explosion. The simulations with MolDStruct and SIESTA are consistent with one-another and they both replicate well the experimental data. Contrarily to Single Particle Imaging, Coulomb Explosion Imaging does not necessarily need hard X-rays and would be feasible with an intense FEL, such as the one being developed in the EUPRAXIA project. With MolDStruct, the relationship between structural information and Coulomb explosions can be studied intensively in simulations, information which can later on be used to support and enhance experiments on molecular sample structures by adding new imaging possibilities and providing better interpretation of the signal.

Scholarship elegibility

yes

Primary authors: KRÜGER, Lais Friederike (Uppsala Unversitet); ANDRÉ, Tomas (Uppsala University); TIMNEANU, Nicusor (Uppsala Universitet); CALEMAN, Carl (Uppsala University, Center for Free-Electron Laser Science, Deutsches Elektronen-Synchrotron)

Presenter: KRÜGER, Lais Friederike (Uppsala Unversitet)