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First insights to refined results: mapping charge transfer in dissociating molecules

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Charge transfer is essential to many complex chemical processes and thus a thorough understanding at the molecular level is desired. One particular aspect concerns the interplay between the positions of nuclei and the probability of charge transfer. During a beamtime at EuXFEL's SQS instrument, we studied how the ability to transfer electrons in dissociating molecules with a rotating fragment changes throughout the dissociation process.
Beyond the fundamental physics, this talk highlights the data analysis journey. We demonstrate how preliminary online and first offline feedback enabled us to steer the experiment, yet how it differs from the post-beamtime refined results. We discuss the role of the EuXFEL data analysis ecosystem using tools such as EXtra-metro, DAMNIT and EXtra in different stages of that journey.

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