Report on the outcomes of a Short-Term Scientific Mission[1]

Action number: CA20129

Grantee name: Oksana Travnikova

Details of the STSM

Title: Data Analysis of Hard X-Ray Induced Fragmentation and Charge Redistribution Dynamics: First Results from the New High-Energy Electron-Multi-Ion Coincidence Setup, MUSTACHE

Start and end date: 18/05/2025 to 29/05/2025

Description of the work carried out during the STSM

The STSM focused on the analysis of electron-multi-ion coincidence data collected using the new MUSTACHE setup, a high-resolution spectrometer developed for studying deep inner shell ionization of high-Z atom-containing molecules, including radiosensitizers. The primary objective of the visit was to gain advanced training in using custom data analysis macros developed by Prof. E. Kukk (University of Turku) within the IgorPro environment and to apply this knowledge to datasets obtained in December 2024 at the SOLEIL synchrotron.

The training covered data calibration, construction of PEPICO (photoelectron-photoion coincidence) and PIPICO (photoion-photoion coincidence) maps, data filtering based on ion charge states, momenta and electron energies, and development and use of macros for multidimensional momentum correlation analysis. A significant portion of the time was dedicated to understanding how these tools can be used to disentangle complex fragmentation and relaxation pathways following hard X-ray ionization.

We primarily focused on two radiosensitizer molecules: 5-iodo-4-thio-2′-deoxyuridine and 5-bromo-4-thio-2′-deoxyuridine. Initial results revealed distinct fragmentation behavior dependent on the halogen present, suggesting that the nature of the halogen significantly influences charge redistribution and subsequent molecular breakup. These findings were discussed in detail and will form the core of a forthcoming publication currently in preparation.

Further work involved the development and testing of macros for analyzing three-ion coincidences and extracting kinetic energy release (KER) distributions. These tools are essential for investigating ultrafast nuclear dynamics occurring during Auger cascades, particularly in small I-containing molecules such as dihalogenated methanes, which were also studied during the same beamtime in December 2024. The ray-tracing simulations were used to compare the experimental ion energy distributions with those predicted based on known setup geometries and fields, enhancing the reliability of the extracted data.

[1] This report is submitted by the grantee to the Action MC for approval and for claiming payment of the awarded grant. The Grant Awarding Coordinator coordinates the evaluation of this report on behalf of the Action MC and instructs the GH for payment of the Grant.

The STSM followed the initial working plan closely, with all scheduled activities completed as intended. No significant deviations occurred. The visit provided a comprehensive framework for current and future analysis, laying the groundwork for several joint publications and follow-up collaborative work.

Description of the STSM main achievements and planned follow-up activities

The main goal of this STSM – to perform advanced data analysis of electron - multi-ion coincidence measurements using the newly developed MUSTACHE setup and to receive training in dedicated analysis software – was fully achieved. The STSM enabled in-depth analysis of electron-ion coincidence data from the first measurements using tender X-rays to investigate halogen-containing radiosensitizer molecules and dihalogentaed methanes, revealing element-specific fragmentation pathways and charge redistribution mechanisms following deep inner-shell ionization.

The training received on custom analysis tools significantly enhanced the grantee's ability to independently process and interpret multidimensional coincidence data. Specific skills acquired include ion momentum correlation mapping, extraction of kinetic energy distributions, various filtering based on the extraction of the different type of information, and application of ray-tracing simulations. These methods will be crucial for analyzing all future datasets acquired with the MUSTACHE setup.

Initial interpretation of the experimental data has already led to clear insights into halogen-dependent electronic and nuclear dynamics. The results from the two radiosensitizers studied are currently being compiled into a scientific manuscript, co-authored with the host group, which is expected to be submitted in the near future. Additionally, another manuscript focusing on ultrafast nuclear dynamics in small I-containing molecules is foreseen after completing data analysis and its interpretation.

This STSM has strengthened the ongoing collaboration between the applicant's research group and Prof. E. Kukk's team. Plans for future joint work include co-development of additional analysis tools, participation in upcoming beamtime proposals, and continued investigation of radiation-induced processes in high-Z-atom containing organic molecules. The insights and tools developed during this mission also contribute directly to the broader goals of the Action, which include fostering deeper understanding of radiation damage mechanisms relevant to medical and biological applications.

Overall, the STSM significantly advanced both the technical capabilities and collaborative network of the grantee, with tangible outcomes in the form of publications, software tools, and long-term research directions.