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

Action number: CA20129

Grantee name: Yihui Yan

Details of the STSM

Title: Stability of porphyrin derivatives embedded in helium droplets upon electron irradiation

Start and end date: 16/09/2024 to 27/09/2024

Description of the work carried out during the STSM

Description of the activities carried out during the STSM. Any deviations from the initial working plan shall also be described in this section.

(max. 500 words)

During the first week of my internship, I worked on enhancing the helium-tagged molecular ion spectrometer, "Toffy2." The improvements involved adding a second pickup chamber to the existing setup, which included a helium nanodroplet (HND) source, a pickup chamber, and a quadrupole time-of-flight mass spectrometer (TOF-MS). A new resistive heating oven was constructed within the second pickup chamber, allowing samples to be heated to several hundred degrees Celsius for evaporation. By the end of the week, we focused on optimizing ion transfer and calibrating the mass spectrometer using ion signals from the HND, successfully improving the instrument's precision and sensitivity.

After achieving optimal vacuum conditions over the weekend, we commenced the second week with an experiment aimed at generating doubly-charged gold (Au) clusters. Au vapor was produced in the resistive oven and ionized via charge transfer or Penning ionization by interacting with the HNDs. Helium gas was introduced into the evaporation chamber, causing the nanodroplets to shrink through collisions, which improved ionization efficiency. Additionally, a secondary electron-impact ionization source was employed to increase the chances of producing doubly-charged Au ions. However, the ion signals were weak, prompting a change in strategy.

Then, we replaced the Au sample with fullerene (C_{60}), a more stable molecule known to provide stronger ion signals. Water vapor was then introduced into the second pickup chamber to investigate the binding energies of multiply-charged C_{60} water clusters. This allowed us to study the ionization behavior of fullerene in combination with water molecules, offering valuable insights into their clustering and bonding mechanisms.

[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.

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

Description and assessment of whether the STSM achieved its planned goals and expected outcomes, including specific contribution to Action objective and deliverables, or publications resulting from the STSM. Agreed plans for future follow-up collaborations shall also be described in this section.

(max. 500 words)

During the STSM period, we successfully completed modifications to the helium-tagged molecular ion spectrometer "Toffy2." A second pickup chamber equipped with a gas inlet system and a custom-made resistive oven was added. The oven was designed using two molybdenum screws as supports and conductors for Ohmic heating. A 1.5mm thick pure molybdenum sheet was bent into a boat shape to hold the sample, while a tubular heat shield made of molybdenum, with a diameter of approximately 20mm, served to contain sample vapor, enhance pickup efficiency, and protect other parts of the device. The gas inlet system, equipped with a pressure controller (Bronkhorst GmbH, FG-001AV-LFU-88-K), allowed gaseous or high-vapor-pressure dopants to be introduced into the pickup chamber.

The experiments targeting Au's doubly-charged clusters were not very successful. Significant production of Au-water clusters likely stemmed from the hydrophilic nature of the molybdenum material, which, upon heating, released water that combined with Au. We attempted prolonged low-temperature baking to evaporate residual moisture without generating Au vapor, which improved the $(Au)_n^+$ signal. However, no doubly-charged Au signal was observed despite optimizing ionization energy and adjusting the ToF signal range and resolution. The low $(Au)_n^+$ signal, around 500 counts per second, may have been due to limited sample quantity and the absence of ion lenses in the new pickup chamber, contributing to the weak signal.

For the detection of multiply-charged fullerene-water clusters, we successfully obtained signals of doubly-charged fullerene-water clusters. Future work will focus on enhancing these signals and exploring the binding capabilities of fullerene with water under multiple ionization states. Additionally, we plan to use a laser beam to merge with the target ions, utilizing messenger spectroscopy to further analyze the ion-photon interactions and binding properties of these clusters. The photo-products will be measured using time-of-flight mass spectrometry, which will provide more sensitive photofragment signals for the detection of target ions.