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

Action number: CA20129 "Multiscale Irradiation and Chemistry Driven Processes and Related Technologies" (MultIChem)

Grantee name: Sreckovic Vladimir

Details of the STSM

Title: Data-Driven Modeling of Molecular Ion Chemistry: Integrating Theory and Machine Learning

Start and end date: 19/08/2025 to 25/08/2025

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)

Recent advances in experimental techniques and computational chemistry have significantly improved our understanding of molecular interactions, particularly collisional and radiative processes. Studying these processes and expanding atomic and molecular (A&M) data repositories like VAMDC and RADAM remains crucial. Demand for accurate molecular data, both experimental and theoretical, is rising across research and industry for advanced modeling.

Machine learning (ML) has shown strong promise in predicting atomic and molecular properties. In astrochemistry, electron-induced reactions in organic films mimic the formation of cosmic ices in the interstellar medium (ISM), where ice-coated dust grains act as "chemical factories" for complex molecules. These grains, typically silicate or carbonaceous cores coated with frozen species like H_2O, CO, CO_2, and NH_3, facilitate reactions central to molecular complexity and prebiotic chemistry.

This STSM studied collisional and radiative processes involving these molecules, generating relevant A&M data for their chemistry and characterization. We calculated and analysed cross sections and rate coefficients, producing datasets that support astrochemistry, lab modeling, and more. To maximize impact, we adopt interoperable, standardized data formats for integration into platforms like VAMDC.

[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.

During the STSM, we computed rate coefficients for collisional and radiative processes involving N_2H^+, NS^+, and diatomic helium ions, with guidance from Professor Felix Iacob. These species are of relevance to astrochemistry and plasma modeling.

The reactions were analyzed using the dipole resonant mechanism, where the processes are driven by the dipole component of the electrostatic interaction between the electron and quasimolecular complexes. During the STSM, we compared results with the data obtained from theoretical methods based on Multichannel Quantum Defect Theory (MQDT).

During this STSM we start on the work on the application of ML algorithms to predict reaction rates based on computed and literature data. Also, we developed a data model compliant with the VAMDC schema, generated a relational database, and wrote Python-SQL scripts to import the data into it. We start enriching existing BG nodes with additional excitation, ionization, and recombination data, thereby enhancing their scientific value.

This mission provides an opportunity to deepen collaboration with Prof. Jakob, aligning with the long-term goals of the project and enabling future co-authored publications and joint conference presentations.

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)

The primary output of this STSM is a curated dataset of rate coefficients for molecular systems involving nitrogen, hydrogen, sulfur, and helium. These data can be relevant for modeling collisional and radiative processes in solid-state astrochemistry, plasma physics, and nanofabrication. Another outcome of this STSM is the conversion of new molecular datasets into a standardized format, ready for integration into the databases.

A significant outcome of this STSM is the initiation of implementing and benchmarking machine learning algorithms to aid in reaction rate prediction. This aligns with the development of computational tools for multiscale modeling (MoU WG3).

As follow-up activity, the results will be analyzed in collaboration with Prof. Iacob, with dissemination planned through a peer-reviewed article in *Data* (an open-access journal dedicated to advancing transparency and reusability in scientific data) as well as a presentation at a conference. Furthermore, the STSM will lay the groundwork for extended research collaboration and the development of future project proposals.

This STSM meets the following Multichem keywords / objectives / deliverables:: - WG1: Irradiation- and chemistry-driven multiscale phenomena: Creation and collection of data for MultIChem database where a comprehensive databank of related quantities (e.g., photon, electron and ion interaction cross sections with bio- and organometallic molecules, nanoparticles, nanostructures and composite structures, chemical reaction rates, diffusion coefficients for different atomic and molecular species, compositions of metal-containing nanostructures grown by FEBID, etc.); - WG2: Intersectoral cooperation on research and innovation and - WG3: Multiscale approach based technological advances: Development of novel computational tools for multiscale modelling. Facilitating communication and cooperation between research groups from different scientific disciplines and countries, such as theoretical and experimental groups in atomic and molecular physics, physical chemistry, biology, material science, -Conference, seminar/webinar and poster presentations.