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: Investigation of collisional and radiative processes: datasets of importance for molecular dynamics

Start and end date: 27/09/2024 to 03/10/2024

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)

As noted in the literature, the knowledge of complicated processes in many systems, including living ones, caused by photons, various particles, etc., is one of the main goals and needs of today's science. These processes may, for example, result in the therapeutic effects of radiation, energy conversion and storage, catalytic activity, or be crucial to technologies for the development of novel light sources. In recent decades, new experimental techniques and computational chemistry methods have gained prominence in the study of molecular interactions and dynamics. Furthermore, one can note the current importance of examining the collisional and radiative processes and the associated A&M data (VAMDC, RADAM, etc). The science community and industry today require access to such molecular data, which includes recommended ones, for further modelling purposes.

In the course of STSM, we investigated collisional and radiative processes of small molecules and provided data useful for characterization and chemistry for such systems. We calculated, and analysed cross sections and rate coefficients for such processes and species in Timisoara with Prof. Felix Iacob, a molecular physics expert. The outcomes, i.e. the generated datasets/databases, can be applied to essential activities such as modelling, industry, synchrotron experiments, and so on.

The reactions have been treated by the dipole resonant mechanism. In this characterization, the processes are caused by the dipole part of the electrostatic interaction between electron and the

[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.

quasimolecular complexes. This method is especially effective when used with the so-called decay approximation During STSM we compared the data obtained using theoretical methods based on the Multichannel Quantum Defect Theory (MQDT) and numerical tools,

In Timisoara with the prof. Felix Iacob we collected existing literature about theoretical and experimental works in the area of research and discussed the outcomes of the aforementioned species' rate coefficients and cross sections. During STSM, we developed a data model that fits the data while still being compliant with the VAMDC schema; generated a relational (MySQL or sqlite) database; and wrote Python-sql scripts to convert the data to the relational database. We are adding additional data to the MolD and ACol nodes, which currently contain excitation, ionization, and recombination data for a variety of species.

The main purpose of this STSM was to extend our collaborative work on the theoretical data featuring processes concerning hydrogen and helium molecular systems with Prof. Felix Iacob from the Faculty of Physics, West University of Timisoara.

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)

In this STMS, we investigated processes and data that can be used in a wide range of applications, including industry, synchrotron experiments, and laboratory modeling. Direct STSM outcome is a new dataset i.e. dataset of rate coefficients for a wide range of parameters for hydrogen and helium molecular systems.

Also, the result of this STSM is the conversion of new molecular datasets in a special format ready to be implemented in the databases. The output of STSM is a draft for the journal Physica Scripta.

As a follow-up activity we plan to submit the abstract at least to one international conference (https://asspectro.ipb.ac.rs/2024/) and plan to extend further cooperation with the host.

This STSM provides an opportunity to extend collaborative work with Prof. Felix Iacob of the Faculty of Physics, West University of Timisoara, in the field relevant to the action.

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.