

SHORT TERM SCIENTIFIC MISSION (STSM) SCIENTIFIC REPORT

This report is submitted for approval by the STSM applicant to the STSM coordinator

Action number: CA20129 MultiChem

STSM title: Prof.Dr. Andrey V.Solov'yov's training, research and dissemination activities at the University of Kent, United Kingdom

STSM start and end date: 03/07/2018 to 08/07/2022

Grantee name: Prof Andrey Solov'yov

PURPOSE OF THE STSM:

The purpose of the action was **to disseminate the knowledge** about the COST Action MultiChem among graduate and PhD students and staff members of the School of Physical Sciences of the University of Kent; **to present possibilities of the multiscale modelling** of the irradiation induced processes by means of the software packages MBN Explorer and MBN Studio developed by the MBN Research Center (MBN RC), Frankfurt, Germany; **to perform hands-on tutorial** at the School of Physical Sciences, University of Kent, Canterbury on *Multiscale Computational Methods for Complex Molecular Systems* by means of the software packages MBN Explorer and MBN Studio; **to discuss on-going experiments** on irradiation induced transformations in various liquid molecular systems deposited on substrates and the possibilities of collaboration in this field of research, to discuss possibilities of **further development of the training activities** in the aforementioned areas of physical, chemical and computational research in a form of one or several training networks; to continue joint **work on the roadmap paper** on multiscale modelling of phenomena in condensed matter systems exposed to radiation which should overview the state-of-the-art theoretical, computational and experimental achievements in the field and outline the main research challenges and directions for investigations for the MultiChem community for the next years.

DESCRIPTION OF WORK CARRIED OUT DURING THE STSMS

The STSM of Prof. A.V. Solov'yov to School of Physical Sciences, University of Kent, Canterbury took place during July 03 - July 08. This mission was hosted by Professor Nigel Mason, OBE, Head of School, and an internationally recognized expert in molecular spectroscopy and fragmentation dynamics applied to radiation chemistry, astronomy, aeronomy and plasma physics.

During this visit Professor Andrey Solov'yov:

- (i) hold the three days' hands-on tutorial on *Multiscale Computational Methods for Complex Molecular Systems* at the University of Kent with MBN Explorer & MBN Studio [1,2,3] and the ways of application of these software packages to modelling of the radiation damage and radiation chemistry processes and material science systems. The tutorial was addressed to graduate and PhD students, postdocs and staff members of the School of Physical Sciences of the University of Kent [4].

MBN Explorer is a software package developed by MBN RC for multiscale simulations of complex molecular structure and dynamics with applications in Physics, Chemistry, Biology, Material Science, and Industry. It is suitable for classical MD, Irradiation Driven MD (IDMD), Stochastic Dynamics (SD) and relativistic dynamic simulations of large biological systems, nanostructured materials, composite materials, gases, liquids, solids and interfaces, with sizes ranging from atomic to mesoscopic dimensions.

MBN Studio is a multitask toolkit with the graphical user interface for MBN Explorer that has been developed by MBN RC to facilitate setting up and starting MBN Explorer calculations, monitoring their progress and examining the calculation results. MBN Studio has a number of built-in tools allowing the calculation and analysis of specific characteristics that can be obtained from output of simulations. A special modeling plug-in allows one to construct a large variety of molecular systems quickly and efficiently;

- (ii) discussed the cooperation between the MBN Research Center and the University of Kent on the multiscale modelling of structure and dynamics of complex molecular systems and radiation physics research;
- (iii) learned about the on-going experimental and theoretical work at the School of Physics University of Kent, especially in the field of irradiation induced and chemical effects caused by metal nanoparticles and other molecular species exposed to irradiation;
- (iv) continued the joint work with Professor N. Mason on the validation of analytical and computational models for structure and properties of radiosensitizing metal nanoparticles;
- (v) continued working on the joint roadmap paper with Professor N. Mason aimed at the dissemination of the knowledge gained by the research community in the research area covered by the COST Action MultiChem and related fields.

DESCRIPTION OF THE MAIN RESULTS OBTAINED

1. There was established a group of researchers at the University of Kent, Canterbury whose work will involve computational modelling by means of MBN Explorer and MBN Studio;
2. The software (MBN Explorer and MBN Studio) will be installed on the local computer cluster (tentatively by the end of July, 2022) and it will be made accessible for members of the School of Physical Sciences, University of Kent;
3. There were established new collaborative links of the MBN RC with the colleagues from both the University of Kent in the field of radiation and astrochemistry;
4. Writing of the joint roadmap paper aimed at the dissemination of the knowledge gained by the research community in the research area covered by the COST Action MultiChem and related fields was continued.

FUTURE COLLABORATIONS (if applicable)

There were **(i)** established collaborations of the MBN RC, Frankfurt am Main, Germany with the the School of Physical Sciences, University of Kent, Canterbury, UK; **(ii)** outlined concrete plans towards the further development of training activities in the COST Action MultiChem research area on interdisciplinary physical, chemical, biological and computational problems in a form of one or several training networks.