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

Action number: CA20129 MultIChem

Grantee name: Prof. Dr. Andrey Solov'yov

Details of the STSM

Title: Development of new modelling activities

Start and end date: 29/05/2024 to 01/06/2024

The purpose of the STSM of Professor Andrey Solov'yov: to ATOMKI, Institute of Nuclear Research was to:

(i) Present the state of the art research and the modelling capabilities of the MBN software to the research community of ATOMKI and the University of Debrecen [1-4].

(ii) Discuss possible theoretical and computational support for radiation induced material modification projects and the development of new modelling activities, particularly in the fields of astrochemistry, radiation chemistry and nuclear/space materials science, focusing on the mechanical and chemical properties of the new materials.

References

1. I.A. Solov'yov, A.V. Yakubovich, P.V. Nikolaev, I. Volkovets, A.V. Solov'yov, *MBN Explorer - a universal program for multiscale computer simulations of complex molecular structure and dynamics*, Journal of Computational Chemistry, v. 33, p. 2412–2439 (2012)
2. I.A. Solov'yov, A.V. Korol, A.V. Solov'yov, *Multiscale Modeling of Complex Molecular Structure and Dynamics with MBN Explorer*, Springer International Publishing, Cham, Switzerland (2017), 447 p., ISBN: 978-3-319-56085-4, ISBN: 978-3-319-56087-8
3. I.A. Solov'yov, A.V. Verkhovtsev, A.V. Korol, A.V. Solov'yov (Eds.), *Dynamics of Systems on the Nanoscale*, Lecture Notes in Nanoscale Science and Technology, Springer Nature Switzerland, Cham, Switzerland (2022), 546 p., ISBN: 978-3-030-99290-3, ISBN: 978-3-030-99291-0 (e-Book)
4. A.V. Solov'yov, A.V. Verkhovtsev, N.J. Mason, R.A. Amos, I. Bald, G. Baldacchino, B. Dromey, M. Falk, J. Fedor, L. Gerhards, M. Hausmann, G. Hildenbrand, M. Hrabovský, S. Kadlec, J. Kočišek, F. Lépine, S. Ming, A. Nisbet, K. Rick-etts, L. Sala, T. Schlathölter, A. Wheatley, I.A. Solov'yov; Condensed matter systems exposed to radiation: Multiscale theory, simulations, and experiment, arXiv:2311.13402 [physics.chem-ph] (submitted to Chemical Reviews).

[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 work carried out during the STSM

The STSM of Prof. A.V. Solov'yov to ATOMKI, Institute of Nuclear Research, was hosted by Dr. Zs. Dombrádi, D.Sc., Director of ATOMKI.

During this visit Professor Andrey Solov'yov discussed:

(i) The new, highly interdisciplinary research field studying the behaviour of condensed matter systems exposed to radiation was discussed. The discussion was focused on several recent advances in the field based achieved at the MBN Research Center and at ATOMKI.

(ii) Particular attention has been paid to the capabilities of theoretical and computational modelling using MBN software to describe radiation-induced phenomena in materials.

(iii) Development of new modelling activities, particularly in the areas of astrochemistry, radiation chemistry and nuclear/space materials science, focusing on the mechanical and chemical properties of new materials.

(iv) On-going experiments at ATOMKI on irradiation induced processes in various materials, e.g. polymeric materials, materials for space applications, collision experiments with astrochemically relevant molecules, and the possibilities for collaboration in computational modelling in this area of research.

(v) The work of the theory group at ATOMKI on collision theory, simulations of particle transport in materials with the GEANT4 code and its possible links with MBN Explorer and MBN Studio.

(vi) Various radiation-induced processes at the material surfaces.

(vii) (vii) Simulations of astrochemistry relevant processes using Stochastic Dynamics implemented in MBN Explorer and their analysis with MBN Studio.

(viii) Further development of the training activities in the related areas of computational physics, chemistry, material science and radiation research in a form of a doctoral training networks, summer schools, on-line tutorials.

(ix) Further development of the cooperation between MBN Research Center and ATOMKI.

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

The STSM main achievements are as follows:

1. This STSM has contributed to broadening and deepening the collaborative relations between the teams of MBN Research Center and ATOMKI, Institute for Nuclear Research in Debrecen.

2. New collaborative links of the MBN RC with the colleagues from ATOMKI in the field of materials research, radiation research, collision physics and astrochemistry have been established.

3. This STSM has benefited the whole MultIChem COST Action through the wide dissemination of its knowledge.

The follow-up activities to the STSM are as follows:

(i) there will be continued cooperation between the MBN RC, Frankfurt am Main, Germany and ATOMKI, Institute, Debrecen Hungary;

(ii) a proposal for a training network within the COST Action MultIChem research area on interdisciplinary physical, chemical, biological and materials science problems will be prepared;

(iii) MBN Research Center will participate in the strengthening of theoretical and computational research activities at ATOMKI.

This STSM is relevant to WG1, which studies irradiation-driven chemical transformations of complex molecular systems exposed to different types of radiation, and to WG2, which aims to validate the scientific results of WG1 at the more complex, technology-relevant level. Specifically, Task 2,4 Optimisation of computational tools for multiscale modelling for the use in technological applications related to nanofabrication and characterisation of nanostructures. It will also serve as a model for WG3, which will complement the objectives of WG1 and WG2 through cross-technology collaboration. The main objective of WG3 will be to advance the existing technological solutions through multiscale modelling.

The discussions held have strengthened the recent collaboration between the MBN Research Center team and the teams at ATOMKI, allowing the combination of theoretical, computational and experimental expertise to study the irradiation-driven processes in various condensed matter systems and to apply this knowledge to related technologies. This achievement is in line with several capacity building objectives of MultIChem, which focus on

(i) the establishment of a pan-European IDC community for the study of collision- and irradiation-induced processes in various molecular, biomolecular and nanoscale systems, and

(ii) the accumulation and systematisation of knowledge gathered by different complementary communities working in the areas related to IDC.