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

**Action number: CA20126**

**Grantee name: Alex Laikhtman**

## Details of the STSM

Title: Surface and plasma treatments of multilayer porous nanoparticles of $WS_2$ and $MoS_2$ for enhancement of their adsorption and adhesion properties.

Start and end date: 07/09/2022 to 21/09/2022

## 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)*

The initial aim of this STSM was to develop and improve the modelling of production and life times of excited species in various gas cold plasma environments, the interaction of these plasma-excited ions and electrons with neutrals in the gas phase and with $MoS_2$/$WS_2$ porous nanoparticles. The goal of this work is to understand the mechanisms of gas plasma excitation. Such an understanding may contribute to optimizing the parameters applied in the plasma treatment processes. A. Laikhtman gave a seminar lecture where he presented in very details both the experimental and theoretical work on hydrogen storage in these nanoparticles as well as their modification with foreign atoms to improve electronic properties and to integrate them with the graphene layers in catalysis applications.

While the presented simulations were based on the density functional theory (DFT) methods, the host group headed by Prof. Manolescu is also specializing in molecular dynamics (MD) calculations. During the extensive discussions, Prof. Manolescu and his colleagues stressed out the limitations of the DFT to the stationary ground states and proposed to use the MD-based modelling to describe the excited states of plasma species and their interactions with nanoparticles.

The initially planned work was significantly extended to the projects conducted by the host group. Namely using Si nanowires for electrical, optical, solar cells applications and as sensors. Si nanowires are grown on the Si wafer substrate using the Ag nanoparticles as the catalyst. The applied method enables to produce these nanowires vertically oriented to the substrate surface. Using different treatments, e.g. plasma and environmental exposure,

[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.

these nanowires exhibit piezoresistive properties which can be modified by such treatments. In order to improve these characteristics, A. Laikhtman suggested to modify the hydrogen plasma treatment previously performed by the host group. In addition, he suggested to extend the characterization of Si nanowires by techniques available in his laboratory: environmental SEM, micro-Raman, AFM.

In addition, A. Laikhtman and the host group discussed the perovskite based on MAPI (methylammonium-lead-iodide) coatings of Si nanowires for solar cells applications. These properties are achieved due to MAPI penetration and filling the pores between the nanowires, but are adversely affected by migration of iodine atoms. A. Laikhtman suggested to use inorganic nanotubes ($WS_2$, $MoS_2$) instead or in addition to Si nanowires. This is due to the fact that they are hollow inside, multi-layered, and have open ends, so MAPI can penetrate inside, and the migration of iodine will be probably limited by interaction with W/Mo and S atoms. The main obstacle, however, is to prepare well oriented nanotubes, although there are works reporting their successful synthesis.

A. Laikhtman extensively discussed the above issues with all senior staff and PhD students of the nanophysics host group. He visited the nanowires synthesis and solar cells characterization laboratories in the Reykjavik University (RU), as well as materials characterization/treatment facilities in the University of Iceland (Prof. Snorri Ingvarsson).

## 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)*

As summarized following the discussions, the host group will assist to use the MD methods to model the excited states in plasma (hydrogen, argon, nitrogen) to find the optimal plasma conditions for the interaction of plasma species with nanoparticles of $WS_2$. The applications are hydrogen storage, plasma cleaning and polishing as well as pores production to open the gate for plasma particles to penetrate the inner layers of the nanostructures. These calculations can be a basis of the research paper.

The host group will send the nanomaterials and perovskites-based nanostructures to the laboratory of A. Laikhtman in HIT for characterization and additional plasma treatments using the available facilities in HIT. The proposed additional experiments include impedance spectroscopy and testing light propagation and interaction.

A. Laikhtman will prepare and send to the RU group the nanoparticles of $WS_2$ to test the characteristics of coating them with perovskites – alone or in combination with vertically oriented Si nanowires. In parallel, A. Laikhtman will coordinate with the nanoparticles synthesis laboratory in HIT to synthesize well-oriented $WS_2$ nanotubes. Various catalytic techniques will be tested for this purpose.

The completed STSM is fully in line with the deliverables and objectives of this COST action. As specifically mentioned in the MoU, its main objective is *the establishment of a collaboration framework between the different research groups in the European Research Area on nanoporous semiconductors and oxide materials and on their applications in health, energy and the environment*. This STSM initialized a true collaboration between two academic nanocenters in different and remote from each other COST countries: Israel and Iceland, when each laboratory currently specializing in a number of porous nanomaterials using different study and preparation methods.

The completed STSM promoted the knowledge exchange within several working groups of the action, namely: **WG1. Advances in Porous Materials and Technologies**, aiming to develop the technologies to produce and functionalize porous materials, research on the material properties, efforts in finding applications and bringing them to the proof-of-concept stage; **WG3. Energy aiming green energy generation and storage**; **WG5. Management and Dissemination**: the host group joined this COST action as a result of the initial contacts between HIT and RU groups at the STSM preparation stage. This effectively included Iceland as a new member country in this action and opened the gates to other research groups and institution in Iceland to participate in action resources for the mutual benefits of all action members. In such a way this STSM ***specifically contributed to the COST declared policy of openness and inclusiveness.***