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

**Action number: CA20126**

**Grantee name: Hanna Sopha**

## Details of the STSM

Title: Single-atom-based nanotubular photocatalysts for photocatalytic water splitting

Start and end date: 15/02/2023 to 16/03/2023

## 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.

During the STSM, deep insights in the preparation, characterization, and application of single atom (SA) photocatalysts were gained.

In detail, the first activities of this STSM were the preparation of Pt SA photocatalysts on sputtered $TiO_2$ layers on FTO ($TiO_2$/FTO) substrates using a dark deposition process frequently used in the laboratory of Prof. Schmuki. For this dark deposition, $TiO_2$/FTO substrates were stored in aqueous, deaerated solutions containing low concentrations of $H_2PtCl_6$ (i.e., 2 mM and lower) in the dark for one hour. In comparison, nanoparticle (NP) decorated $TiO_2$/FTO substrates were prepared using a similar approach to achieve porous and highly photocatalytic substrates. However, instead of using dark deposition the substrates were kept under UV irradiation for one hour. These SA and NP photocatalysts were characterized using SEM and XPS. Afterwards, the photocatalysts were employed for water splitting experiments as well as for the photocatalytic degradation of organic dyes.

Furthermore, as this STSM was planned as the beginning of a cooperation between the groups of Prof. Schmuki in Erlangen (Germany) and Dr. Macak in Pardubice (Czech Republic), $TiO_2$/FTO substrates as well as $TiO_2$ nanotube (TNT) layers were decorated with Pt using atomic layer deposition (ALD), already before the STSM by the group of Dr. Macak in Pardubice, with different ALD cycle numbers with the aim to produce Pt SAs by ALD on the different $TiO_2$-based substrates. These samples were taken to Erlangen by the grantee (Dr. Hanna Sopha) and investigated as well. Similar as for the SA photocatalysts using the dark deposition process, characterization was carried out using SEM and XPS. The ALD Pt SA decorated porous and non-porous $TiO_2$ substrates were further employed for

[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.

hydrogen evolution reaction experiments.

By now, these results are rather preliminary and additional experiments have to be carried out within the future cooperation.

## 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.

The main achievements described in the STSM application were reached. The goal of this STMS was to gain knowledge in the SA catalyst preparation using the dark deposition process frequently employed in the labs of Prof. Schmuki, as well as the characterization and the application of the SA catalysts for water splitting and hydrogen production as a green energy source (fitting into WP3 – Energy of the COST Action). The deep knowledge gained will facilitate the future cooperation between the two groups in Pardubice, Czech Republic, and Erlangen, Germany.

For follow-up activities, it is planned to optimize the ALD process and possible post-treatments for the Pt SA catalysts prepared using ALD. As for the moment, mainly flat $TiO_2$ substrates were used for the catalysts for an easier evaluation and modulation of the reactions. In the future also porous substrates, i.e. $TiO_2$ nanotube layers, will be used, which is in accordance with the COST action. For these, the ALD process needs to be further optimized as on the $TiO_2$ nanotube layers NPs are formed more easily than on the $TiO_2$/FTO substrates. Additionally, investigations will be carried out to stabilize the SAs deposited by ALD on the different porous or non-porous $TiO_2$-based substrates to prepare even more efficient and stable catalyst for hydrogen production.

It is expected that from the work carried out within the 30 days of this research stay and the future activities planned to accomplish the started work, several publications in high-impacted journals will derive within the next two years.