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

Action number: CA20126

Grantee name: Francisco Javier Fernández Alonso

Details of the STSM

Title: Development of structures based on the infiltration of TMDs in porous silicon

Start and end date: 04/09/2023 to 14/10/2023

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.

In relation to the original proposal, work has been done on the synthesis of $TaSe_2$ using IBD in the receiving group, as well as the infiltration of this material in porous silicon, synthesized in the applicant's group at the Autonomous University of Madrid, to maximize the specific surface area. As of the date of issuance of this report, we are still characterizing the nanostructures obtained.

Due to the progress of the research carried out in both groups, within the framework of the COST action, in addition to the originally proposed topic, work has been done on two other topics, which are briefly explained below:

- **Synthesis of black TiO_2 nanotubes for applications in Li-ion batteries (LIBs), as well as in PEC cells and in dye degradation**: Titanium dioxide (TiO_2) nanostructures have been widely used in several photocatalytic applications due to their advantages of low cost, chemical stability, and relatively high photo-activity. However, applications of TiO_2 have been restricted in the ultraviolet range because of the wide band gap. Broadening the light absorption of TiO_2 nanomaterials is an efficient way to improve photocatalytic activity. Thus, there is interest in developing structures based on black TiO_2 for applications in PEC cells or applications in photocatalysis, such as dye degradation. Likewise, due to its excellent capacity retention, anatase is considered an excellent candidate as an anode in Li-ion batteries. However, the poor rate capability of TiO_2 electrodes, caused by the low electrical conductivity and Li diffusion coefficient, strongly hinders its practical application in high-power LIBs. It has been reported that through the hydrogenation of TiO_2 it is possible to obtain improved fast lithium storage compared to pristine samples.

At the STSM, TiO_2 nanotubes have been synthesized by electrochemical anodization. These structures present a very high specific surface area. These nanotubes have been reduced to black TiO_2 in the laboratory of the grantee at the Autonomous University of Madrid.

[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.

- Synthesis of the 2D material hematene through liquid exfoliation of natural iron ore hematite for its application in photocatalysis and hydrogen production: With the advent of graphene, the most studied of all two-dimensional material, many inorganic analogues have been synthesized and are being exploited for novel applications. Balan et *al.* reported the possibility of obtaining hematene through liquid exfoliation of natural iron ore hematite, as well as improved photocatalytic activity in the visible when hematene is loaded on titania.

In the STSM, the liquid exfoliation method described in the original article has been reproduced using the means available in the recipient group. The results obtained have been characterized using techniques available in the recipient group (SQUID, Raman and XRD), as well as others available in the grantee group (UV-VIS, XPS).

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.

In relation to the topic of the original proposal, it remains to characterize the synthesized nanostructures, which will be done in the coming weeks. The final objective is to transfer this technology to diagnostic applications in medicine, which is within the scope of both WG1 (Advances in Porous Materials and Technologies) and WG2 (Health) of this COST Action

Regarding the black TiO_2, currently, it is planned to study the possible synergistic behaviour between TiO_2 nanotubes and carbon nanotubes for LIBs in collaboration with Prof. Carmen Morant at the Autonomous University of Madrid. In addition, we want to study new structures based on TiO_2 nanotubes through loading with plasmonic NPs, doping, etc., for PEC cells, in collaboration with Prof. Apolinario at the University of Porto, as well as for applications in photocatalysis, in which the grantee is nowadays working. All of the above is within the scope of WG1 (Advances in Porous Materials and Technologies), WG3 (energy), and WG4 (environment) of the COST action.

In relation to the exfoliation of hematene, it is planned to study structures based on different semiconductors loaded with this 2D material to study their photocatalytic properties or applications in hydrogen production. Currently, Dr. Apolinario, from the receiving group, works with porous structures based on Fe_2O_3, while the grantee works with porous structures of Ta_2O_5, materials in which we plan to study the incorporation of hematene. All the above is within the scope of WG1 (Advances in Porous Materials and Technologies), WG3 (energy), and WG4 (environment) of the COST action.

Furthermore, during the STSM the grantee has seen first-hand the facilities available to the receiving group and has been able to present the facilities available at the Autonomous University of Madrid. In addition to the collaboration initiated within the framework of the STSM, and which is expected to continue, the receiving group has shown interest in starting new collaborations, for example, to be able to carry out measurements with IBA techniques in the Materials Microanalysis Centre of the Autonomous University of Madrid.

It is expected to be able to present the results that emerge from the collaboration between the receiving group of this STSM and the candidate's group at the UAM in different international congresses and meetings. In addition, it is expected to publish the results of the work developed within the framework of this collaboration in scientific journals. In any contribution to a conference or publication related to the work developed in this STSM, the financial support of the COST action to carry it out will be acknowledged.