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

Action number: **NanosSpace COST Action CA21126**

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Details of the STSM

Title: Click-Chemistry Functionalization of Carbon Nanostructures for Advanced Nano-Carbon Studies
Start and end date: 8/03/2026 to 21/03/2026.

Description of the work carried out during the STSM

During this STSM, the focus was on the synthesis and surface functionalization of Carbon Dots (CDs) with amino and sulfonyl groups, serving as sources of Nitrogen (N-CDs) and Sulfur (S-CDs) doping. These groups modulate the optical and electronic properties of the nanoparticles and provide reactive sites for further chemical modifications. Special attention was given to applying click chemistry on the CD surfaces. Amino and sulfonyl functionalities enable the introduction of azide or alkyne groups, which can undergo highly selective conjugation reactions with various molecules, including fluorophores, biomolecules, or polymers. **Figure 1** illustrates this strategy for CDs decorated with carboxylic groups (-CO_2H).

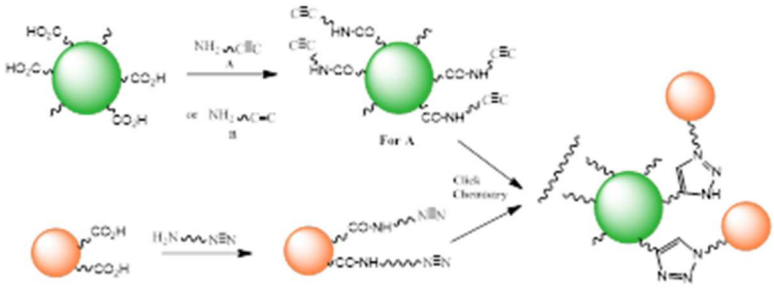


Figure 1. Schematic representation of the reaction carried out in this STSM with CDs

Other synthetic approach, a little bit more complex reaction was carried out using S-CDs to obtain the thiol (-SH) compound by reduction of the sulfonyl surface group (-SO_3^-) with I_2 and Ph_3P, which later will be reacted with 1,2,4, triazole as probe to obtain the S-Triazole bond. Same was done directly with N-CDs and we are waiting for the characterization by XPS to probe the surface decoration by these different approaches.
In other context, the product obtained by the reduction of the sulfonyl nanoparticles, were requested to be used in Li@batteries. In this context, S-CDs and S-containing functional groups, such as sulfonyl moieties, offer promising solutions to enhance charge transport and provide active sites for anchoring polysulfides, thereby improving the electrochemical stability and cycling performance of the batteries. Additionally, the incorporation of sulphur functionalities through controlled surface chemistry such as the

[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.

formation of triazole derivatives via click reactions can further tailor the interaction between the carbon nanostructure and sulphur species.

This work demonstrates a versatile approach to engineering CDs as modular nanoplatforms, combining heteroatom doping and surface chemistry to tune their properties and enable targeted functionalization for sensing applications.

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

The STSM successfully established a robust methodology for the synthesis and surface functionalization of Carbon Dots (CDs) incorporating N and S heteroatoms. These functionalized CDs, bearing amino and sulfonyl groups, enabled fine tuning of their optical and electronic properties while providing reactive sites for further chemical modification. A key achievement of this work was the use of these heteroatom doped CDs as versatile platforms for the generation of triazole derivatives via click chemistry. The introduction of azide/alkyne functionalities on the nanoparticle surface allowed the efficient implementation of azide/alkyne cycloaddition reactions, leading to well defined triazole functionalized nanomaterials. This strategy highlights the potential of CDs as modular scaffolds for the controlled development of advanced functional architectures.

The resulting materials exhibit promising applicability across multiple fields. Their tunable fluorescence and surface properties make them suitable candidates for sensing, with special emphasis on their use as functional coatings for optical fibers, enabling the development of advanced optical sensing platforms. In addition, the presence of S@containing functionalities opens new opportunities in the field of energy storage, especially in Li@S batteries, where such groups can contribute to improved charge transport and stabilization of polysulfide intermediates.

As a follow-up, future work will focus on optimizing the synthesis and click functionalization processes to enhance the efficiency, stability, and structural control of the triazole derivatives. Further efforts will also address the integration of these materials into optical fiber systems and their evaluation under real sensing conditions. In parallel, their potential role in energy storage applications will be explored in more detail. The collaboration established during the STSM is expected to continue, leading to joint publications and the development of new research proposals.