SAFE AND SUSTAINABLE BY DESIGN GRAPHENE/MXENES HYBRIDS

Safe and Sustainable by Design (SSbD) Functionalized MXenes: Environmental Impacts Comparison through Life Cycle Assessment (LCA)

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INTRODUCTION & OBJECTIVES

- MXenes are a class of advanced 2D materials composed of layered transition metal carbides, carbonitrides and nitrides produced from layered ternary materials known as $M_{n+1}AX_n$ or MAX phases by selective etching the A-layers.
- SAFARI project aims to enable the SSbD production and utilization of MXenes, covering the whole supply chain, from precursors' preparation (MAX phases) to final applications (conductive inks, electromagnetic interference (EMI) shieldings and biosensors) (Figure 1).
- A key step is the functionalization of MXenes, which enables the tailoring of their surface chemistry to achieve the desired properties and performance characteristics for their intended applications. In SAFARI, titanium-based MXenes (Ti MXenes) were functionalized using metallic nanoparticles (NPs) (Cu, Ag and Ni) and organic motifs (PVA, PPy, PANI, EDOT, APTES and PEDOT:PSS) via an ultrasonication assisted process (U/S) at 1:1 ratio functionalizing material / Mxene, except for APTES functionalization at 2:1 ratio functionalizing material / Mxene.

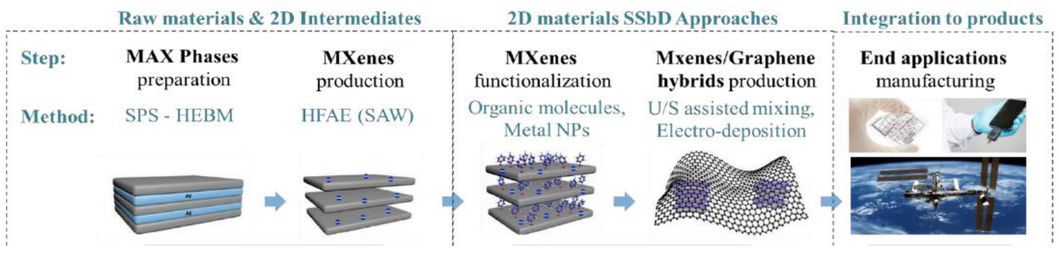


Figure 1.– SAFARI´s SSbD MXenes supply chain.

- The objective of this study is to determine the environmental impacts of functionalized Ti MXenes production process via LCA assessments in order to identify hotspots and improvement opportunities, thereby supporting the innovation process.

METHODOLOGY

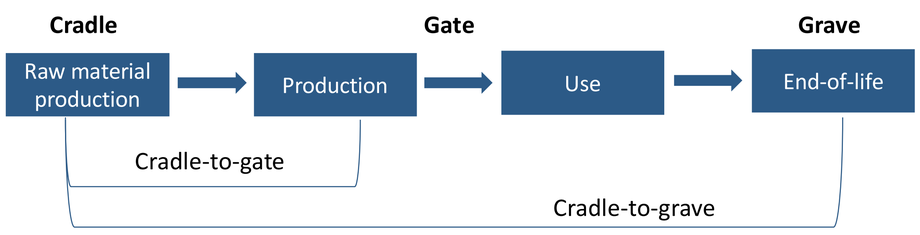


Figure 2.– Scope selected for LCA : Cradle-to-Gate.

To determine the environmental impacts, a Life Cycle Assessment (LCA) was carried out following ISO 14040/14044 and PEF methodology. The software SimaPro v10.1 with the database Ecoinvent 3.10 and the Environmental Footprint v3.1 method were used.

The functional unit was defined as 1 g of functionalized Ti MXenes manufactured and the scope was Cradle-to-Gate (Figure 2).

LCI data consisted of primary data obtained from the production process data provided by CREATIVE NANO PC (CNANO) partners. This data included inputs, outputs, wastes and energy requirements involved in the production processes.

The goal is to identify the primary environmental impacts associated with the functionalized Ti MXenes materials production.

RESULTS & DISCUSSION

Ag functionalization process shows the highest environmental impact, followed by EDOT, PANI, PPy, APTES, Cu, PVA, Ni and PEDOT:PSS functionalization processes.

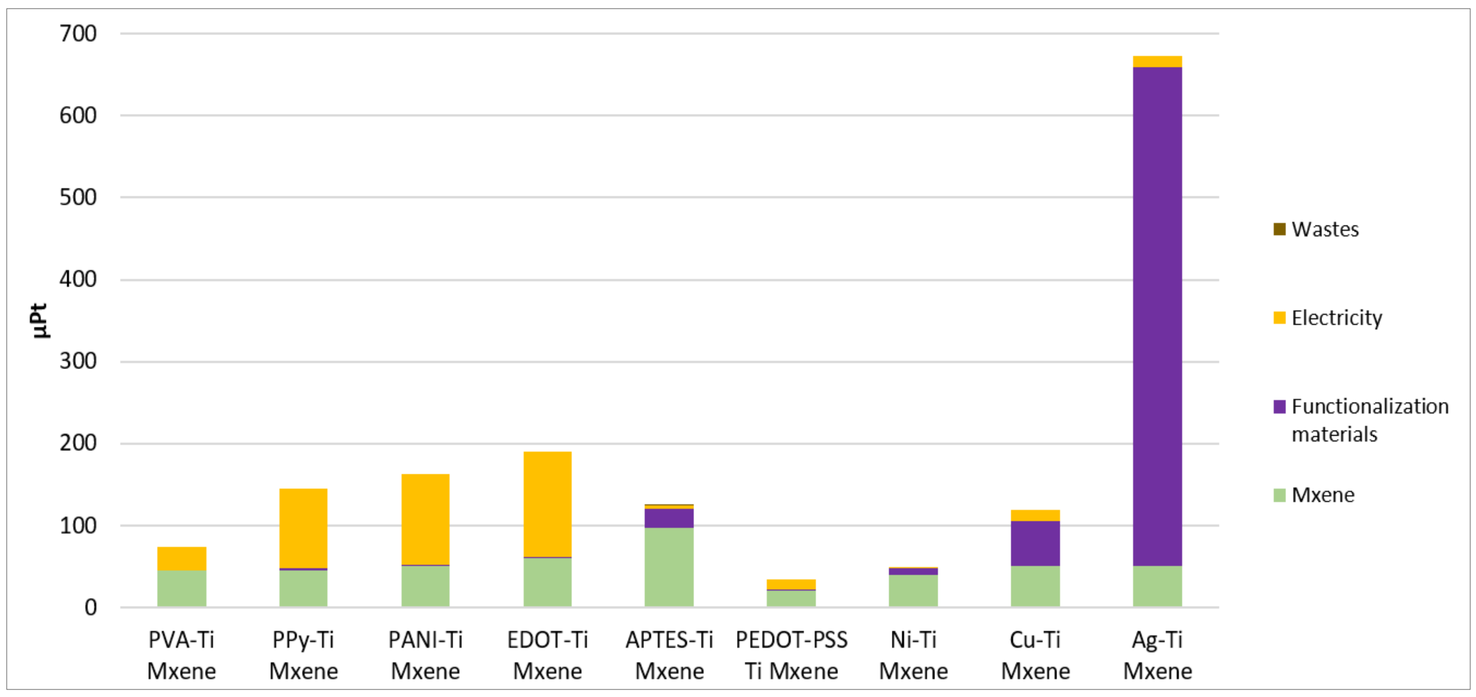


Figure 3.– Functionalized Ti MXenes Environmental impact.

PVA = polyvinyl acrylates
PPy = poly pyrrole
PANI = polyaniline
EDOT = 3,4-ethyelenedioxytiophene
APTES = 3-aminopropyl)triethoxysilane
PEDOT:PSS = poly EDOT with polystyrene sulfonated

Metallic NPs functionalization

- Ag functionalization: 90% of the impact is due to functionalization materials, being silver nitrate the most contributing one (87% of the total impact). Remaining 10% mainly connected to the upstream process to produce the MXene.
- Cu functionalization: impact is due almost equally to the MXene production and the functionalization materials (43% and 46% of the total impact, respectively).
- Ni functionalization: MXene production is the most contributing activity (80% of the total) followed by the functionalization materials (18%).

Organic motifs functionalization

- PVA functionalization: 61% of the impact is due to upstream process to produce the MXene while energy consumption accounts for 39% of the impact .
- PPy, PANI and EDOT functionalizations: impact is primarily due to energy consumption (67%, 68% and 68% respectively) followed by the upstream process to produce the Mxene (31%).
- APTES functionalization: MXene production is the most contributing activity (77% of the total), followed by functionalization materials (19%) being ethanol the most contributing one (18% of the total impact).
- PEDOT:PSS functionalization: MXene production as the most contributing activity (60% of the total), followed by energy consumption (38%).

CONCLUSIONS

The upstream impacts related to the production of the MXenes are the key driver of the environmental performance in many of the scenarios. Consequently, increasing the mass fraction of the functionalizing materials – i.e. reducing the ratio of MXenes in the formulations – would improve the environmental performance. Energy consumption is the primary cause of environmental impact for PPy, PANI and EDOT functionalizations. It is recommended to continue working on obtaining higher energy efficiency and selecting more sustainable sources.

ACKNOWLEDGEMENTS

GRAPHENE FLAGSHIP

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