Innovative photocatalysts integrated in flow photoreactor systems for direct CO_2 and H_2O conversion into solar fuels

Deliverable 5.1

Safety recommendations on the selection of the components to develop the new photocatalysts

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1. Introduction

In addition to the appropriate mechanical and physical properties that newly developed materials should present to allow their use in the areas of interest, the potential impact that they represent for the human health and the environment is another critical factor that should be considered before their implementation. The present report provides a comprehensive review of the current available literature regarding the toxicity of the main components that are being considered to be part of the catalysts that will be developed in NEFERTITI. Thus, the potential hazards of each component and its toxicological profile are discussed in this report individually. The materials reviewed are specified in Table 1.

Table 1. Individual components reviewed from a toxicological perspective in this report.

Deliverable	Catalyst	Individual components
Potential 2D porous materials for the simultaneous photocatalytic conversion of CO_2 and H_2O into syngas (D2.1)	porphyrin-perylene/Au NPs porphyrin-perylene/RuO_2 NPs	Perylene Sn Zn Ni Al Sb Porphyrin Au NPs RuO_2 NPs
Potential photocatalysts for the alcohol generation from syngas (D3.1)	TiO_2-Ni TiO_2-Cu TiO_2-Fe TiO_2-Zn CuCoAlloy NPs TiO_2-RhMn NPs Fe_5C_2/Cu-ZnO-Al_2O_3	TiO_2 NPs TiO_2 surfaces Ni Fe Cu Zn Rh NPs, Mn NPs, Fe_5C_2 NPs ZnO/Al_2O_3 Cu

Finally, and based on the information compiled for each individual element, preliminary safety recommendations on the selection of the components to develop the new photocatalysts are provided.

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2. Conclusion

Based upon the information presented in the previous sections, it is evident that the support material used for the fabrication of photocatalyst – COF, Perylene and Porphyrin are non-toxic to human health and environment. The metals selected that can be incorporated in the core of the photocatalyst can be categorized into mainly three types – inert or not required by the human body, essential or required by the human body and toxic. The inert materials include Tin, Nickel, Aluminium and Titanium dioxide while the essential metals are Zinc, Iron and Copper. The toxic metal in the present list of components was only Antimony. However, there are limited toxicity studies on Antimony and its mechanism.

It should also be noted that toxicity of metals depends upon duration, dosage of exposure, the chemical combination or susceptibility. In case of occupational health hazards, where workers are exposed to high levels of metal concentration, or accidental ingestion of high concentration of metal usually results in health complications. For example, exposure to high concentrations of zinc chloride fumes can be lethal. Some metals in combination with other chemical moieties are found to be toxic. For example, organo-tins and nickel in some forms are toxic. Some of the metals can also compete for the cellular binding sites and can increase or decrease the toxicity. For example, Zinc can compete with iron for cellular binding sites and can prevent redox cycling of iron as it does not have redox activity and reduce the iron-mediated oxidation of lipids, proteins, and DNA.

Toxicity of nanoparticles have also been discussed in the sections. Nanoparticles possess unique properties which are different from their bulk counterpart. For example, bulk TiO_2 is an inert material which is used in various food products. However, nano-TiO_2 is active and can cause adverse health effects. Overall, there has been conflicting and inconsistent results upon the toxicity of nanoparticles. The fact that nanoparticle toxicity depends upon shape, size, synthesis method, functionalization, and biological model, it is difficult to analyze the safe/recommended limits of nanoparticles. Therefore, additional data is required to conclude on the safety of nanoparticles.

In summary, the uncertainty regarding the potential adverse consequences on human health from exposure to nanoparticles, together with the lack of information of the hazard effects of compound mixtures (for example, in the case of metals, many research works are focused on the study of the organisms´ responses to these elements individually), make it difficult to provide specific recommendations on the selection of the materials. Thus, the toxicological assays that will be performed in the second stage of task 5.3 will shed light about the potential hazards of the selected catalysts empirically, providing a preliminary evaluation of their impact over the human health and the environment. Finally, it is worth noting that, based on precautionary principles, it is highly recommended the implementation of control

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measures as strategy to mitigate or prevent the potential risks associated to the exposure to the catalysts and their different components, as well as the selection of appropriate treatment and disposal options after their use to minimize potential adverse effects to the environment.

3. Safety recommendations for the components:

Metal fumes are toxic and may cause respiratory disorders or metal fume fever. If any fabrication process generates metal fumes or dust, do not inhale, and use mask or similar respiratory barrier. Avoid fumes generated from zinc, nickel and titanium dioxide – as they are associated with asthma, bronchitis or pulmonary and nasal cancer. Avoid inhalation of perylene derivatives and organic tin. Perylene when used as a pure component does not pose any toxicity. Avoid high temperature if aluminum dust or fumes are generated, it may lead to fire hazard.

Special care should be taken when handling Antimony – it is carcinogenic and has potential for organ toxicity. Contact with skin may induce "antimony spots". Certain compounds of nickel are potential carcinogenic and teratogenic. Thus, use of gloves is highly recommended when using nickel and antimony. Some people are reported to have skin allergy when in contact with tin, nickel, aluminum and iron. Porphyrin may also cause mild irritation when in contact with skin. In such cases, gloves should be used while handling.

Zinc, iron, and copper may cause eye irritation. Wear eye protection when using these. Materials such as COF and nanomaterials should be handled carefully as these are new materials, thus toxicological profile is not well defined. Nanomaterials have the potential to penetrate through skin barrier, thus, gloves should be worn at all times during handling and avoid inhalation. Since size is the main factor in determining the toxicity of nanoparticles rather than the chemical composition. The safety recommendation remains the same for all the nanoparticles and COF.

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