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PeroCUBE – High-Performance Large Area Organic Perovskite devices for lighting, energy and Pervasive Communications

Deliverable 7.1

Risk-Benefit assessment of the use of Perovskites in PeroCUBE devices

WP 7 – Human health risk assessment and life cycle assessment

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Contents

Executive Summary

This deliverable presents a quick tier-0 qualitative assessment of the use of perovskites in perovskite-based devices. It is the output of T7.1 and includes a qualitative assessment of the risks and benefits of these devices when compared with reference or 'benchmark' products.

Need for the Deliverable

The overall objective of WP 7 is to assess the potential human health and environmental risks and to provide a life cycle assessment to balance the risks and benefits of the application of perovskite-based devices in energy harvesting and lighting applications. In line with a tiered approach, a qualitative assessment is first needed so that a quick scan of risks and benefits of these devices can be made and relevant 'red flags' (related to the potential risks) can be identified timely. This allows a pro-active approach towards the elimination of any potential risk and thus ensures sustainable development of the devices along their innovation value chain, i.e. safety-by-design.

Objectives of the Deliverable

The objectives of this deliverable include:

- presentation of the results from the qualitative risk-benefit assessment of perovskite-based devices using LICARA Innovation Scan tool.
- preliminary identification of the aspects which may aid these devices in further propagating within the innovation value chain without any concern for the risk(s) over their life cycle.

The devices which are considered for the assessment are perovskite-based photovoltaic cells (PePV) on both flexible and rigid substrates, perovskite-based light emitting diodes (PeLED) on both flexible and rigid substrates and perovskite-based light fidelity system (PeLiFi).

Outcomes

In the present tier-0 qualitative risk-benefit assessment of perovskite-based devices over their entire life cycle, we found that the assessed devices, i.e. flexible PePV, rigid PePV, flexible PeLED, rigid PeLED and PeLiFi, have consistently low risk and moderate benefit scores when they are compared with their conventional counterparts. For instance, flexible PePV qualitative benefit score is equal to 0.39 (out of 1) and qualitative risk score is equal to 0.25 (out of 1) when compared to OPV. Similarly for rigid PeLED, these scores are 0.33 and 0.19 respectively when compared to OLED. These low risk and moderate benefit scores put the devices in a transit 'yellow zone' of LICARA Innovation Scan, which means that these perovskite-based devices are promising developments and have the potential to be sustainable over their entire life cycle. However, they need additional benefits or added values for them to lie in the LICARA Innovation Scan's 'green' zone which implies a clear go-ahead with their further development in the innovation value chain. The light emitting bracelet has been kept excluded from the present assessment because its feasibility, technical requirements and specifications still need to be determined. Therefore, insufficient information was available for the assessment.

For all applicable devices, the additional necessary benefits have been identified and reported below in the decreasing order of their importance:

1. More control (easy-to-tailor) over in-situ synthesis of the perovskite crystalline thin films during manufacturing phase
2. Higher life time of use of the perovskite-based device
3. Higher efficiency of use particularly for PeLED devices
4. Use of metal halide compounds other than that of lead, e.g. tin-halides, during manufacturing phase
5. Synthesis of perovskite using less hazardous (i.e. environmental and human friendly) solvents
6. More knowledge over potential emissions from these devices during end-of-life stage

Next steps

The next step will include moving towards a higher tier quantitative assessment by using a hotspot scan that will focus on the quantitative release estimations of components from perovskite-based devices into indoor and environmental compartments over their full life cycle.

1 Introduction

The objective of WP7 is to assess the potential human health risks and to provide a life cycle assessment to balance the risks and benefits of the application of perovskites in lighting and energy harvesting applications. To achieve these goals, a tiered approach is followed going initially from a qualitative approach (with relatively low input needs and higher uncertainty) to a full quantitative life cycle assessment (LCA) at the end of the project, when the applications will be better defined.

The initial qualitative approach (tier-0) is based on the LICARA Innovation Scan which has been developed by TNO[1] for the preliminary but swift assessment of benefits and risks of innovative products. The tool addresses the three main life cycle stages of a product: manufacturing, use and end-of-life and qualitatively assesses the (environmental, economic and societal) benefits as well as the (environmental, public health, consumer and occupational) risks. The LICARA Innovation Scan is an online tool that will become publicly available (Q1 2021) as part of TNO's DIAMONDS platform via https://diamonds.tno.nl/#licara.

During this project, two main types of innovative products or devices will be developed:

- Perovskite-based PV (PePV) cells in the form of large area panels on both flexible and rigid substrates
- Perovskite-based LED (PeLED) devices in the form of large area panels on both flexible and rigid flexible substrates

These devices will be integrated and demonstrated for the following applications:

- Energy harvesting applications through PePV
- Lighting applications through PeLED
- LiFi applications through perovskite-based LiFi (PeLiFi) which will be demonstrated with the creation of different devices aimed to reach an effective communication between servers and devices, and developing a device capable of reproducing high quality multimedia in streaming.
- Wearables: A bracelet providing info by a PeLED display or a watch with PePV on its dial to harvest solar energy

To assess the devices and their demonstrators, it is first necessary to know their manufacturing process to a certain extent and a choice has to be made regarding to which processes or products they need to be compared. This information has been gathered through interviews with the project consortium partners responsible for developing the devices and upscaling their manufacturing process. The collected information is provided in the following section.

1.1 Perovskite-based Photovoltaic (PePV)

The PePV is a type of solar cell or a photovoltaic that uses organo-metallic compounds to produce electricity from sunlight by photovoltaic effect. The perovskites used in this project are certain lead halide compounds potentially treated with phenethylamine. The PePVs act as energy harvesting

[1] LICARA nanoSCAN developed by EMPA and TNO (van Harmelen et al., 2016) was used to develop the LICARA Innovation Scan for the risks and benefits of the use of non-nano hazardous substances.

devices, i.e. devices which are able to capture energy from external sources (e.g. sunlight) and make it available for low power applications or small wireless autonomous devices, like those used in wearable electronics, such as watches. The latest example with a potential application of PePV can be the recently launched wrist watch by Swiss watch brand Tissot with a touch-screen interface powered by solar energy. The watch dial contains tiny solar sensors that capture solar energy and store it an accumulator. With this scope in mind, for the purpose of risk-benefit assessment, PePV will be assessed on the basis of their comparison with other existing organic PV (OPV) and amorphous silicon-based PV devices as these are the kind of devices that are currently being used for similar energy harvesting purposes and are likely to be substituted by PePV in the future.

1.2 Perovskite-based Light emitting diode (PeLED)

The development of high-efficiency, high-colour purity, and low-cost light emitters are highly demanded for their use in television, mobile phones, lighting and other electronic devices. Organic LED (OLED) have a very high luminous efficiency, but low colour purity that provides a limited natural colour range. High material cost, complex colour-tuning process, and low charge carrier mobility of OLED are other drawbacks. Organometal halide-based PeLED, having perovskite as direct bandgap semiconductor for electroluminescence, is capable of much higher colour-purity at a lower cost compared to OLED. They have an optical bandgap that can be tuned in the visible to infrared regions, which makes them very promising for a range of optoelectronics applications. With this scope in mind, for the purpose of risk-benefit assessment, PeLED will be assessed on the basis of their comparison with OLED as OLED are currently being used for light emitting purpose and are likely to be substituted by PeLED in the future.

1.3 Perovskite-based Light Fidelity system (PeLiFi)

LiFi is wireless communication technology which utilizes light to transmit data and position between devices. It is a light communication system that is capable of transmitting data at high speeds over the visible light, ultraviolet, and infrared spectrums. The technology is similar to WiFi: while WiFi uses radio frequency to induce a voltage in an antenna to transmit data, LiFi uses the modulation of light intensity to transmit data. LiFi has the ability to safely function in areas otherwise susceptible to electromagnetic interference (e.g. aircraft cabins, hospitals, military). A PeLiFi system consists of PeLED on one end to simultaneously transmit light and data from the server and a perovskite-based photo detector (i.e. router) on other end to receive the data and provide it to the user (working with a laptop). The photodetector is also a PeLED device, as PeLED can be used to emit light but can also absorb light in a specific wavelength. The use of perovskites in LiFi communication makes the technology cheaper to use on a mass scale and ensures fine tuning to receive any wavelength of the transmitted light waves which is currently not possible in existing LiFi systems. With this scope in mind, for the purpose of risk-benefit assessment, PeLiFi will be assessed on the basis of their comparison with existing LiFi which uses Gallium Nitride in light transmitting LED and Si in photo detector. This type of LiFi is currently being used and is likely to be substituted by PeLiFi in the future.

1.4 Perovskite-based wearables

A light emitting bracelet is the perovskite-based wearable that serves as a demonstrator for the perovskite-based technology and the devices using it. The bracelet will be processed utilizing an in-mould integration technology where a flexible foil containing the light emitting PeLED areas, printed conductors and the driving electronics will be integrated into one seamless part via injection moulding process. However, the feasibility, technical requirements and specifications of such wearable still need to be determined which does not allow its risk-benefit assessment and hence it is not covered in this deliverable.

2 Methods

2.1 LICARA Innovation Scan for risk-benefit assessment

The initial qualitative risk-benefit assessment of the perovskite-based devices has been carried out on the basis of the LICARA Innovation Scan tool. This tool was developed by TNO particularly within the framework of PeroCUBE project on the basis of the LICARA nanoSCAN (van Harmelen et al., 2016). The LICARA nanoSCAN, was originally developed by TNO and EMPA in the framework of the EU FP7 LICARA project for the assessment of nanomaterials and nano-enabled products. However, we noticed that the substances used in the PeroCUBE devices are not (only) nanomaterials, so there was a need to adapt the LICARA nanoSCAN to be suitable for non-nano chemicals. In addition, the online LICARA nanoSCAN was heavily outdated and could no longer be maintained. Therefore a new improved online version has been developed by TNO that will be sustainable for the future and suitable for more broader innovative products, called the LICARA Innovation Scan. Details about the technical implementation are covered in section 6 Appendix I.

The new LICARA Innovation Scan guides the decision-making process about new products by:

- scanning both the benefits and risks over the product's life cycle in comparison to a conventional product or technology with a similar functionality;
- estimating economic, environmental and social opportunities;
- identifying the specific risks for consumers, workers, the public and the environment;
- supporting interpretation of the results, reflected in a consistent argumentation about the weaknesses and strengths of the product;
- giving guidance on next steps;
- using little quantitative data;
- combining state-of-the-art know-how in Life Cycle Assessment and Risk Assessment;
- integrating existing tools like Stoffenmanager®, Precautionary Matrix and NanoRiskCat that are backed by renowned agencies or private institutions;
- using a modular approach.

Each of the perovskite-based devices are individually scanned for their risks and benefits. In each scan, the perovskite-based device is compared with its conventional counterpart or benchmark. The tool is designed in a modular way and contains eight sections or boxes, as shown in

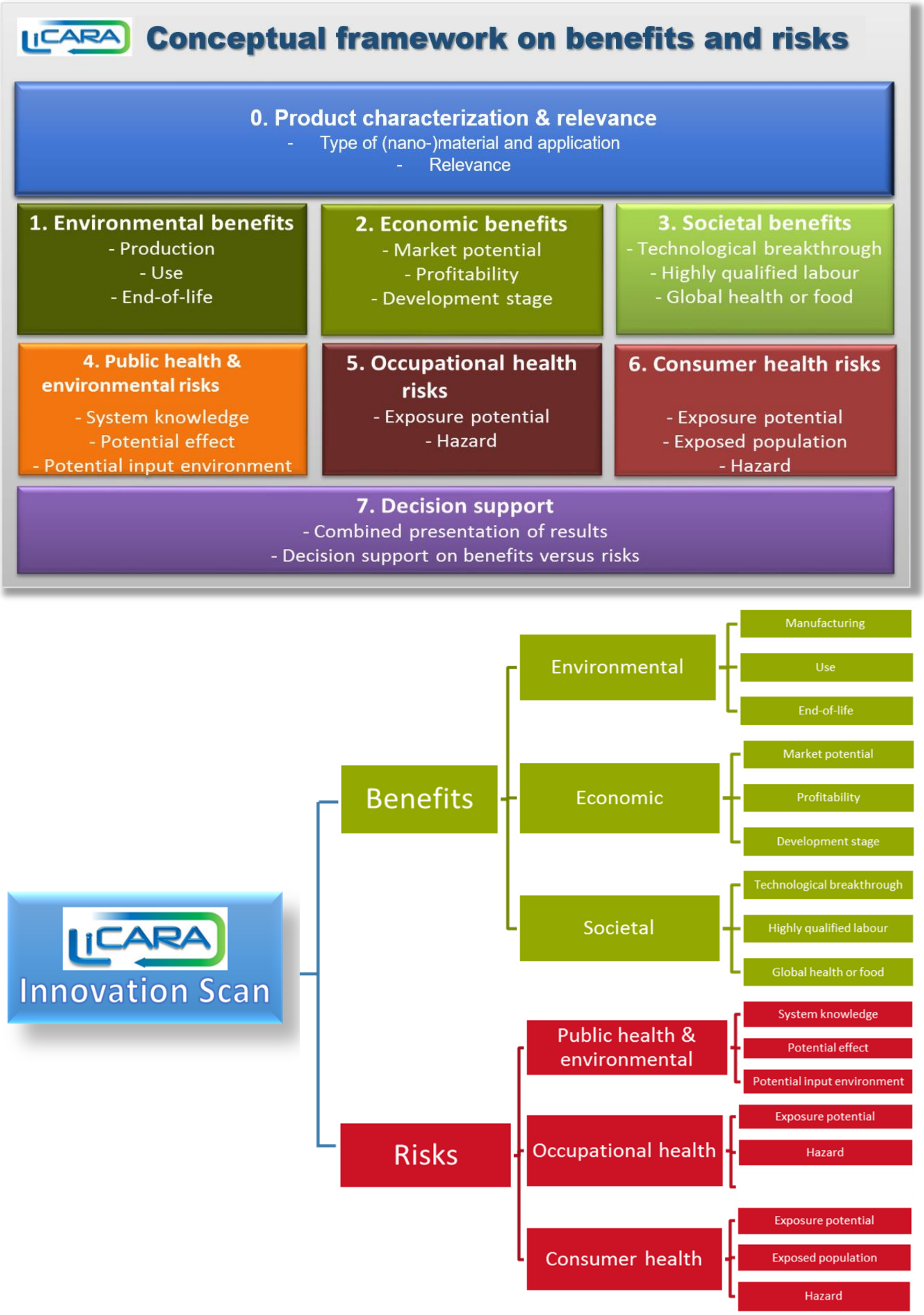


Figure *1* (a) and (b). Each box is relevant to a specific aim. The scan starts with the blue Box 0 (

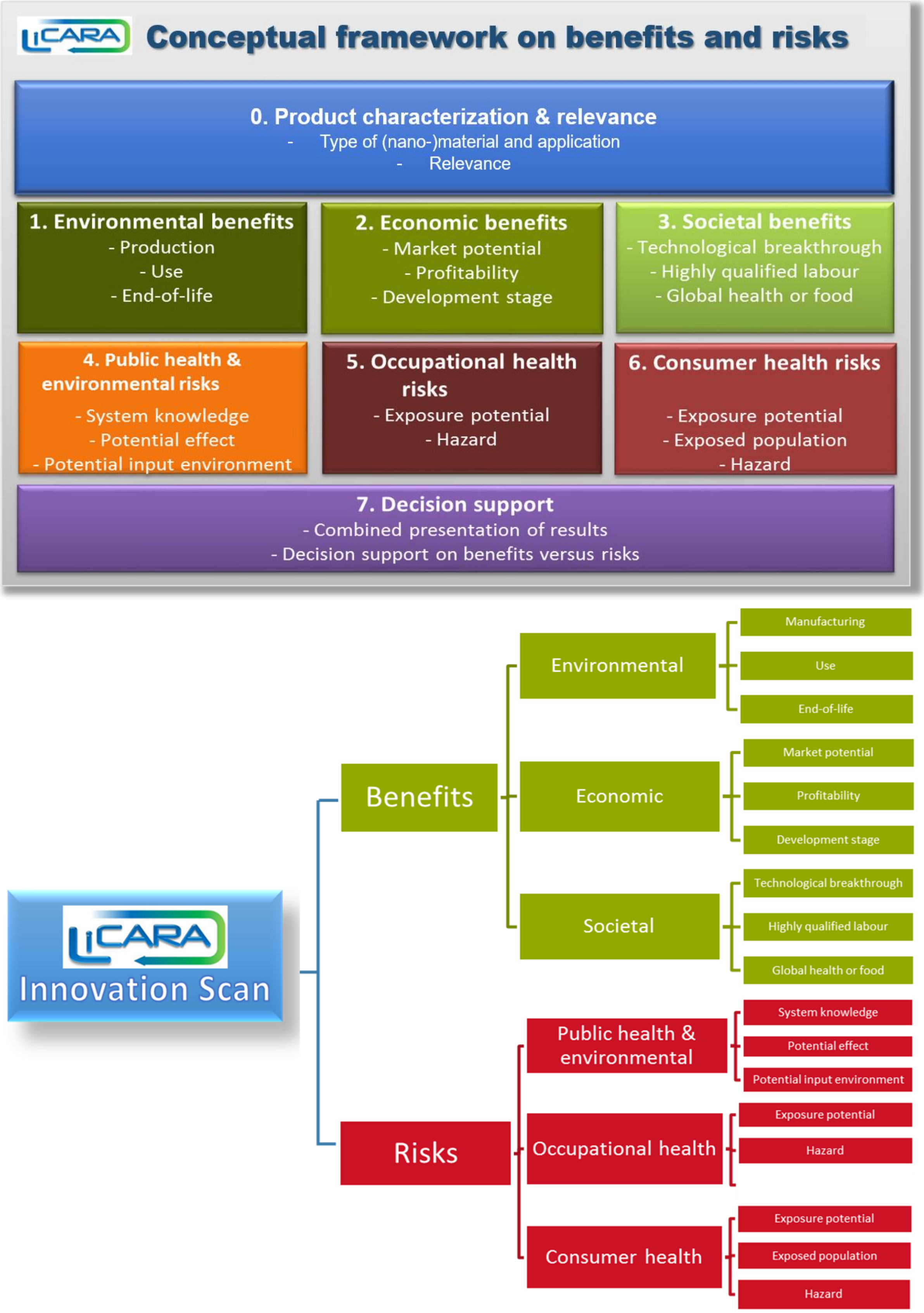
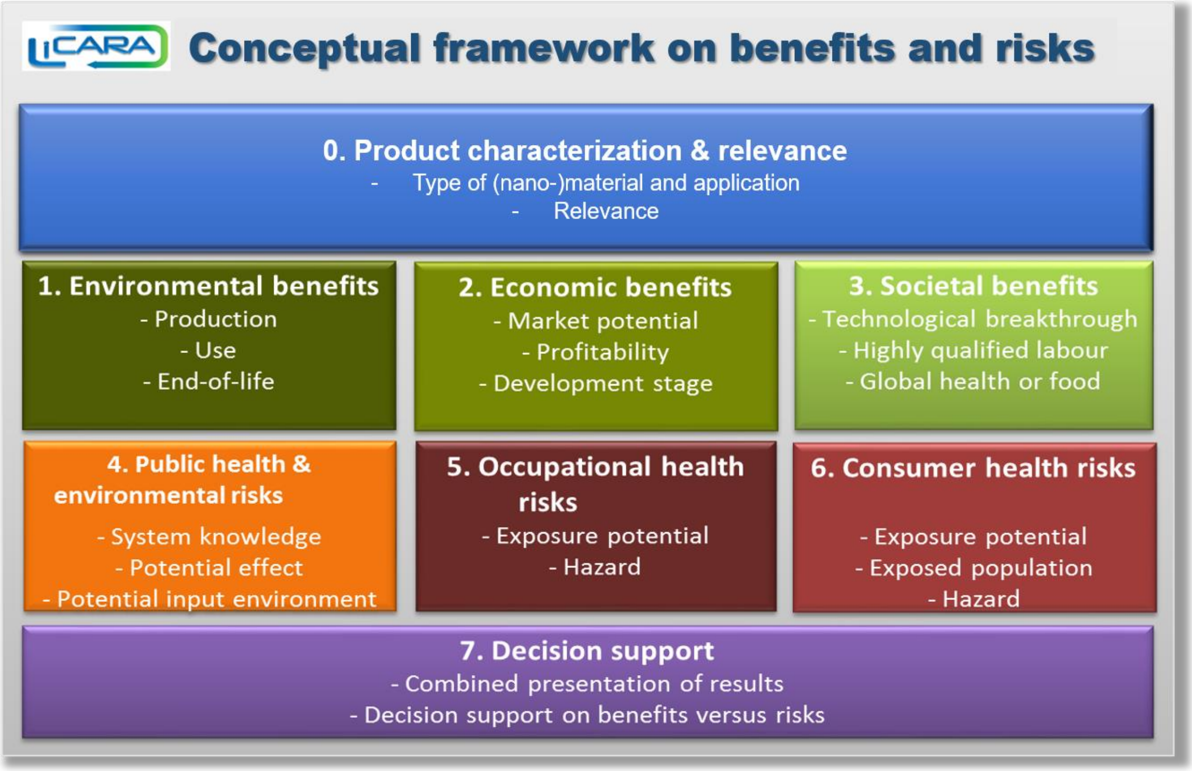


Figure *1* (a)) which helps to characterize the product and identifies its conventional counterpart to compare with. Subsequently, three types of benefits (environmental, economic and societal benefits;

second-row green Boxes 1–3) and three types of risks (public health and environmental, occupational health, and consumer health risks; third-row red Boxes 4–6) are assessed. Each box can be used independently to assess its particular benefits or risks. The subjects covered within each type of benefit or risk are shown in



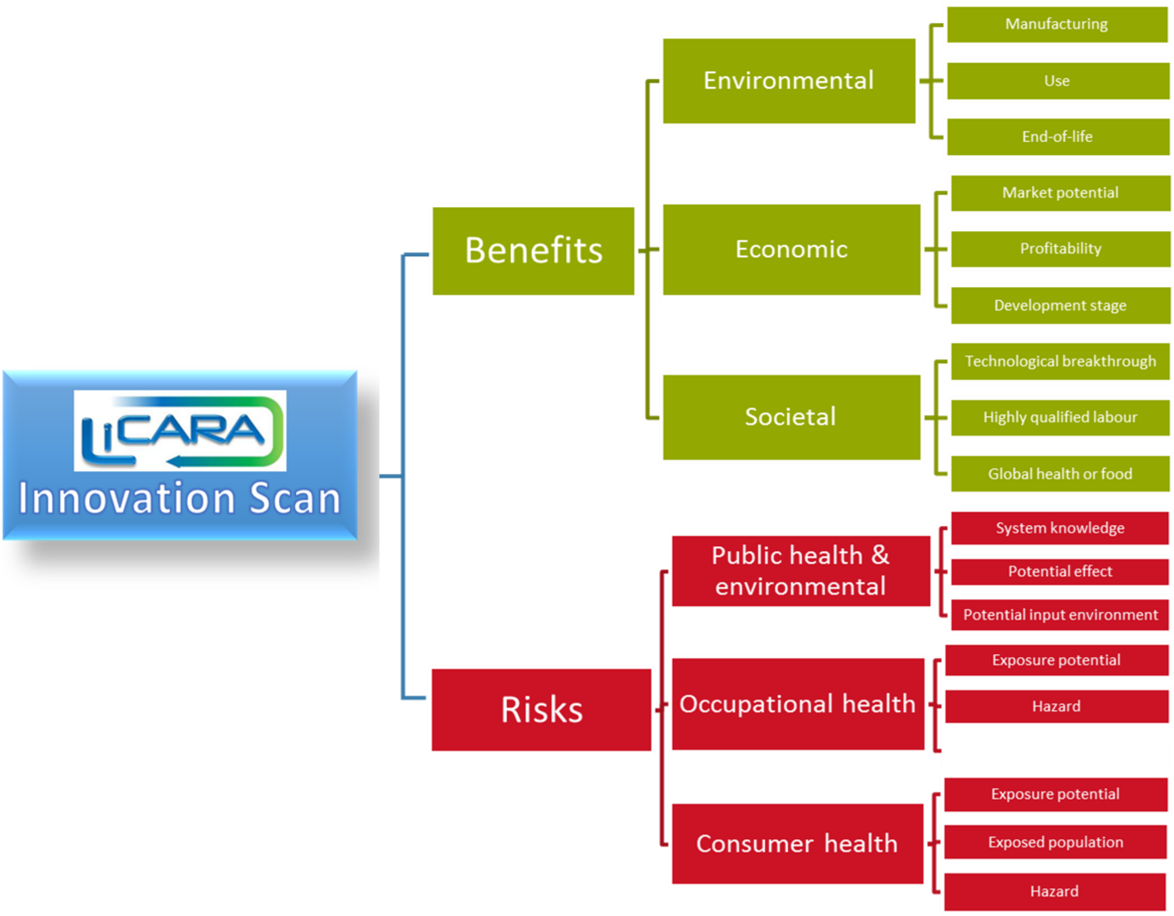


Figure *1* (b) which contain a series of questions/fields with product related data that needs to be entered. The questions involved are qualitative and semi-quantitative and can thus be answered without detailed materials and technology expertise. Purple Box 7 in

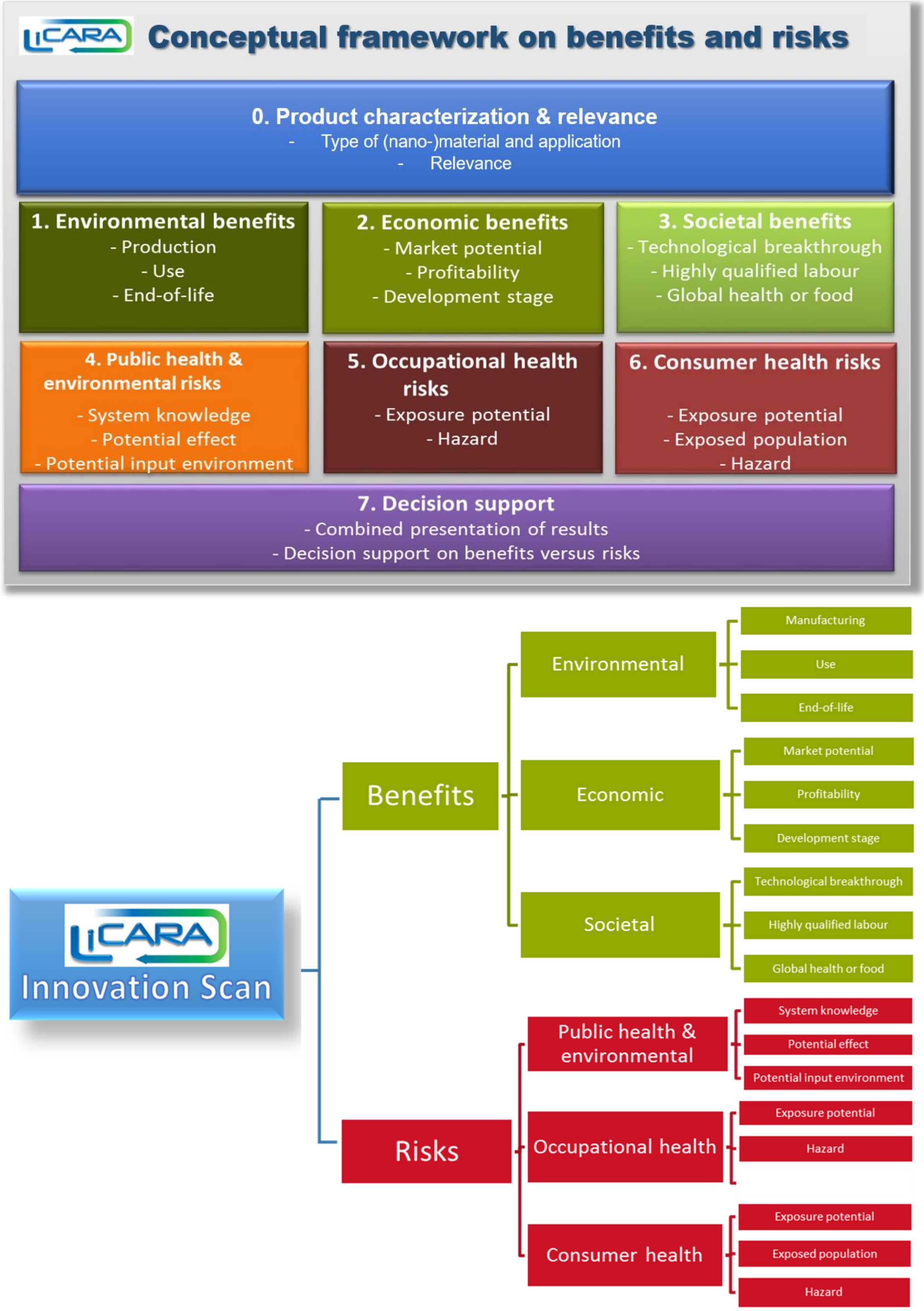


Figure *1* (a) finally integrates and evaluates the overall synthesized result. Of course, this step can only lead to a truly valid decision support for an innovative product, if all the benefit and risk boxes have been completed.

The final result of LICARA Innovation Scan is essentially an overview of a product's strengths and weaknesses, including uncertainties and knowledge gaps and their importance. This supports manufacturers and their stakeholders in their decision making on further assessment, research, development and production of a particular product. The tool delivers the final result on the basis of the principles of Life Cycle Assessment (LCA), Risk Assessment (RA) and Multi-Criteria Decision Assessment (MCDA). LCA is suited to assess the environmental benefits of a new product over its full life cycle, in comparison to a reference product (mainly Box 1). RA is used to assess the risks (based upon hazard and exposure) of certain activities or processes (Boxes 4–6). MCDA is used as a method that is particularly applicable when decisions need to be made in the face of uncertainty and a paucity of quantitative data. This is especially the case when developing new innovative products, like perovskite-based devices.

In order to take full advantage of all the relevant existing know-how and experiences concerning the assessment of innovative products, LICARA Innovation Scan is based upon parts of a number of existing tools: Swiss precautionary matrix which scopes product characterization in Box 0 and public health and environmental risks in Box 4, Stoffenmanager® which scopes occupational health risks in Box 5, and NanoRiskCat which scopes consumer health risks in Box 6. These three tools are briefly described in the following sections.

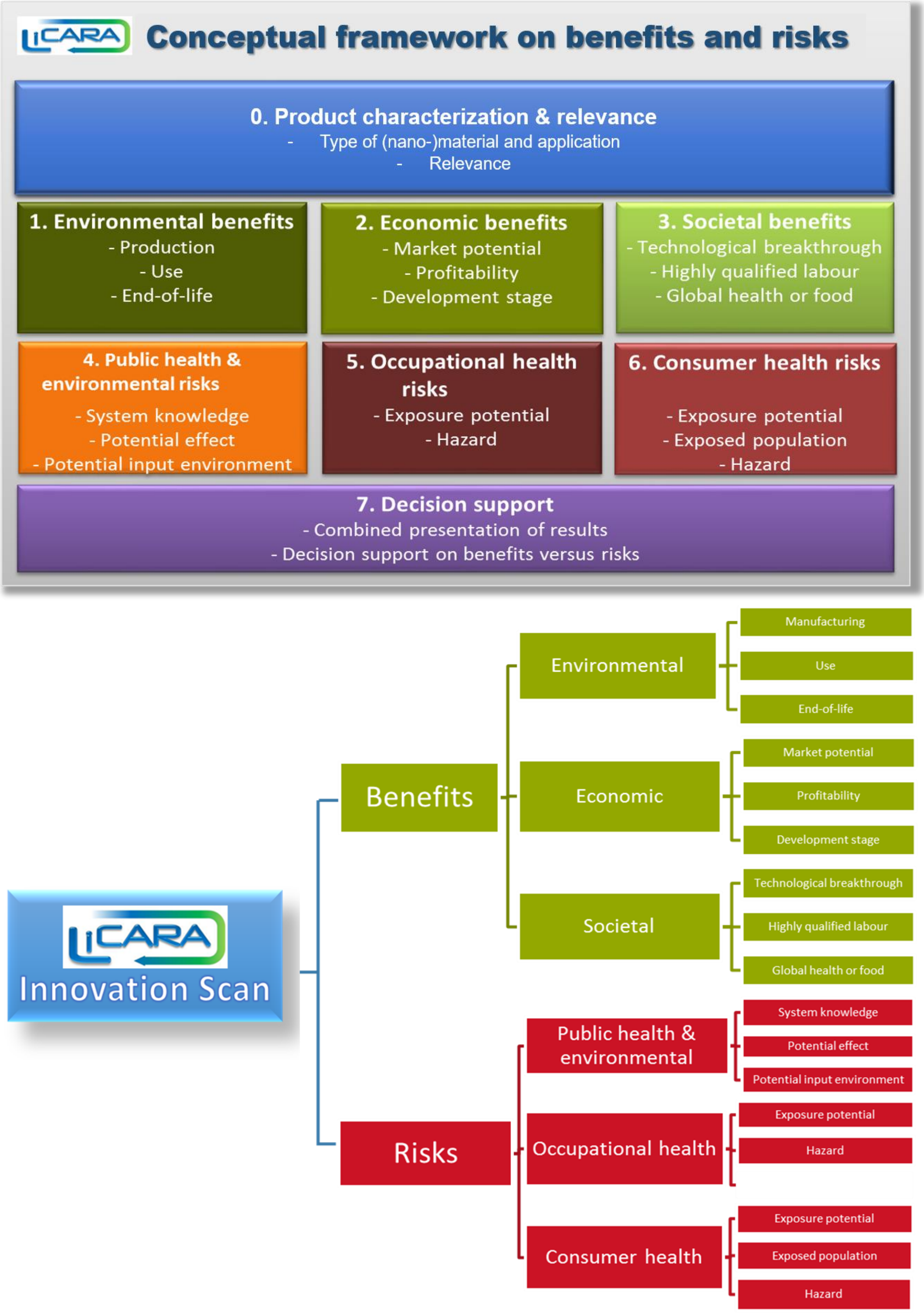


Figure 1: **(a)** Overall structure of LICARA Innovation Scan to assess the benefits and risks; **(b)** subjects covered within each type of benefit or risk.

2.1.1 Swiss precautionary Matrix

Swiss precautionary matrix, also known as Precautionary matrix, is a method which was originally developed for assessing the nano-specific health and environmental risks of nanoproducts (Höck et al., 2013). However, the structured assessment of the precautionary matrix remains same for materials/products other than nanomaterials and nanoproducts or, in the present context, perovskite-based devices and their composing components. LICARA Innovation Scan assesses public health and environmental risks in Box 4 through a series of 9 questions which are based on the precautionary matrix tool and embedded in LICARA Innovation Scan. These questions assess gaps in knowledge about the background and future life, potential effect and potential emission into the environment of the product and its components. The tool applies a scoring system attributing equal weights to each underlying question which is different from the scoring system of the Precautionary matrix (Höck et al., 2018; van Harmelen et al., 2016).

2.1.2 Stoffenmanager®

The qualitative module of Stoffenmanager® is a web-based free-to-use risk banding modelling tool, available at https://stoffenmanager.com/. It was developed to help companies without specific expertise in chemical risk assessment to prioritize their potential risks of chemicals and to indicate the types of exposure controls that could lower these risks. Such a tool classifies exposure situations into risk, control or priority bands, based on classification systems for the hazards of the substances and the exposure and controls in the situations (Marquart et al., 2008). Unlike the Precautionary Matrix tool, Stoffenmanager® (selected) questions, which assess occupational health risks, are not embedded in LICARA Innovation Scan: it asks the users to use the web-based Stoffenmanager® tool to independently obtain a Stoffenmanager® qualitative risk score and enter that score in Box 5.

In the web-based Stoffenmanager® tool, the user manually enters data. It is also possible to enter data from a database with product information, using a standard exchange format. However, in the context of the PeroCUBE project the information and data was collected form the project partners and entered manually in the web-based tool. The following information has to be entered:

1. Name of the product
2. Publication date of the Safety Data Sheet (SDS)
3. Whether the substance is a solid or a liquid
    a. For a solid: the dustiness
    b. For a liquid, the vapour pressure
4. Supplier of the product
5. Departments in which the product is used
6. Composition of the product, according to the SDS
7. Hazard categories (i.e. symbols according to the SDS)
8. Personal protective equipment (PPE) and ventilation needed (according to the SDS)
9. Risk and safety phrases [R/S phrases for the product (i.e. not for the individual components), according to the SDS]

Based on the entered information, Stoffenmanager® assigns hazard severity band from A to E (A being least hazardous and E being most hazardous) and exposure probability band from 1 to 4 (1 being lowest exposure and 4 being highest exposure) to the substance and scenario being assessed. The hazard band of each substance is based on the hazard-phrases entered. For this purpose, the division of R-phrases in hazard bands of COSHH Essentials is used. An overview of the hazard bands can be found in the documentation on COSHH Essentials at http://www.coshh-essentials.org.uk. The exposure model used for exposure banding in the Stoffenmanager uses the method based on information about the work tasks and environment and consists of three key elements: the intrinsic emission of the materials; the undergone handling or processing of the substance/material; and present occupational hygiene control, such as local exhaust ventilation. These elements are combined to qualitatively estimate the exposure level (Cherrie et al., 1999).

Stoffenmanager® combines the results from the hazard and exposure banding steps to produce risk bands or 'priority band'. The combination of hazard and exposure into priority or risk bands in the Stoffenmanager is presented in Figure 2. The classification of situations into priority or risk bands is based on the bands of hazard and exposure. Allocation into risk bands is done in such a way that exposure to very high hazard substances, such as carcinogenic substances or substances that lead to respiratory sensitization, would lead to a high priority, unless the exposure is very limited (leading to medium priority). The intention is to ensure that these substances and their use and control are considered specifically and in more detail by the user and to encourage the substitution by less dangerous substances. Also, very high exposures should generally lead to high priority, unless the hazard of the substances is very low. The further allocation is done to ensure a generally increasing risk band with increasing levels of the exposure and/or hazard bands.

		Exposure Bands			
		1	2	3	4
Hazard Bands	A	3	3	3	2
	B	3	3	2	1
	C	3	2	2	1
	D	2	2	1	1
	E	1	1	1	1

Figure 2: Priority bands in the Stoffenmanager. Hazard: A = lowest hazard and E = highest hazard. Exposure: 1 = lowest exposure and 4 = highest exposure. Overall result: 1 = highest priority and 3 = lowest priority.

2.1.3 NanoRiskCat

The consumer health risk assessment in LICARA Innovation Scan is done on the basis of NanoRiskCat which is also a nanomaterial based tool like Precautionary Matrix tool and focuses on their potential for exposures and effects during their use, particularly as nano-enabled products (Hansen et al., 2013). However, the selected questions that originate from NanoRiskCat and used in LICARA Innovation Scan can also be applied to materials/products other than nanomaterials, as is the case with perovskite-based devices. These questions mainly correspond to the determination of exposure potential of the consumer product, in particular, location of the material being assessed in the product (over the surface or in the bulk etc.) and the potential size of exposed population. The hazard assessment part is taken from Stoffenmanager® and is therefore the same as for occupational health. The combination of four exposure levels and the five hazard levels result in a risk which is scored similar to that of the occupational health risk assessment.

2.2 Manufacturing of perovskite-based devices

To manufacture perovskite-based devices, specific blends of perovskites precursors are incorporated in ink formulations which, during the process of manufacturing perovskite-based devices, convert to lead halide perovskite in the form of a layer. An ink formulation needs to be optimized within laboratory conditions to obtain high quality perovskite films and good contact among layer interfaces conforming the device. The best performing ink formulation(s) are subsequently to be transmitted for upscaled manufacturing process by means of:

- Roll-to-roll manufacturing on flexible substrates,
- Sheet-to-sheet on rigid substrates,
- Spin coating techniques on rigid substrates.

In this case, it is expected that some of the ink formulation components used during the laboratory development phase will be adapted according to the necessities of the scaled-up manufacturing processes.

For the purpose of the present tier-0 risk assessment of the perovskite-based devices, they will be assessed for their risks and benefits. Focussing on their manufacturing, rather than laboratory scale synthesis, gives more reliable insight of the risks and benefits of these devices when they are market-ready. The information regarding the upscaling of the manufacturing process and the manufacturing process of already existing comparable devices has been gathered by means of desktop research and by means of interviews with the partners, to ensure that all the information considered for the LICARA Innovation Scan is as accurate as possible.

2.2.1 PePV and PeLED manufacturing on flexible substrates

The manufacturing of PeLED and PePV on flexible substrates will be carried out by VTT. At first, the partner will start with small scale fabrication (1cm^2) an then will scale up the manufacturing to panels of 10 cm^2. The manufacturing on flexible substrates takes place by roll to roll (R2R) manufacturing technology. Roll to roll manufacturing technology is the process of printing or applying coating on a flexible material starting with a roll and the re-reeling it to create an output roll after all the layers have been deposited on the substrate.

The process followed follows these steps (Kim et al., 2020; Välimäki et al., 2013):

- A thin layer of Indium Tin Oxide is deposited on a flexible PET substrate by means of vacuum sputtering which is known to be a high energy consuming process;
- A layer of Zinc oxide is added by gravure printing;
- The perovskite ink layer is added on top;
- The entire structure is ‘sandwiched’ between two layers of silver (acting as electrodes) and then encapsulated within transparent plastic layers to protect the “active layer” from atmospheric agents like water (more details in section 3.3).

The added silver layer is composed of silver micro- and sub-micro particles which are potentially prone to release when subjected to stress upon the breach in encapsulation layer. In comparison with the manufacturing of a conventional organic PV and commercially available OLED, a number of observations specified below (detailed in section 3.1.1) are important for the purpose of this deliverable.

Manufacturing process and functionality

The manufacturing of a perovskite-based device (PePV or PeLED) is more complicated than that of their conventional organic counterparts. The perovskite layer in perovskite-based devices are "synthesized" from (commercially) available perovskite precursor ink at the moment of printing (i.e. in-situ synthesis of perovskite crystalline thin films). Existing commercial OLED and OPV solutions, on the other hand, are already synthesized before the printing process (i.e. no-situ synthesis from the precursor), thus more reproducible. Due to this particular aspect, it is harder to control the process at this stage and to guarantee consistency and replicability of the final manufactured perovskite-based device.

The formulations of perovskite solutions to be applied on a substrate to manufacture PePV and PeLED are different in terms of the molar concentration of perovskites: the concentration of perovskites is around 1-1.2 M in case of PePVs and it is around 0.4 M in case of PeLEDs.

The existing commercially available organic PV precursors are stable but expensive. In contrast perovskites are considerably cheaper.

The efficiency of existing OPV generally lags behind the efficiency of PePV. Whether PeLED are also more efficient compared to existing OLEDs is a question that needs to be answered in due time.

The stability or lifetime of PePV lasts in the order of months. However, for PeLEDs, the stablity is much shorter, in the order of hours.

Substance-intrinsic and process risks

The solvents used in the process (e.g. o-Xylene and Dimethylformamide (DMF)) are a source of concern for toxicity hazards during the manufacturing process. They are known to cause allergy, asthma symptoms, skin damage and serious eye irritation upon exposure. These solvents are also used during the manufacturing of "conventional" OLED and organic PV. The additional toxicity hazard in the manufacturing of the perovskite-based devices is mainly posed by the presence of lead halides in the perovskite which are known to be reprotoxic (i.e. causing interference in some way with normal reproduction) and ecotoxic amongst other harmful effects.

The residual solvents left after the manufacturing are blow dried inside a ventilated oven and generated vapors are entrapped inside a filter which is disposed-off by a specialized company.

The solvents and perovskite-based inks are handled inside fume hoods and the operating worker (varies from 1 to 2 in numbers at a time) is equipped with gloves, safety glasses, protective jackets and full face respirators.

The main "source" of waste derives from a small amount of ink present in the ink reservoir of the printer (~50 ml) which is estimated to contain <100 mg of Pb content at the end of manufacturing process. The excess amount of the ink is added in the reservoir to ensure enough supply of the ink during roll-to-roll printing.

A secondary source of waste is represented by the trimmings derived from cutting the PePV and PeLED from the roll. These trimmings might have some contamination from the perovskites and thus contain traces of lead. This is approximately estimated to be 3% of the PeLED and PePV area.

The work benches are wiped clean at the end of the process to ensure that no Pb content is left on the surfaces.

The pilot-scale fabrication are done in a 109 m^3 volume room equipped with local exhaust ventilation. Only 1-2 operators carry out the task within their breathing zone (i.e. distance head-product <1m) while wearing full face respirator masks and no one else is present around them within a distance of 1m during the entire duration of the task, i.e. there are no bystanders.

2.2.2 PePV and PeLED manufacturing on rigid substrates

The manufacturing of PePV and PeLED on rigid substrates will be carried out by the partner CSEM. As in the case for VTT, at first small scale devices will be produced (1cm^2) and then an upscaling to 10 cm^2 will be carried out. The manufacturing of the devices will occur by Sheet to sheet (S2S) manufacturing technology. In S2S manufacturing, different materials can be deposited (e.g. by means of vapour deposition) on a rigid substrate (e.g. glass) that is continuously moved forward at a constant speed. In the case of the perovskite-based devices, manufactured by CSEM, the following steps are followed:

- At first, a layer of nickel oxide is deposited on a glass substrate by means of vacuum sputtering.
- The perovskite ink is deposited on the nickel oxide layer by means of spin coating until a desired layer thickness is obtained. Spin coating can be carried out on areas up to ~10 cm^2. However, it is unlikely that spin coating will be used for scaled-up production. The use of vacuum deposition during S2S manufacturing is a more likely option which is also suitable for depositing perovskite layer.
- Similar to devices with flexible substrate, layers of silver are added which act as electrodes and then the entire structure is encapsulated within plastic layers for the protection of perovskite layer from environmental agents (humidity, oxygen etc.).

In comparison with the manufacturing of other thin film PVs (such as amorphous silicon PV or gallium arsenide PV) and commercially available OLEDs, similar observations can be made for the manufacturing process and functionality, and substance-intrinsic and process risks of perovskite-based devices with rigid substrates as in the case of their flexible substrate counterparts (described in section 3.1.1). There are, however, some exceptions and additional observations that stand out which are described below.

Manufacturing process and functionality

The solution-based in-situ synthesis of perovskite crystalline thin films for perovskite-based devices is carried out mostly at room temperature. As this working temperature does not require any external energy input, an overall lower energy consumption is implied compared to that of amorphous silicon based PV cells manufacturing.

Substance-intrinsic and process risks

The use of toxic solvents and lead halides, as described earlier in section 3.1.2, remain absent in the case of the manufacturing of amorphous silicon PV. This makes the process of PePVs manufacturing more hazardous than that of silicon-based PVs.

The pilot-scale fabrication is carried out inside a 50-100 m^2 mechanically ventilated room. The previous tasks related to perovskite ink handling are done within the conformity of glove boxes which are situated in 600 m^2 sized clean room. Only 1-2 operators carry out the task within their breathing zone (i.e. distance head-product <1m) while wearing full face respirator masks and no one else is present around them within a distance of 1m during the entire duration of the task, i.e. no by stander.

3 Results

Based on the information presented in Section 2.2, LICARA Innovation Scans were done for each of the three perovskite-based devices, i.e. PePVs, PeLEDs and PeLiFi. Separate scans were done for both flexible and rigid substrates. For each of the six scans, their comparative risk-benefit analyses were done with respect to their conventional counterparts: for flexible PePV, the conventional counterpart is flexible OPV; for flexible PeLED, the conventional counterpart is flexible OLED; for rigid PeLED, the conventional counterpart is rigid OLED; for rigid PePV, the conventional counterpart is amorphous silicon PV; and finally for PeLiFi, the conventional counterpart is commercially available Gallium Nitride and silicon based LiFi systems. These scans have been done with the assumption that the perovskite-based devices are already on the market (industrial production). Thus, the results should be interpreted as the risk-benefit analysis of these devices when industrially manufactured based on the current knowledge of the partners. The current knowledge of the partners has several unknowns and uncertainties which induces a similar level of uncertainty in the accuracy of the final analysis results. Within due course of the project, the partners are expected to extend their knowledge and experience about the perovskite-based devices manufacturing processes, thereby reducing the knowledge uncertainty which in turn would make the results more accurate. This clearly underpins the rationale behind the choice of the Tiered approach in WP7.

3.1 Comparative scan of flexible PePV vs. flexible OPV

In Figure 3 (a) and (b), the benefits and risks of flexible PePV (with respect to flexible OPV) are presented for each of their three categories (dark-coloured bars) and the underlying issues/subjects involved in them (light-coloured bars). The category result is given by the average of the underlying scores.

The error bar, shown as a blue line for e.g. environmental benefits during end-of-life in Figure 3 (a), represents the uncertainty/lack of knowledge on a specific aspect (i.e. questions answered as 'Unknown'). In these cases, a worst case scenario has been used in the calculations (e.g. highest risk, worse performance in comparison to the benchmark).

The relative risks posed by PePV are presented on a scale varying from 0 to 1 in Figure 3 (b). Scores below 0.3 indicate 'low risks'. This means that all three categories of risk are low for PePV. The potential effect of the PePV upon their release into the environment however exceptionally scores 0.5 and lies in the ‘medium’ category (i.e. between 0.33 and 0.67). The PePV is not expected to pose any ‘high risk’ as neither of the three risk types score more than 0.67.

For benefits in Figure 3 (a), the situation is somewhat different: the PePV can be better, but also worse than the flexible OPV. The benefits are presented on an axis ranging from -1 to 1, where -1 indicates the lowest, negative benefit (i.e. in all aspects worse than the flexible OPV) and 1 indicates the highest possible, positive benefit (i.e. in all aspects better than the flexible OPV). Thus, a score of 0 means 'neutral', as good as the flexible OPV. The environmental benefits of the PePV stands at a net score of -0.17. This negative environmental benefit or ‘environmental loss’ in developing PePV is mainly associated with the use of hazardous lead halides, more difficulty due to the hard-to-control in-situ synthesis of the perovskite crystalline thin films during manufacturing and lower life time of use of PePV. Moreover, harmful emissions during end-of-life stage of the PePV are unknown at this moment which adds uncertainty to the overall environmental benefit (shown as error bars). It is expected that during the course of the project, the partners will be able to increase the lifetime of the perovskite-based devices.

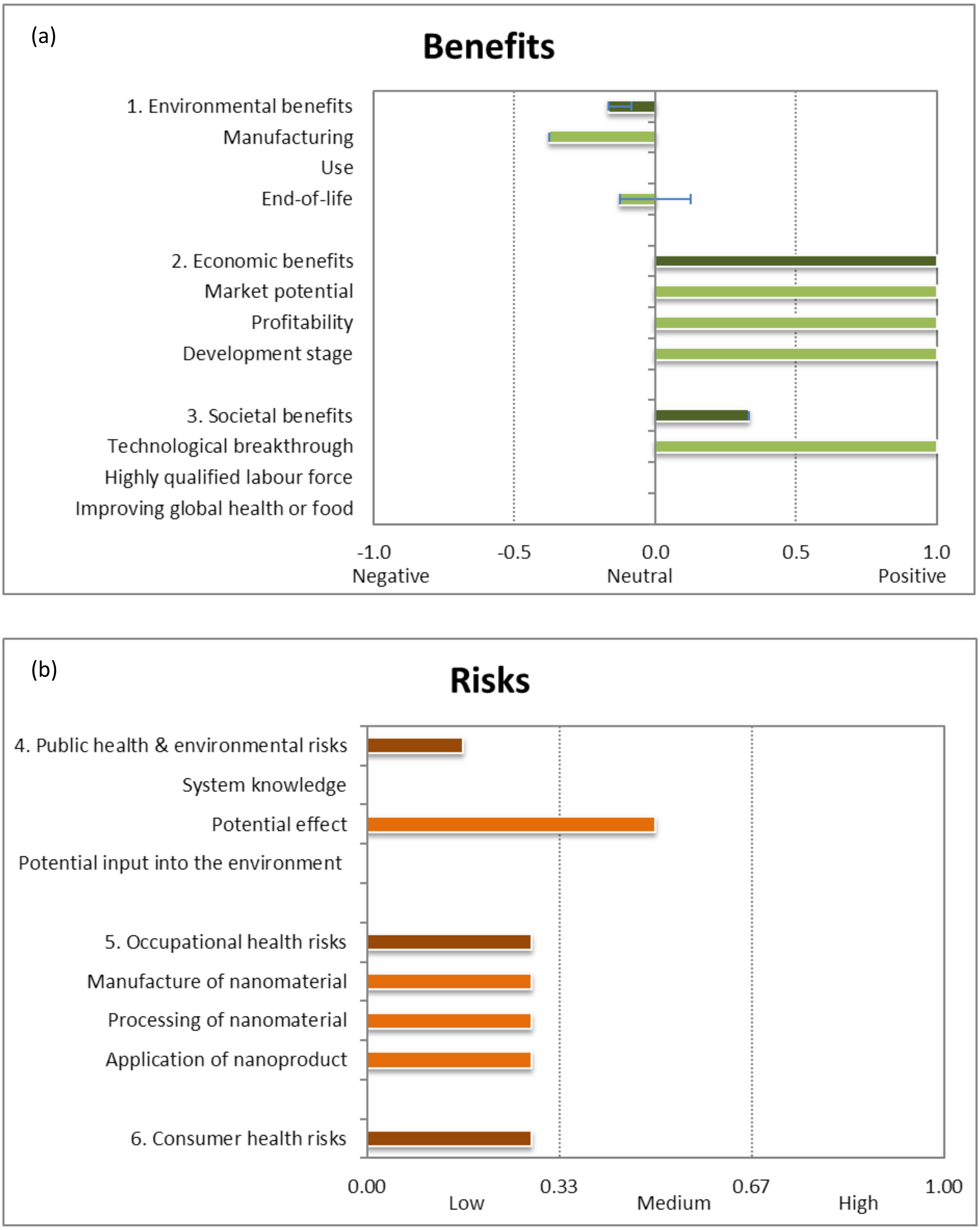


Figure 3: Comparative scans of **(a)** benefits and **(b)** risks of flexible PePV over flexible OPV.

At the same time, it has to be observed during the project that not all the perovskite-based devices have to contain lead, but can also be based on other compounds such as tin (Sn) halides. Compared to tin, lead has higher uptake ability by plants which suggest serious contamination issue when lead is used and leakage occurs (EU Directive 2014; Li et al., 2020). Moreover, tin is abundant in nature, poses low health risks, and Sn-perovskite has a crystal structure similar to Pb-perovskite (Giustino and Snaith

2016; Toshniwal and Kheraj 2017). These improvements will certainly improve the environmental benefits of PePV and other perovskite-based devices as discussed in later sections.

In contrast, both economic and societal benefits associated with PePV are already positive and stand at 1 and 0.33 respectively. This is due to the fact that PePV is expected to be significantly cheaper and more energy efficient than OPV. It should be noted that a low time-to-market (i.e. <1 year) for PePV is considered here within 'development stage' in coherence with our aforementioned assumption that the perovskite-based devices are already on the industrial manufacturing stage which leads to such a high economic benefit. If the time-to-market is high (e.g. >5 years), the net economic benefit score will drop to 0.33 because of the inherent uncertainties of a product with high time-to-market. In terms of cost and efficiency, the low time-to-market has no effect.

In terms of societal benefits, the development of flexible PePV can be considered a clear technological breakthrough (=1, as its cheaper price with expected higher efficiency of use will aid in improving energy requirements) but it is considered as good as flexible OPV in improving global health or food situation. The development of PePVs also do not contribute much in the substantial improvement of a highly qualified labour force which more or less remain same as is for flexible OPVs. Therefore a score of '0' is attributed for both subjects.

To evaluate both the benefits and risks of a product, it is assumed that each benefit and risk category is equally important. Total underlying risks and total underlying benefits are presented in a graph in Figure 4 where both benefit and risk are equally important and each is being represented on its own normalised axis. The benefits on the horizontal axis are net benefits which have a moderate overall score varying from 0.39 to 0.42. The risks on the vertical axis carry a low overall score of 0.25 and are outweighed by the benefits (i.e. positioned slightly to the right of the diagonal from (x,y) = (0,0) to (x,y) = (1,1)). The quick qualitative tier-0 risk-benefit assessment puts the development of the PePV in transit 'yellow zone' which signifies that distinguishing the added value of the flexible PePV from that of flexible OPV is infeasible for the moment with current state of benefits and risks. Other benefits are thus required for the PePV development so that it deserves to go ahead (i.e. towards 'green zone') or risks need to be reduced. The benefits and risks are expected to be related primarily with the environmental aspect of the flexible PePV, i.e. more control over in-situ synthesis of the perovskite crystalline thin films, use of metal halide compounds other than that of lead, e.g. tin-halides during manufacturing phase, higher life time of use of the device and, more knowledge on potential emissions during end-of-life stage of these PePVs.

If needed to be prioritised, control over in-situ synthesis of the perovskite crystalline thin films should be put at the highest priority as it will give the development of perovskite-based flexible PV the heaviest 'push' towards the 'green zone' signifying a clear go-ahead in the further stages of innovation value chain. Other required benefits that follow in the decreasing order of their influence over the push towards green zone include higher life time of device use, use of metal halide compounds other than that of lead and more knowledge over potential emissions during end-of-life stage.

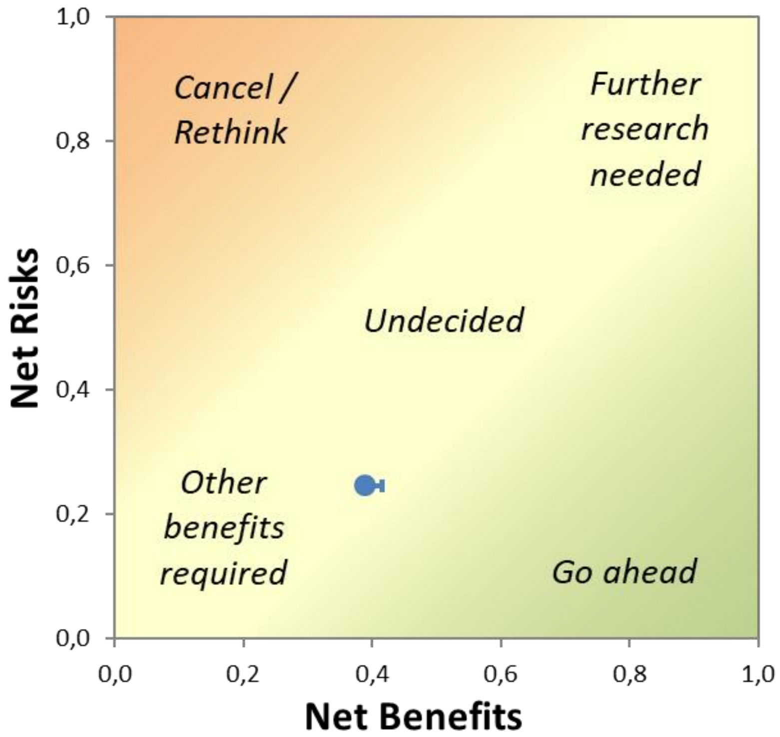


Figure 4: Risk-benefit assessment of the development of flexible PePV over flexible OPV.

3.2 Comparative scan of rigid PePV vs. amorphous silicon-based PV

The development of a rigid PePV over its conventional counterpart, i.e. amorphous Si-based PV entails low environmental loss or benefit as its score varies from -0.04 to 0.04 in Figure 5 (a). The main distinction can be observed for environmental benefits during manufacturing where the environmental loss/benefit is null as compared to flexible PePV and PeLED where the environmental loss are higher (0.38 for both, see Figure 3 (a) and Figure 7 (a)). The energy consumption of the manufacturing process of a rigid PePV is also lower which adds to environmental benefit. The manufacturing process complexity of rigid PePV however remains similar to that of the amorphous Si-based PV which does not add any attribute to the manufacturing phase or process. On the other hand, hazardous solvents (e.g. dimethylformamide, hexane, o-xylene) and lead halides are actively used during the manufacturing of rigid PePV which are absent in case of amorphous Si-based PV. The potential emissions from rigid PePV during end-of-life stage are also presently unknown. These factors overall lead from very low environmental loss (=-0.04) to low environmental benefit (=0.04) in case of rigid PePV. The screening of the rest of the benefits and risks (shown in Figure 5 (b)) remain same as observed earlier in case of flexible PePV.

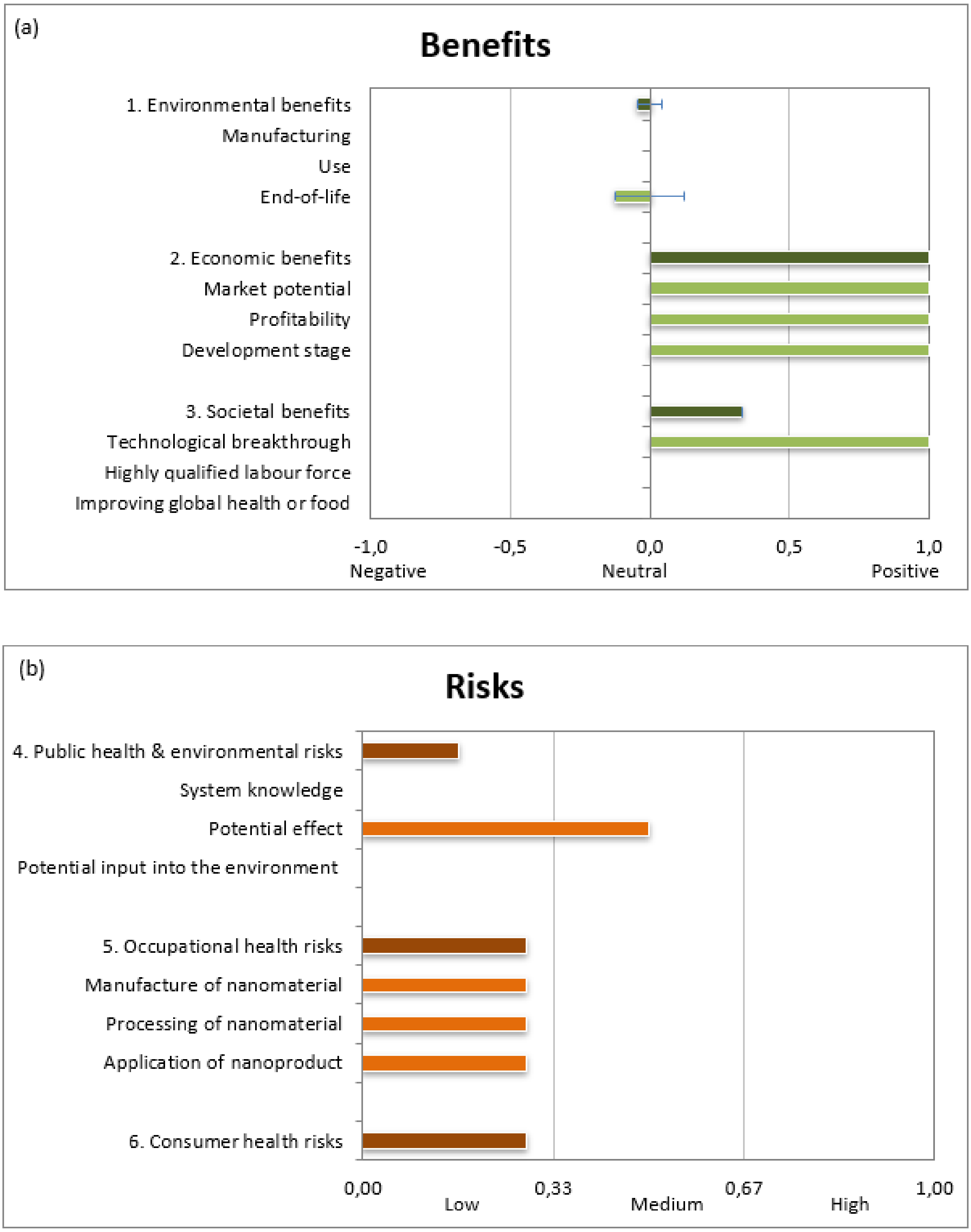


Figure 5: Comparative scans of **(a)** benefits and **(b)** risks of rigid PePV over amorphous silicon-based PV.

With the aforementioned better environmental performance of rigid PePV over its conventional counterpart as compared to flexible PePV, the risk-benefit assessment of rigid PePV in Figure 6 shows a higher overall benefit which varies from 0.43 to 0.46 (higher than flexible PePV). The risk level also remains low (=0.25) and similar to flexible PePV. The benefits outweigh the risks (i.e. positioned right of diagonal) but are still moderate (not enough value) which puts the rigid PePV development in the transit 'yellow zone'. By putting the highest priority on increasing life time of device use, followed by the use of alternate metal halide compounds and solvent which are less hazardous than presently used during manufacturing and finally more knowledge certainty about the emissions during end-of-life stage, the development of rigid PePV system will move to the 'green zone' with more certainty in the decision to go ahead. The partners, notably CSEM, are already working on the use of alterative less hazardous non-carcinogenic solvents. The obtained results so far on the feasibility of their use show promising outcomes which will be considered in the next phase of the project.

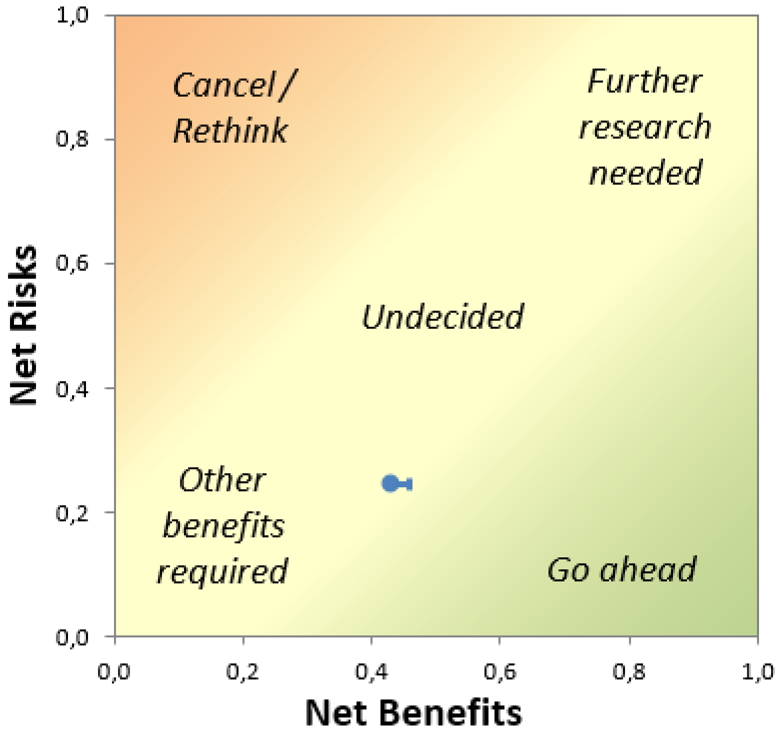


Figure 6: Risk-benefit assessment of the development of rigid PePV over amorphous Si-based PV

3.3 Comparative scan of PeLED vs. OLED (flexible and rigid)

The benefits scan of PeLED over OLED is shown in Figure 7 (a) which is applicable for both of its flexible and rigid substrates. The environmental benefits score varies from -0.33 to -0.13. The main reason for this low score can be attributed to the unknown efficiency of use of these PeLED devices compared to OLED which decreases the environmental benefits score during the use phase and assigns an uncertainty to it. Rest of the benefit scores (and the subjects within these benefits) remain same as that of PePV in Figure 5 (a). Similarly, the risks shown in Figure 7 (b) also remain same.

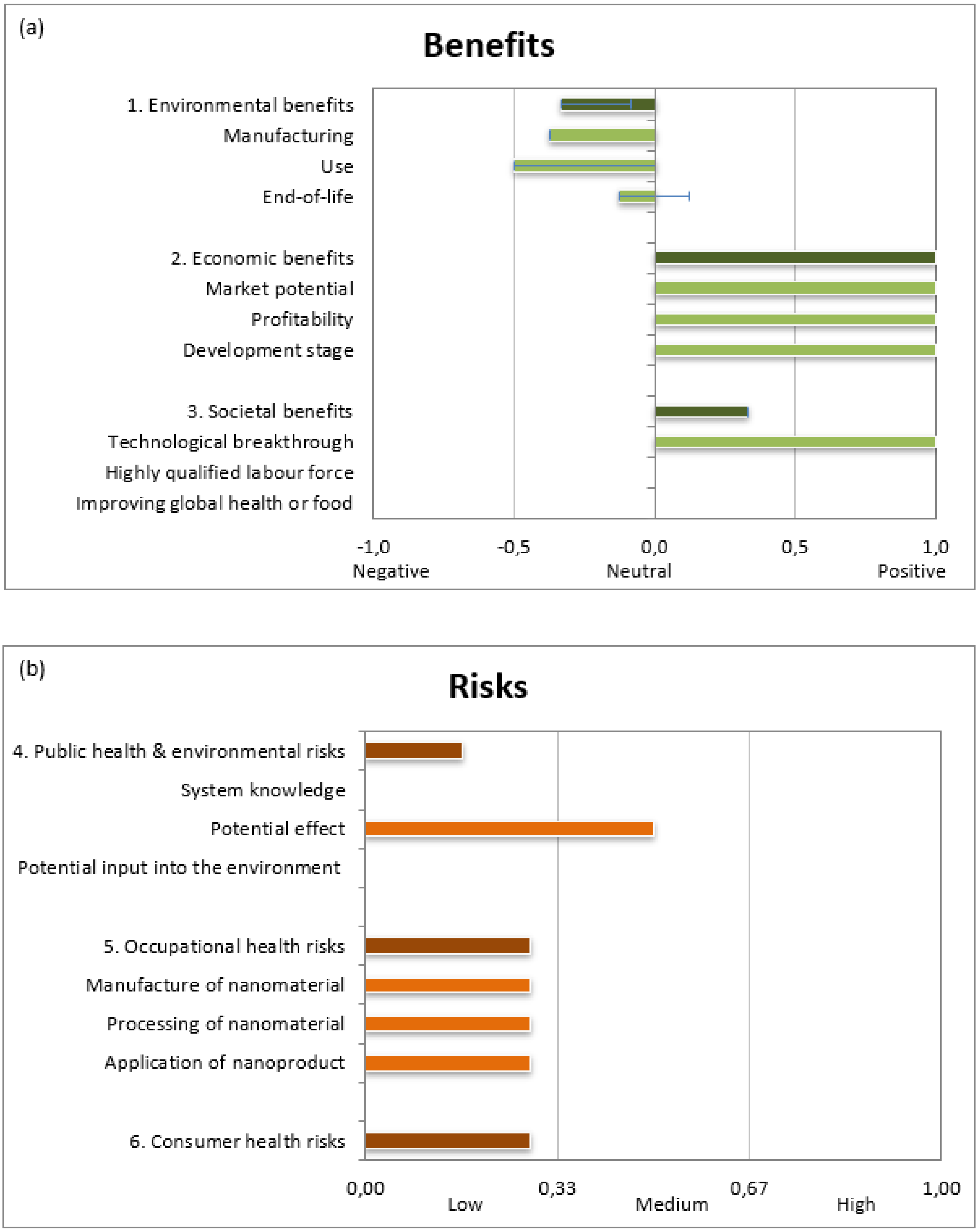


Figure 7: Comparative scans of **(a)** benefits and **(b)** risks of flexible PeLED over flexible OLED

The scans from Figure 7 (a) and (b) lead to the risk-benefit assessment which is shown in Figure 8. The overall benefit score varies from 0.33 to 0.4 which is a moderate benefit score but outweighs risk lying at 0.25 (i.e. slightly right of the diagonal). This shows that although the implied risks in PeLED development are low, it still requires more benefits, particularly higher life time and efficiency of use, as well as more certain knowledge of emissions during end-of-life stage, for a clear decision on whether the development of PeLED deserves to go ahead. The order in which these required developments are mentioned is also the same as their influence on obtaining the clear decision to go ahead. Therefore, most efforts should be put on increasing the life time and efficiency of use of PeLED. In the due course of the project, it is expected to have more knowledge on other factors of PeLED too, which will move the risk-benefit analysis to a more certain decision.

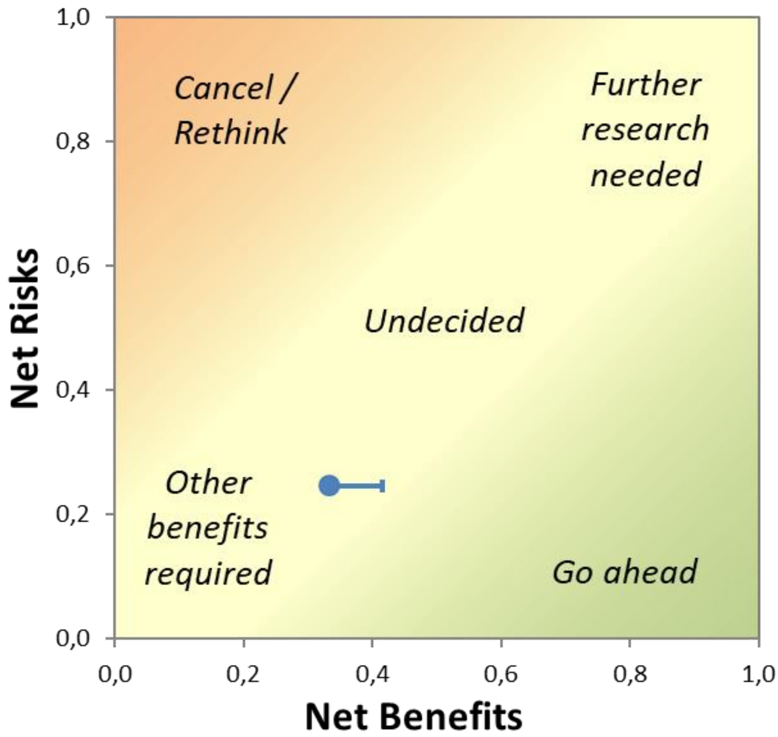


Figure 8: Risk-benefit assessment of the development of PeLED over OLED applicable for both of its flexible and rigid substrates

3.4 Comparative scan of PeLiFi vs. conventional LiFi

The environmental benefits or losses of the development of a PeLiFi over conventional LiFi is dominated by the fact that the former involves the use of aforementioned hazardous solvents and lead halide during its manufacturing which impart a hazardous characteristic to its manufacturing phase. The corresponding score in the scan is thus equal to -0.38, as shown in Figure 9 (a). A higher efficiency but lower life time of use renders the environmental benefit of PeLiFi during its use phase to be neutral. The scores corresponding to the environmental benefit during end-of-life stage and to the other two benefit types remain the same as for aforementioned perovskite-based devices. The scan of the risks in Figure 9 (b) yields the same result as was observed in previous cases. Therefore, as expected, public health and environmental risks stand at 0.17 and both occupational and consumer health risks stand at net score of 0.29 (low risks).

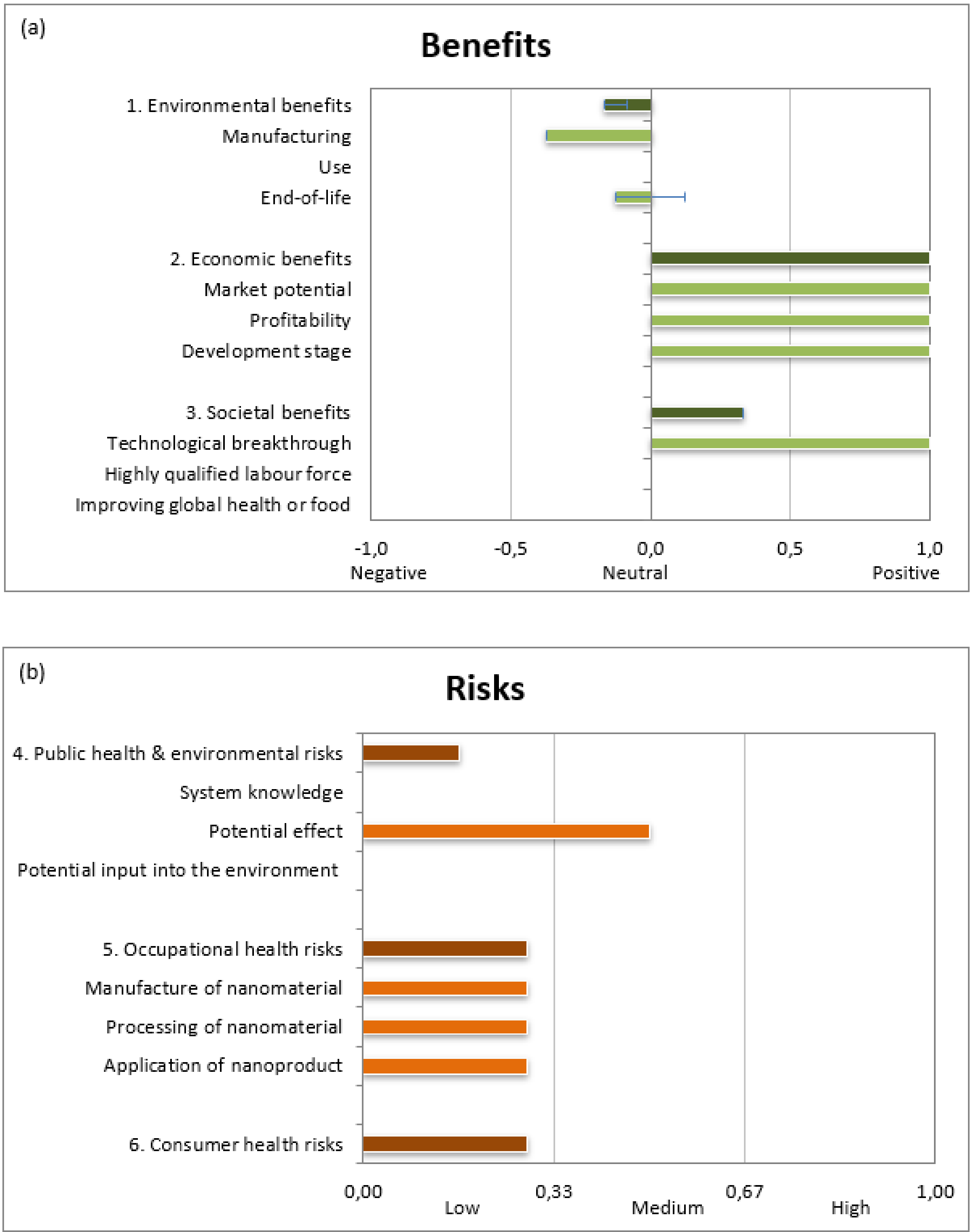


Figure 9: Comparative scans of **(a)** benefits and **(b)** risks of PeLiFi over conventional LiFi system

The risk-benefit assessment in Figure 10 puts PeLiFi development over conventional LiFi system at an overall moderate benefit score varying from 0.39 to 0.42 and risk score equal to 0.25 (low). This shows that PeLiFi can be a promising development over conventional LiFi system but it requires more benefits so that it can deserve to go ahead. This can be achieved primarily by adding following environmental benefits (in the decreasing order of their significance): obtaining higher efficiency of use, use of alternate less hazardous metal halide compounds and solvents during manufacturing, and more certainty in the emissions estimate during its end-of-life stage.

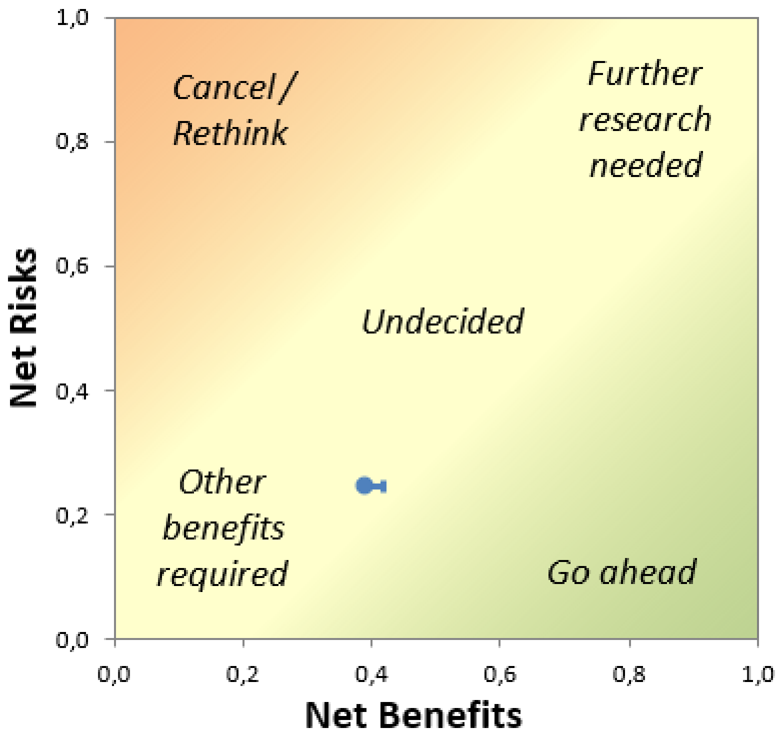


Figure 10: Risk-benefit assessment of the development of PeLiFi over conventional LiFi system

4 Discussion and Conclusions

Based on a general conceptual framework, LICARA Innovation Scan tool can support decision-making by evaluating the benefits and risks over the life cycle of the perovskite-based devices compared to their reference products. It is a new tool which has been developed from LICARA nanoSCAN whose use is specific to the assessment of only nanomaterials and nano-enabled products. Considering the scale of the perovskite-based devices and their components, a generic model was thus necessary that can go beyond the nano-specific dimensions to suit the innovative products in general.

During the initial phase of information gathering on the manufacturing processes and features of perovskite-based devices, we observed that a lot of information on the perovskite-based devices was already available with the partners due to their past experiences of working with the same or similar devices. Nevertheless, some information was known in a qualitative way and several unknowns and uncertainties were present in their knowledge, e.g. uncertain PeLED efficiency, unknown potential emissions etc., which are typical of an early stage of a project. In addition, several input parameters have been scored by using expert judgement only (opinion-wise). The tool proved to be useful to derive the risk-benefit analysis even with such qualitative and few information.

The average time needed to fill in the tool was <1 h which is reasonable for any SME developing an innovative product. The information could be relatively easily filled in the tool by choosing the qualitatively categorised answers from a dropdown menu to the simply worded questions. Therefore, there is no specific expertise needed to work with the tool, except for its Stoffenmanager® component which may require the (basic) knowledge of certain technical terms in occupational hygiene and epidemiology.

In the present tier-0 qualitative risk-benefit assessment of perovskite-based devices, we found that all five assessed devices, i.e. flexible PePV, rigid PePV, flexible PeLED, rigid PeLED and PeLiFi, have consistently low risk and moderate benefit scores when they are compared with their conventional reference devices. For instance, the qualitative benefit score for flexible PePV is equal to 0.39 (out of 1) and qualitative risk score is equal to 0.25 (out of 1) when compared to OPV. Similarly for rigid PeLED, these scores are 0.33 and 0.25 respectively when compared to OLED. These low risk and moderate benefit scores put the devices in a transit 'yellow zone' of LICARA Innovation Scan which signifies that these perovskite-based devices are promising developments and have the potential to be sustainable over their entire life cycle. However, they need additional benefits or reduced risks for them to lie in the LICARA Innovation Scan's 'green' zone which signifies a clear go-ahead with their further development in the innovation value chain. The needed benefits and reduced risks have been identified to be mainly associated with the environmental aspect of these devices and these are generally as following in the decreasing order of their significance to put the device developments in the green zone.

1. Controlled (easy-to-tailor) in-situ synthesis of the perovskite crystalline thin films during manufacturing phase,
2. Higher life time of use of the perovskite-based device,
3. Higher certainty in the efficiency of use, particularly for PeLED devices,
4. Use of metal halide compounds other than that of lead, e.g. tin-halides, during manufacturing phase to mitigate the hazard,
5. Synthesis of perovskite using less hazardous (i.e. environmental and human friendly) solvents,
6. Knowledge over potential emissions from these devices during end-of-life stage.

In due course of the project, more quantitative information with lesser uncertainty will be generated in relevant work packages of the project which will replace product knowledge limitations and expert judgements that underpin the present tier-0 assessment. This may result in elevation in risk levels which remain hidden or undetected in the present assessment. Therefore, a higher tier (tier-1) quantitative assessment will be necessary which will be done using a hotspot scan. The hotspot scan will focus on the quantitative release estimations of components from perovskite-based devices into indoor and environmental compartments over their full life cycle. This will be followed by a tier-2 quantitative human health risk assessment which will make use of relevant exposure scenarios for workers, consumers, and general public as well as information on the hazardous properties of the substances used and released during manufacturing, use and disposal. It will be further complemented with a cradle-to-grave life cycle assessment of selected perovskite-based devices to ensure their sustainable development.

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6 Appendix I: Technical implementation of LICARA Innovation Scan

6.1 Sustainable approach

After their initial development within a project, it always remains a challenge to keep an online tool properly maintained in the years after the project has been completed. To alleviate this, TNO has developed an online platform, called DIAMONDS, that can be used as a generic backbone for scientific tools. Tools developed on this generic backbone can become more sustainable as the overall maintenance is shared and tools can benefit from the generic building-blocks of the platform.

LICARA nanoSCAN was originally developed in Excel. An online version was developed once but never properly maintained. As changes to the original LICARA nanoSCAN were needed for the Perocube project, we have chosen to implement the novel version in a more general and sustainable fashion as part of the DIAMONDS platform. To reflect the fact that the novel version is no longer nano-specific, we have named it LICARA Innovation Scan.

The new LICARA Innovation Scan was built in a modular fashion by augmenting some of the generic building blocks and adding a new integrating component. In essence, the LICARA Innovation Scan consists of a set of questions (captured in a Questionnaire Module), a set of algorithms (captured in a Script Module), a set of visualizations (captured in a Visualization Module) and a new integrating component (captured in a Scan Module) that brings all components together. Due to this generic approach, it was possible to develop two new online tools using the same building blocks, i.e. the newly created online LICARA Innovation Scan (for innovative products in general) as well as a new online version of the original LICARA nanoSCAN (for nano-specific products).

6.2 Resulting implementation

6.2.1 Registration and login

On the initial landing page (https://diamonds.tno.nl/#licara) a LOGIN/REGISTRATION button is available in the top-right corner. This button brings up a login page, which is depicted in Figure 11. Registered users can directly login, but first-time visitors first need to register a DIAMONDS account. A link to the registration form is provided on the login-page which is depicted in Figure 11.

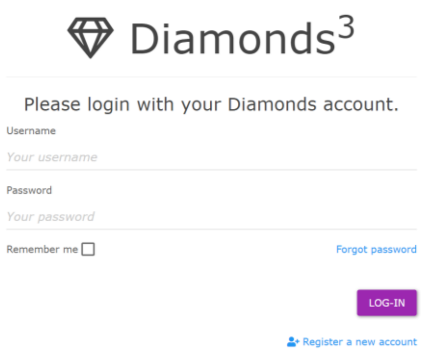

Figure 11: Screenshot of login with registration link.

6.2.2 Starting with defining a new scan

After login, users can choose between performing a traditional LICARA Nanoscan or performing the new LICARA Innovation Scan that is relevant for the PeroCube assessments.

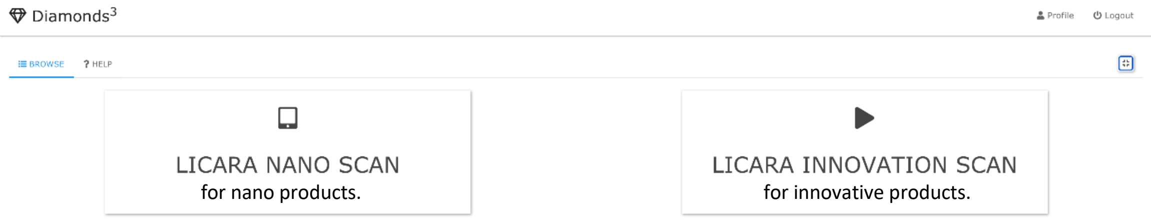

Figure 12: Screenshot of choice between original LICARA Nanoscan or new LICARA Innovation Scan

After this choice, the user is presented with all his/her previous runs that have been saved as depicted in Figure 13 . The user can decide to select one of the available previous runs or start a completely new run. When starting a completely new run, the user can provide a name and this run will be saved. In future visits, this run will now also be available in the list of available runs. The subsequent experience is similar to having selected one of the available previous runs, except that in the latter, the previously provided answers to the questions are loaded and presented as pre-filled answers in the subsequent pages.

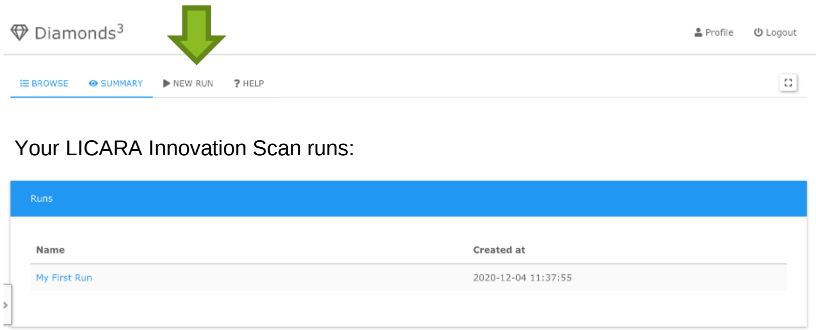

Figure 13: Screenshot of page with previously saved runs which you can select. A green arrow indicates the possibility to start a new run

Before starting the actual innovation scan, three introduction pages are presented to the user. These introductory pages can always be revisited at a later time by clicking on the “INTRODUCTION” Tab. The first introduction page explains what the LICARA Innovation Scan is and is depicted in Figure 14. The second and third introduction page explain more about the underlying framework and the scientific basis. Throughout the tool, users can choose to navigate through all pages in chronological order by using “<- BACK” or “SAVE & NEXT ->” buttons at the bottom. Alternatively, users can click on the top tabs to quickly navigate through the main components (“INTRODUCTION”, “INNOVATION SCAN”, “RESULT” and “?HELP”) and/or click the underlying subpages presented as numbered steps just below the top tabs (depicted as a line with numbered solid circles consisting of (1) Introduction; (2) Overview and (3) Scientific basis in Figure 14).

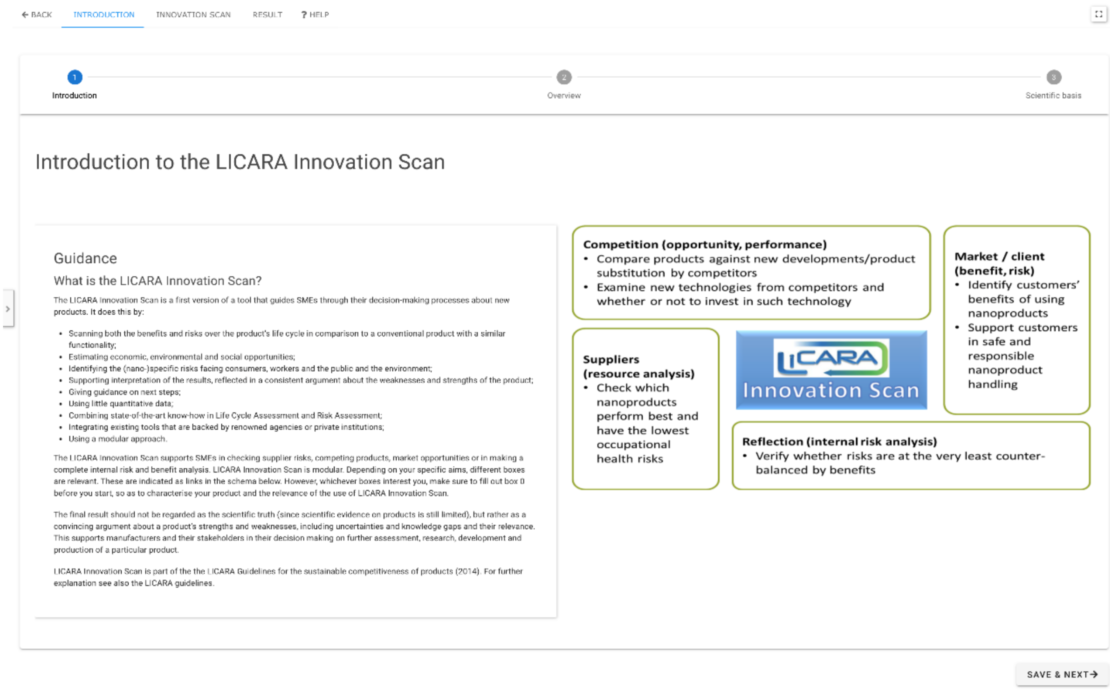

Figure 14: Screenshot of the first page of the introduction pages. This page provides basic introductory information about what the LICARA Innovation Scan is. Tabs at the top allow quick navigation through main components. Blue underlined “INTRODUCTION” tab indicates “INTRODUCTION” as the currently active component. Directly below the top Tabs, the available steps of the currently active component are shown as a line with numbered circles. Blue solid “1” circle and bold “Introduction” indicates “1 Introduction” as the currently active step. The content of this step is shown in the main panel At the bottom a gray “SAVE & NEXT ->” button allows the user to finalize this step and move to the next step.

After the three introductory steps of the “INTRODUCTION” component follows the second “INNOVATION SCAN” component. This component guides the user through seven steps corresponding to the first seven boxes described in section 2.1 and shown in

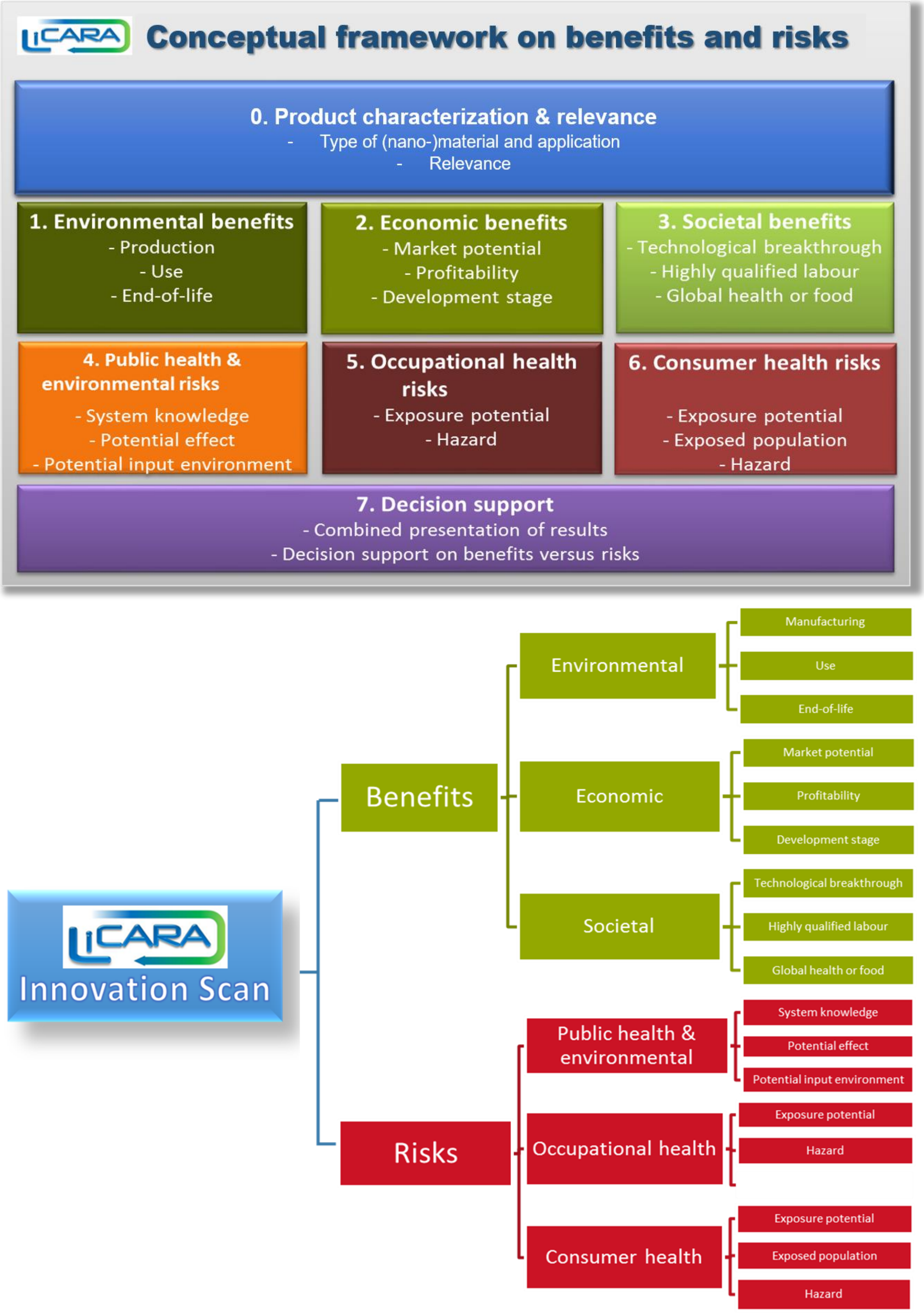

Figure *1* (a). In each step, the user can fill in information for a number of questions with mostly predefined options and see their effect on the resulting scores for that particular step. The user can then save the results and continue with the next step. However, due to the modular nature, the user is also allowed to jump between steps in the order to his/her liking. The seven steps are:

- Step 1 “Product characterization & relevance”.
- Step 2 “Environmental Benefits”
- Step 3 “Economic Benefits”
- Step 4 “Societal Benefits”
- Step 5 “Public Health & Environmental Risks”
- Step 6 “Consumer Health Risks”
- Step 7 “Occupational Health Risks”

Step 2 is an example of a step in which all questions can be answered by tabular answering options and is depicted in Figure 15. The resulting scores of each step are presented in a panel shown in the middle at the right of the page that can be kept open or collapsed according to the user’s preference. Directly after changing any answer the scores will be updated to reflect the new situation. Alternatively, Step 3 is an example of a step in which all questions can be answered by selecting from a list of options in a dropdown box and is depicted in Figure 16.

All the resulting scores are integrated and visualized in the third “RESULTS” component and is depicted in Figure 17. All benefit scores are visualized in an horizontal bar-graph with dark green bars for the three main benefits (“environmental”, “economic” and “societal”) and light green bars for the underlying elements. All risk scores are visualized in an horizontal bar-graph with dark orange bars for the three main benefits (“public health & environmental”, “consumer health” and “occupational”) and light orange bars for the underlying elements. A risk-benefit analysis is visualized by positioning the innovative product in a diagram reflecting net benefit on the x-axis and net risk on the y-axis.

Finally, for convenience, the fourth “? Help” component provides additional help pages explaining how to use the tool.

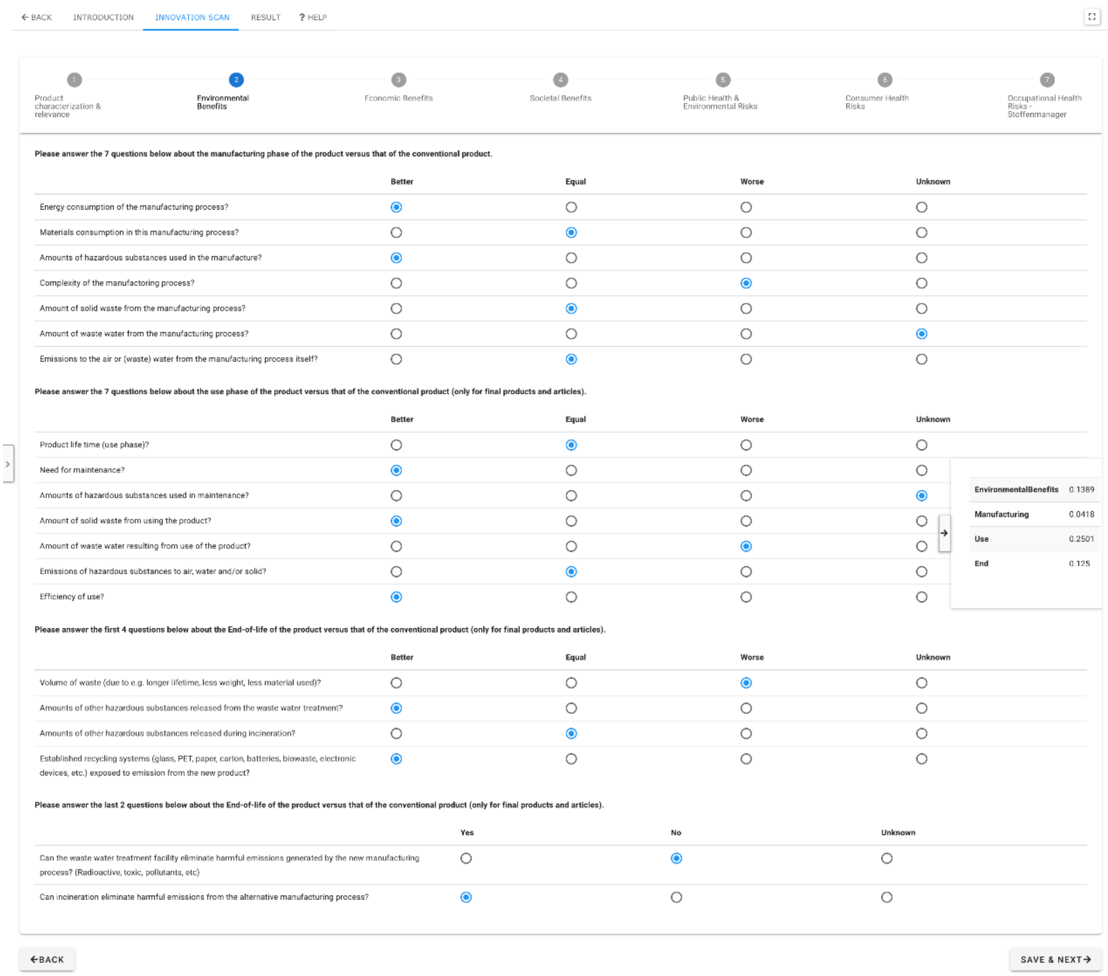

Figure 15: Screenshot of Step 2 “Environmental Benefits” of the “INNOVATION SCAN” component. This page shows four blocks of questions with tabular formed answering options. In the middle at the right a moving panel shows the four resulting environmental benefit scores.

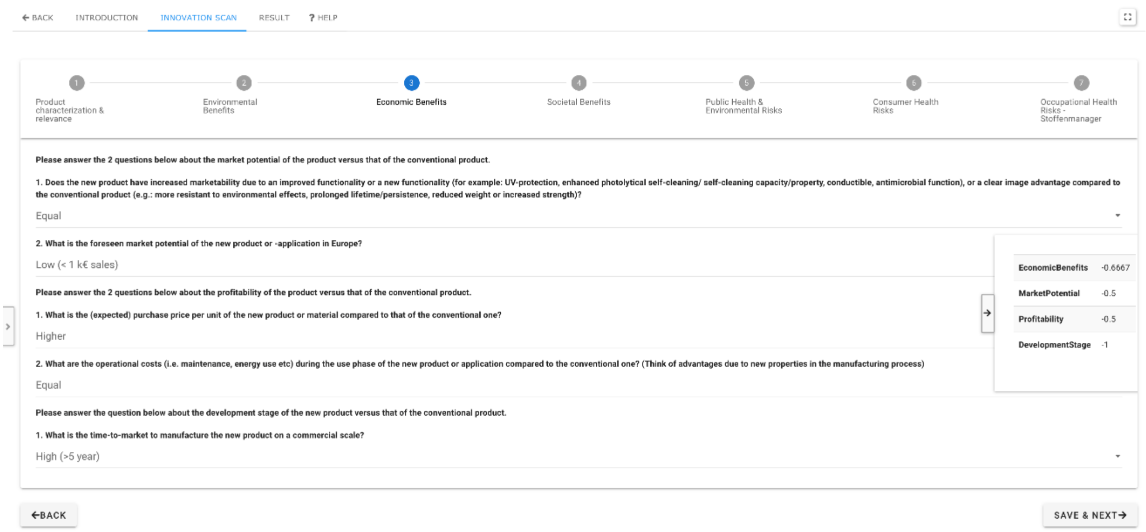

Figure 16: Screenshot of Step 3 "Economic Benefits" of the “INNOVATION SCAN” component. This page shows five questions that can be answered using dropdown boxes. In the middle at the right a moving panel shows the four resulting economic benefit scores.

Figure 17: Screenshot of Result Component with the final integrated results visualized in two bar diagrams and one final risk-benefit diagram accompanied with explanatory text panels.

6.3 Dissemination

To present basic background information about the tool for visitors that do not need to login, we have created a landing webpage at https://diamonds.tno.nl/#licara as depicted in **Figure *18***. More detailed information for interested visitors is available as depicted in **Figure *19***.

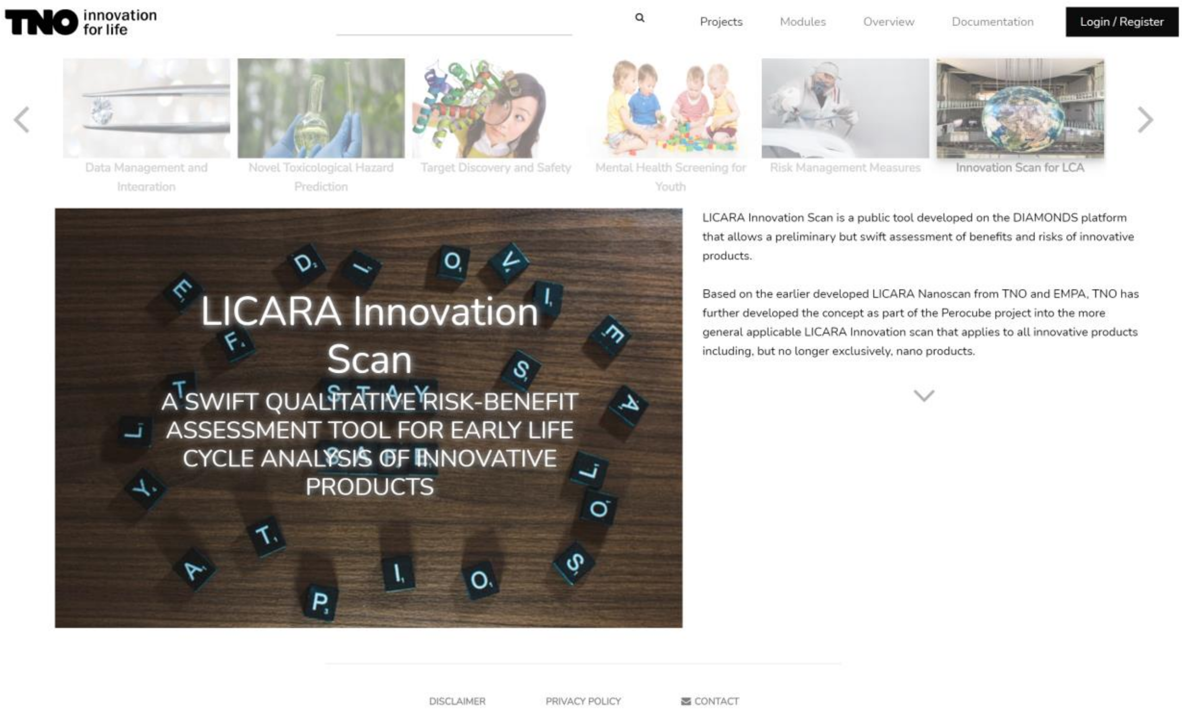

Figure 18: Screenshot of initial landing page (for which no login is required) with url: https://diamonds.tno.nl/#licara.

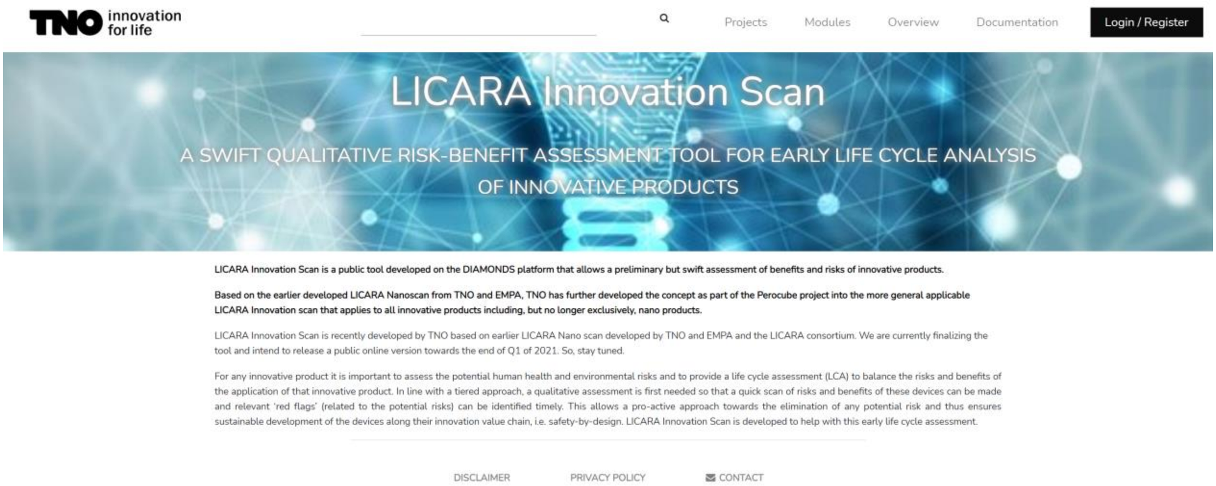

Figure 19: Screenshot of background information (for which no login is required).

The tool will be launched and become publicly available at end Q1 2021. At that time account registration instructions will be published on the information page. In addition, a press release announcing the launch and other PR activities via the PeroCube dissemination channels (website, briefing) are anticipated.