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“Advanced Materials” for innovative solar cell technologies

Part II: Sustainability assessment and significance in the circular economy

Summary

To estimate the environmental sustainability of “advanced materials” (AdMs) in innovative solar cell technologies (emerging photovoltaics, EPVs), it is necessary to consider the entire life cycle. Life cycle assessments (LCAs) can identify those materials in a product that contribute the most to environmental damage in relation to the entire product when compared to the other materials used. This offers the opportunity to optimise the product in terms of sustainability. LCAs of EPVs carried out so far are hardly comparable because of different assumptions and system boundaries; they also have limitations, especially because of missing data. When compared with conventional photovoltaic (PV) technologies, EPVs can generally have a lower demand for energy and a shorter energy payback time because of simpler manufacturing methods and less demand of materials. When compared with solar glass or the (precious) metals or “critical raw materials” used for the electrodes, the AdMs assessed in the LCAs showed minor environmental impacts, primarily because they are used in relatively small quantities. EPVs have not yet reached marketability; consequently, no corresponding recycling technologies have been developed yet. Separating the composite materials represents a major challenge in recycling. Ideally, not only environmental compatibility (“prevention through design”, also known as “safety by design”) but also recyclability (“design for recycling”) should be taken into account already at the design stage. Furthermore, consideration should also be given to finding a suitable compromise between highest efficiency, best stability, cost-effectiveness, and sustainability (“sustainability by design”).

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Introduction

The production of energy is one of those human activities that cause great environmental damage. Greenhouse gas emissions from the burning of non-renewable fossil fuels lead to global warming and environmental pollution, with over-exploitation of mineral resources and raw materials resulting in the destruction of the environment, loss of biodiversity, and political and social problems. One of the most promising alternatives to power generation from fossil fuels is photovoltaics. The sun provides many times more energy per year than is consumed worldwide.^{1,2} Photovoltaic systems emit no CO₂ during their service life and operate silently. Despite all the advantages, however, it cannot be assumed *a priori* that solar cell technologies are generally environmentally friendly and sustainable. This also applies to innovative solar cell technologies (emerging photovoltaics, EPVs) based on so-called “advanced materials” (AdMs) that were presented in part I of the dossier.³ After traditional silicon-based photovoltaics and thin-film solar cells (e.g. based on cadmium telluride), these third-generation photovoltaic systems offer new fields of application, e.g. in the field of building-integrated photovoltaics or for portable electronic devices and other consumer goods because of their low manufacturing costs as well as light and flexible construction (see also³).

These EPVs include organic solar cells whose light-absorbing layers consist of semiconducting polymers, dye-sensitized solar cells with a porous layer of nanoscale titanium dioxide coated with dye molecules, perovskite solar cells whose active layer consists of lead halides, and quantum dot solar cells with semiconductor layers containing heavy metals. EPVs are still largely under development, with research being conducted on a variety of different materials and material combinations to achieve the best efficiency, the greatest possible stability under prevailing environmental conditions, and a long service life, respectively (see also³).

To determine the environmental impact of such innovative solar cell technologies, it is necessary to consider the entire life cycle: from extraction of the raw materials, production of materials and components for individual cells and complete modules, the use phase right through to their disposal at the end of the service life.

Environmental sustainability assessment of EPVs

The most commonly used method to assess environmental sustainability of a product is through **Life Cycle Analysis (LCA)**. This is a quantitative, product-related method that makes it possible to estimate not only the use of energy and chemicals but also the environmental impact over the product’s entire life cycle whilst also making them comparable with those of other products. LCAs are standardised according to the ISO 14000 series and in principle cover all four stages of the life cycle: acquisition or extraction of the raw materials, processing and manufacturing of materials, application, and the end-of-life phase. However, since it is very elaborate to obtain information on environmental impact during all stages, the scope of an LCA is usually narrowed by selecting individual stages during a product’s life cycle. There is also a degree of flexibility regarding the choice which environmental impact is to be analysed.⁴

To assess environmental sustainability, LCAs for photovoltaics (PV) usually draw on the following **indicators**:

- **“Cumulative energy demand” (CED)**
This is the total consumption of energy during a PV life cycle, i.e. both the direct energy consumption (electricity for the production of the solar cells or modules) and the indirect energy consumption (the energy embedded in the materials, i.e. the energy that is used for the extraction or production of the basic (raw) materials).

■ **“Greenhouse gas (GHG) emissions” or “global warming potential” (GWP)**

A measure for a chemical compound’s relative contribution to the greenhouse effect. It indicates how much a specific mass of a greenhouse gas (GHG) contributes to global warming compared with the same mass of CO₂.

■ **“Energy Payback Time” (EPBT)**

This is the time that a solar cell requires to produce the energy required for its manufacture.

In an LCA, the environmental impact of a product or an individual solar cell or an entire PV system is analysed using different methods for different **impact categories**. These include, for example:⁵

- Ecotoxicology (marine, freshwater, terrestrial)
- Human toxicology (carcinogenic, non-carcinogenic)
- Land use
- Resource depletion (water, fossil, mineral)
- Acidification (soil, water bodies)
- Eutrophication (land, water)
- Particulate matter
- Ionising radiation
- Climate change
- Depletion of the ozone layer

Additional impact categories are also possible. The ISO standard does not specify which impact categories are to be investigated, leaving the choice to the compilers of the LCA.⁵ The required data for LCAs on PV technologies are mostly taken from (commercially) available databases (also referred to as life cycle inventories, LCIs⁶) and, if necessary, supplemented by the analysts’ own assumptions, using primary data from published studies or unpublished company data on specific processes.

Comparing different LCAs of PV systems with each other is generally difficult because analysts can freely choose from a variety of environmental categories and methods that are to be investigated.⁷ In addition, system boundaries are also defined differently, and mostly only the first two stages are investigated, namely the acquisition of raw materials and the manufacturing phase (“cradle-to-gate” LCA). Only few LCAs also cover the end-of-life phase (“cradle-to-grave” LCA). Creators are also free to choose the so-called functional unit, i.e. the reference value. In most cases, the units used for this purpose are power in “kWp”⁸, amount of electricity produced in “kWh” or 1 m² area of the solar cell. Primary data, e.g. consumption of electricity or chemicals, are scarce or incomplete for some manufacturing processes, and there is a general lack of data for the disposal or recycling phase. Often, LCAs also use secondary data from other analyses.

There are major differences with regard to the indicators, parameters, and impact categories analysed. Consequently, some studies only use the key figures EPBT or CED. Amongst the environmental categories, the most frequently calculated ones are the greenhouse gas emissions or the global warming potential. With regard to assessing environmental impact, different methods exist.⁹ In some LCAs, the results are displayed in normalised form; this makes comparison with results of other studies even more difficult.⁷ Another point of criticism of the LCAs on PV systems carried out so far is that they do not provide a complete picture of potential environmental impact and health effects because these often do not consider the latest developments. Examples include the expanding markets in emerging countries such as China, India, and Malaysia, but also the different types of systems such as off-grid PV systems, large-scale systems in desert areas, building-integrated systems, and technological innovations.¹⁰ In the context of EPVs, LCAs are also subject to great uncertainties as development is often still at the experimental stage, meaning only laboratory data can be used. At present, it is difficult to assess how commercial production might affect the results of LCAs. Industrial production has the potential to reduce environmental damage because production in the laboratory is less efficient in terms of use of materials and energy than commercial production.⁷

LCAs for EPVs have so far been carried out on the basis of the most commonly used materials. The majority of innovative, environmentally friendly materials, such as natural or organic dyes, have not yet been evaluated because data on energy and chemical consumption for production is mostly still lacking.¹¹ The end-of-life phase also plays a decisive role in LCAs for PVs in general although this has only been considered in a few studies to date because specific data and information on recycling processes are missing. In some LCAs it was assumed that inorganic materials can be landfilled, plastics can be incinerated, and some materials, especially metals and glass, can be recycled. In any case, the possibility of recycling significantly reduces environmental damage caused by PVs, especially where toxic materials such as cadmium or lead are concerned.⁷

A general crucial factor in LCAs of PVs is the estimated product service life because important parameters such as EPBT depend on it. Since solar cells emit virtually no emissions during their service life: the longer their service life during which they produce electricity, the better their environmental profile in LCAs. The service life of silicon-based solar cells is currently around 25 to 30 years. However, there are no reliable data on the performance of EPVs under real-life application conditions as of yet, only estimates from

laboratory tests or pilot studies.⁷ To date, however, the service life of all types of EPVs still appears to be far below that of silicon-based PVs because EPVs are susceptible to environmental factors such as temperature, humidity, light, and heat. Nevertheless, in some LCAs a service life is assumed to be similar to that of silicon-based solar cells. Strictly speaking, however, this falsifies results and is currently not yet realistic.⁷

Despite all the limitations, LCAs are an important method to identify those materials in a product that contribute the most to environmental damage caused by the entire product when compared to the other materials used. This allows for the identification of problematic materials, such as (1) materials that require a lot of energy during their manufacture, (2) those whose extraction is particularly harmful to the environment or whose availability is limited, as well as (3) materials that pose a risk to the environment or human health. This provides the opportunity to optimise a product in terms of environmental protection and sustainability.

Life Cycle Analyses for EPVs

In the LCAs conducted so far, EPVs have shown to have a lower demand for energy and a shorter EPBT when compared with conventional PV technologies. This is because of their efficiency, their low production costs, and their environmental friendliness. Negative environmental impact because of heavy metal content in the active layers is negligible compared with silicon-based commercial PVs.¹² This is due to the fact that the semiconductor layers are in the nanometre range, i.e. only relatively small amounts of materials are used for these layers. The largest share by mass (more than 90 percent by weight) in EPVs is apportioned to the glass substrate on which the layers are deposited. For this reason, LCAs carried out to date have shown that e.g. solar or safety glass has the greatest environmental impact: because of the high demand for energy during the production of the glass and the rare earth metals for the transparent electrode.⁷

Solar cell components, such as the electrode, can consist of so-called “critical raw materials”.¹³ Raw materials are considered “critical” when originating mostly from other than EU countries and for which global competition is becoming increasingly fierce. Economic significance and risk to supplies are the two most important parameters when determining whether a raw material is classified as “critical”. The EU sources 98% of rare earths from China, 98% of the demand for borate from Turkey, and 71% of platinum and an even higher proportion of platinum group metals such as iridium, rhodium, and ruthenium from South Africa.¹⁴ The EU is 75-100% dependent

on imports for most “critical raw materials”. Resource security can only be achieved if measures are taken to diversify the supply. Primarily, only those raw materials should be used for which there is no risk to supply, and those materials which can be recovered as part of the circular economy. The European Commission publishes a list of “critical raw materials” to design a better supply policy. This list is reviewed and updated every three years.¹⁵

The environmental impact of **organic solar cells** correlates strongly with the use of fullerene derivatives such as phenyl-C61-butyric acid methyl ester (PCBM) used as an absorber layer because this material is the one with the highest input of energy. The production of fullerenes¹⁶ is very energy-intensive because, amongst other things, during synthesis from graphite, only approximately 30% fullerenes can be obtained, with the remainder accumulating as soot.¹⁷ “Cradle-to-gate” LCAs of 15 different materials that can be used as active layer in organic solar cells showed that fullerenes and their derivatives have the highest CED.¹ Other materials such as polymers or “small molecules”¹⁸ perform better. A more detailed analysis showed that functionalised fullerenes have a higher CED than non-functionalised ones. Whilst pure C₆₀ fullerenes, which are produced by pyrolysis, have an energy consumption of 12.7 GJ/kg, energy consumption increases to 64.7 GJ/kg for PCBM because of additional steps during synthesis.¹⁷ The silver used as electrode material also shows up in LCAs as one of the main materials responsible for environmental impact in many categories.¹⁹ Especially the mining of silver, which is associated with sulphurous and acidic waste water, causes major environmental damage.

In the production of **dye-sensitized solar cells**, the use of glass as a substrate and platinum as an electrode is particularly problematic from an ecological point of view. LCAs have shown that glass substrates coated with indium tin oxide (ITO) are mainly responsible for dye solar cells’ high energy consumption and their environmental impact. In these applications, glass has the largest share by mass, with its production consuming lots of energy, whilst indium ranks high amongst “critical raw materials” affected by insecurity regarding supply.¹ A coating with fluorine-doped tin(IV) oxide shows less environmental impact. Replacing glass as a substrate with the plastic polyethylene terephthalate (PET) reduced environmental impact in an LCA in all categories examined, with the EPBT for this variant being the lowest with 0.73 years.²⁰ However, PET is not as temperature resistant as glass, necessitating the use of lower coating temperatures, which can result in poorer performance. Unlike glass, PET has the advantage that solar cells can be manufactured using cost-effective “roll-to-roll”

processes, producing solar cells that are light and flexible, which expands their fields of application.²¹ Dye-sensitized solar cells with organometallic dyes based on ruthenium show the best efficiency. However, this dye can only be produced through multistep reaction, using problematic solvents and expensive chromatographic purification processes.²² Consequently, this dye is responsible for a large share of the environmental impact in a “cradle-to-gate” assessment of dye solar cells.¹ Because of the very small quantity used, the dye is nevertheless less problematic in terms of environmental damage than, for example, the electrode material platinum which is one of the “critical raw materials” whose primary mining is associated with major environmental damage.¹¹

Instead of ruthenium-based dyes, many organic dyes that are abundant in nature can be used. These include for instance anthocyanins, which are responsible for the red, blue, and violet colours of many plants and fruits, as well as tannins, carotenoids, flavonoids or the green plant pigment chlorophyll.²² Environmental benefits of natural dyes include biodegradability, low manufacturing costs, and reduction in the use of precious metals and “critical raw materials”.¹¹ Nevertheless, even organic dyes are not *a priori* sustainable. The dye itself or the solvents required for its production can be toxic and/or expensive, and by-products can be environmental pollutants, too.¹¹ The organic dyes tested to date also perform relatively badly because of the low interaction between the dye and the semiconductor surface.

In **perovskite solar cells**, the materials that show the greatest environmental impact in LCAs are also the glass used, the gold used as electrode material, and other precious metals such as silver or platinum. In the manufacturing processes, deposition of the back contact and the electrolyte deposition as well as the preparation of the solar glass substrates are the areas with the greatest environmental impact.⁷ According to the LCAs conducted to date, the lead halide semiconductor layer of perovskite solar cells is not the material with the greatest concerns regarding toxicity for humans and the environment because of the small amounts used. The perovskite layer’s thickness is less than 500 nm, with the lead content of a perovskite solar cell being less than 1 g/m².²³ However, LCAs cannot directly assess the complex interactions between chemicals and biological systems.²⁴ The toxicity of lead should therefore not be underestimated, and any unintentional release prevented. This can be done primarily through suitable encapsulation material and specialised recycling systems. Because of its toxicity, the use of lead has already been limited or completely banned in many applications in the EU. The EU directive “Restriction of Hazardous Substances Directive” (RoHS)

sets the permitted concentration for lead at 0.1 percent by weight or 1,000 ppm.²⁵ The restriction applies to “homogeneous material”²⁶ in a product. Whether the lead-containing perovskite layer in the solar cells can be considered such homogeneous material is still a matter of debate. In any case, the directive does not cover ground-mounted PV systems, it only affects consumer products. If perovskite solar cells were to be used in e.g. portable electronic devices, and the lead-containing perovskite layer to be classified as homogeneous material, their use in consumer products would then be prohibited because the lead content would exceed 0.1 percent by weight. Moreover, the lead content could also be the reason for restrained consumer behaviour and influence the decision to purchase such products.¹ Since lead halides are watersoluble, there are concerns that these could leach out of damaged solar panels or into landfill and enter the environment and groundwater.²³ However, in order to assess potential harm to the environment, more data are necessary.²⁷

So far, only one single LCA has been carried out on **quantum dot solar cells**. This LCA has shown that, when compared with conventional thin-film solar cells based on cadmium telluride, quantum dot solar cells have less environmental impact because fewer materials are used. However, the energy required to produce the quantum dots (QDs) is higher than for alternative absorber materials.²⁸ Moreover, almost nothing is known about the behaviour, stability, and fate of QDs in the environment, nor about their metabolism in vertebrates or excretion routes.²⁹ However, the results of the few rodent and *in vitro* cell culture studies conducted so far suggest that the nanoscale QDs may pose an environmental and health risk under certain conditions.²⁹ When using QDs made of lead sulphide (PbS), there is a risk that toxic lead ions may be released.³⁰ In general, however, the risk of human exposure is considered to be low because of the very small quantities used.³¹

Significance of AdMs in the circular economy

At present, EPVs in the so-called end-of-life phase (EoL) do not yet play a role in terms of quantity because they have not reached marketability yet. It is therefore obvious that no recycling technologies have yet been adopted or newly developed for EPVs on a pilot or industrial scale. Once, and in line with silicon-based solar cells, a minimum EoL quantity³² for recycling has been established, recovery of the glass substrates on which EPVs are built, as well as recovery of the metals such as copper, silver, gold, indium, tin or aluminium could be of economic interest. The recovery of indium, tin or titanium, which are contained in the

transparent electrode or in the active layers of EPVs (see also³), will play a very important role in recycling in the near future, since the EU has classified these materials as “critical raw materials”.¹⁴ The greatest challenge in the recycling of solar cells is to separate composite materials so that secondary raw materials obtained from individual fractions can be recovered in the purest form and in the most energy-efficient way possible. In most cases, solar cells are hermetically encapsulated in plastic films made of ethylene-vinyl acetate copolymers (EVA) or in epoxy resins to protect the active layers from environmental exposure to e.g. oxygen or water (vapour) ingress in the long term. The separation process of this composite material is also called delamination. In the future, mechanical, chemical or thermal separation processes that are already applied to silicon-based solar cells could be adapted for EPVs.

Mechanical crushing processes, such as shredders, metal separators, screens or optical separation processes are used to separate the glass substrate, which in turn can be fed into flat glass recycling. During these processes, it is especially important to ensure that the recovered glass fractions are not excessively contaminated with metal residues (e.g. aluminium, lead, copper or silver), which can significantly disrupt the glass recycling process. Depending on the composition of the material and the level of contamination, the individual fractions obtained during mechanical separation can be further treated by chemical etching techniques. The metallic fractions can be fed into hydro- or pyrometallurgical processes either directly after the mechanical pretreatment or after further chemical treatment. The fine fractions or residues resulting from the separation processes are subjected to thermal treatment depending on the organic carbon content and heavy metal contents before the resulting solid combustion residues are deposited in so-called residual material landfill sites.

Delamination of the glass-plastic-metal composite can also be carried out by means of thermal processes. The organic components (plastic films, silicone adhesions, etc.) are either burnt under oxidative conditions or thermally recycled using pyrolysis (under oxygen depletion) to obtain pyrolysis gas. The remaining metallic or inorganic components can in turn be fed into metallurgical processes to recover metal alloys of different qualities. In the future, novel physical separation processes, such as so-called high-voltage fragmentation (HVF), could also be used on the composite materials. HVF has already been used to process the so-called black mass³³ of lithium-ion batteries, with the current collector foil made of aluminium being separated by pulsating voltage.³⁴ Compared with conventional mechanical separation technologies, HVF cur-

rently involves relatively high operating as well as investment costs because of the voltage required.³⁵ One promising, innovative, and cost-effective separation process is the physical separation of the composites using high-intensity light pulses that require little energy.³⁶

In summary, currently used recycling processes are very elaborate and costly, often using a combination of mechanical, chemical, and thermal processes, with the choice depending on economic and recycling efficiency. In the future, the recycling industry faces major challenges, especially regarding the recovery of “critical raw materials” as well as AdMs from EPVs, such as the transparent electrode made of ITO or fluorine-doped tin (IV) oxide, from the complex material composites. In terms of the circular economy, existing recycling processes must be adapted or new innovative processes must be developed. Another approach would be to pay attention to recyclable materials already during the design phase (also called ecodesign or “design for recycling”). For example, flexible, biodegradable and thus recyclable EPVs have already been developed.³⁷ Furthermore, secondary raw materials, such as “critical raw materials” recovered from old electrical devices, printed circuit boards of PCs or from other waste streams, could also be used more intensively in the production of solar cells.³⁸ With this in mind, in order to be able to guarantee a sustainable circular economy in the future, manufacturing costs and legal frameworks (extended manufacturer responsibility) will be of great importance, as will be a compromise between material quality, service life, and efficiency of a solar cell. A new mindset with regard to “sustainability by design” could also take place in that EPVs could be used more often in the future, since e.g. organic solar cells use relatively small quantities of “critical raw materials” when compared with conventional thin-film technologies (e.g. Cu(In,Ga)Se₂ or GaAs semiconductors) and silicon-based solar cells (Si wafers).

Recommendations for the development of EPVs with low environmental impact

Refining EPVs requires a compromise that takes into account the most suitable material in terms of sustainability, the highest attainable efficiency and service life, and economic efficiency. Only materials that are non-toxic, inexpensive, and sufficiently available in the long term should be selected. Moreover, they should be obtained from waste wherever possible and be reusable or recyclable.¹¹ The following measures in particular could help make EPVs more environmentally friendly and sustainable:

- Research into alternative electrode materials to replace rare and expensive materials such as gold, silver, and platinum, which are responsible for most environmental damage and impact.¹⁹
- “Critical raw materials” such as platinum, ruthenium or indium as well as complex, expensive, and complicated manufacturing processes should generally be avoided.¹¹
- Lead-containing semiconductor materials should be replaced to prevent environmental and health risks that cannot be quantified at present. Such replacements would also prevent possible negative consumer behaviour as well as restrictions because of potential legal regulations.¹
- Alternative encapsulating materials, for instance biodegradable plastics, should be developed to replace PET.¹⁹ However, because of their low resistance to environmental factors, these would currently only be suitable for products with a short service life.
- The “Green Chemistry” principle should be applied, especially with regard to the solvents used.¹
- Consideration should be given to the entire life cycle already at the design stage of a PV technology – from the manufacturing to the disposal phase (“sustainability by design”).¹⁹
- Recycling should already be considered at the design stage (“design for recycling”). Developing environmentally friendly processes to separate individual layers (delamination) without the use of problematic solvents is essential.²³

However, alongside measures in the field of research and development, the sustainability of EPVs can also be promoted through the development of appropriate political frameworks:

- Regulation of the end-of-life management by establishing a take-back system to increase material recovery, thereby reducing environmental impact. In this context, it is important to pay attention to the possible uses of EPVs, as treatment obligations in waste legislation may differ: e.g. EPVs in buildings must be disposed of differently than portable electronic devices. Extended manufacturer responsibility should be applied, but without generating a competitive advantage for other forms of power generation.

- Recovery, especially of lead and TiO₂, though currently not advantageous for economic reasons, would be welcomed for ecological reasons. Recycling the glass used makes sense from both an ecological and an economic point of view.¹
- The production of solar systems should be relocated to countries with high environmental standards (e.g. because of strict emission standards or high technological efficiency). Installation and operation should take place in countries with high solar irradiation to maximise environmental benefits of PV technology.¹⁹
- Specific regulations for nanomaterials or AdMs used may be needed if there is a risk of release into the environment.²³
- Although the importance of environmental sustainability of solar cell technologies is known to research, there is still a danger that this goal will be sacrificed for higher energy yields. It is worth promoting research that bridges the gap between basic research and economic feasibility. Environmental as well as social sustainability should be continuously reviewed and monitored to facilitate future developments in the sense of “sustainability by design”.⁴

Conclusion

EPVs offer new fields of application and can be more environmentally friendly and sustainable than conventional silicon-based PV systems because they use less amounts of materials and their manufacturing requires less energy. However, some EPV materials are problematic where both environmental protection and human health are concerned, and there are opportunities for optimisation in terms of sustainability. Since EPV technologies are only just evolving, the possibility of intervening through targeted research funding or regulation is still possible. It would therefore be desirable to find a compromise between highest efficiency, best stability, costeffectiveness, and environmental sustainability already early during research and development. In terms of a circular economy, recyclability should already be taken into account at the design stage in order to be able to recover valuable metals, “critical raw materials”, and materials such as glass and plastics.

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Owner: Austrian Academy of Sciences; legal person under public law (BGBl 569/1921 idF BGBl I 31/2018); Dr. Ignaz Seipel-Platz 2, A-1010 Vienna

Editor: Institute of Technology Assessment (ITA); Apostelgasse 23, A-1030 Vienna; www.oew.ac.at/ita

Mode of publication: The NanoTrust Dossiers are published irregularly and contain the research results of the Institute of Technology Assessment in the framework of its research project NanoTrust. The Dossiers are made available to the public exclusively via the Internet portal “epub.oew”: epub.oew.ac.at/ita/nanotrust-dossiers/

NanoTrust-Dossier Nr. 57en, February 2022:
epub.oew.ac.at/ita/nanotrust-dossiers/dossier057en.pdf

ISSN: 1998-7293

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