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INVITED FEATURE ARTICLE

Life cycle assessment of functional materials and devices: Opportunities, challenges, and current and future trends

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Abstract

Functional ceramics such as piezoelectrics, thermoelectrics, magnetic materials, ionic conductors, and semiconductors are opening new frontiers that underpin numerous aspects of modern life. This widespread usage comes with a responsibility to understand what impact their mass production has on the environment. Life-cycle assessment (LCA) is a tool employed for the identification of sustainable materials pathways through the consideration of environmental burdens of materials both during fabrication and as a final product. Although the LCA technique has been widely used for the evaluation of environmental impacts in numerous product supply chains, its application for environmental profiling of functional ceramics is now gaining attention. This paper presents a review of current developments in LCA, including existing and emerging applications with emphasis on the development and fabrication of functional materials and devices (FM&D). Selected published works on LCA of functional ceramics are discussed, highlighting the importance of adopting LCA at the design stage and/or at laboratory stage before expensive investments and resources are committed. Drawing from the extant literature, we show that the integration of environmental and sustainability principles into the overall process of FM&D manufacturing, in a way that anticipates foreseeable harmful consequences while identifying opportunities for improvement, can aid the timely communications of key findings to functional materials developers. This guides the orientation of research, development and deployment, and provides insights toward the prioritization of research activities while potentially averting unintended consequences. It is

Abbreviations: (H)LCA, (hybrid) life-cycle assessment; (T)EC, (tantalum) electrolytic capacitor; AP, acidification potential; c, cancer effects; CED, cumulative energy demand; DSSC, dye sensitized solar cells; EP, eutrophication potential; EPBP, energy payback period; ESB, erbia-stabilized bismuth; ESR, equivalent series resistance; ETP, ecotoxicity potential; FAETP, freshwater aquatic ecotoxicity potential; FSETP, freshwater sediment ecotoxicity potential; FTO, fluorine-doped tin oxide; GRI, Global Reporting Initiative; GWP, global warming potential; HTP, human toxicity potential; IO, input-output; IP, ionizing radiation; IPPC, Intergovernmental Panel on Climate Change; KNN, potassium sodium niobate; LCC, life-cycle costing; LCI, life-cycle inventory; LCSA, life-cycle sustainability assessment; MAETP, marine aquatic ecotoxicity potential; MLCC, multilayer ceramic capacitor; MSETP, marine sediment ecotoxicity potential; NBT, sodium bismuth titanate; nc, noncancer effects; ODP, ozone depletion potential; OSC, organic solar cell; PEG, polyethylene glycol; PM, particulate matter; POCP, photochemical ozone creation potential; PSC, perovskite solar cell; PV, photovoltaic; PZT, lead zirconate titanate; RDP, resource depletion potential; REACH, Registration, Evaluation, Authorisation and Restriction of Chemicals; RoHS, Restriction of Hazardous Substances Directive; SCEnATi, Supply Chain Environmental Analysis Tool-*intelligence*; SLCA, social life-cycle assessment; SOFC, solid oxide fuel cell; SSB, solid-state battery; TAETP, terrestrial ecotoxicity potential; TENG, triboelectric nanogenerator; WEEE, Waste Electrical and Electronic Equipment; X7R, “Temperature stable” ceramics, which fall into Class II of the Electronic Industrial Alliance materials.

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intended that the review presented will encourage the materials science community to engage with LCA to address important materials design, substitution, and optimization needs.

KEYWORDS

life cycle assessment, functional materials, sustainability

1 | INTRODUCTION

Functional materials have the capability of performing functions other than in a load-bearing capacity. Examples include piezoelectrics, thermoelectrics, magnetic materials, ionic conductors, and semiconductors. Their applications underpin many aspects of modern life through energy generation and storage, information and communications technology, multicomponent sensors, healthcare, military defence, and transportation.^{1–3} Functional materials and devices (FM&D) are continually being integrated into electronics and expected to operate in diverse conditions to meet the expectations of consumers.⁴ Accordingly, modern society has witnessed high growth and development through the discovery and applications of this unique set of materials.⁵ Although the global community acknowledges the need to implement sustainable systems,⁶ research and production of these materials continues without complete consideration of the associated environmental impacts.⁷ As the world's population continues to rise, the environmental burden of these materials will grow. The materials science and engineering community are therefore obliged to act on this challenge, not only because of its importance, but because they are in the best position in terms of knowledge and expertise. Advances in functional materials must therefore be augmented with sustainability principles such that products and services are developed with an optimal balance between quality of life and environmental burden. The pertinent question therefore becomes; “how can we ensure that new FM&D yield less environmental impact?”

To provide a genuine answer to the above question, one fundamental technique which all functional materials scientists must apply is life-cycle assessment (LCA). Since the turn of the century, LCA has been put into practice through implementation in world policy.⁸ LCA is a structured framework for the assessment and estimation of environmental impacts associated with the life cycle of a material, product, or service. It is a well-established computational technique used for identifying, quantifying, and assessing the associated environmental impacts throughout the entire value chain of an activity, product, or process.^{9,10} Through the adoption of LCA, environmental impacts can be taken into consideration in the design of a product, thereby: (a) identifying potential environmental hotspots^{11–14}; (b) comparing different features

of specific products or processes^{15–17}; (c) establishing credible procedures for environmental benchmarking^{18,19}; (d) optimizing the environmental impacts of products²⁰; (e) enhancing design policies for sustainable consumption and production^{10,21}; and (f) determining a baseline of information on an entire system for current or predicted practices.^{22–24}

This paper presents a review of current developments in LCA, including existing and emerging applications with a focus on the fabrication of FM&D. This is aimed at supporting decisions that are informed by environmental consideration in areas pertaining to product development and procurement, environmental policy decision making and final choices made by consumers. It is intended that the review presented will encourage the functional materials science community, not to view LCA as a tool borrowed from another discipline, but rather a method with which to engage to address design and optimization questions.

Different LCA methods are proposed and implemented throughout the literature. This review describes some of these techniques and their implementation within the spectrum of functional ceramics and related devices. An overview of relevant LCA methodologies is first presented in Section 2; data collection is discussed in Section 3, within which an exemplar LCA for the environmental assessment of multilayer ceramic capacitors (MLCCs) is outlined; Section 4 reviews the literature surrounding the application of LCA to pertinent FM&D, and the sustainability of these materials and devices is then discussed in Section 5. Section 6 describes the use of LCA in policy and environmental regulation and Section 7 outlines the limitation of the application of LCA in this area. Finally, important future work is outlined in Section 8.

The LCA studies reviewed in this manuscript are relevant to a range of FM&D; an industrial sector for which few such studies has been performed. The environmental impacts of energy generation and storage technologies are discussed, specifically solar cells, fuel cells, batteries, and triboelectric nanogenerators (TENGs) along with the environmental impact of lead free (in comparison with lead-based) piezoelectrics and multilayer ceramic (in comparison with Ta electrolytic) capacitors. The results of each LCA are not provided with the aim of comparison against each other, but as individual results to highlight their own environmental impacts within their functional abilities.

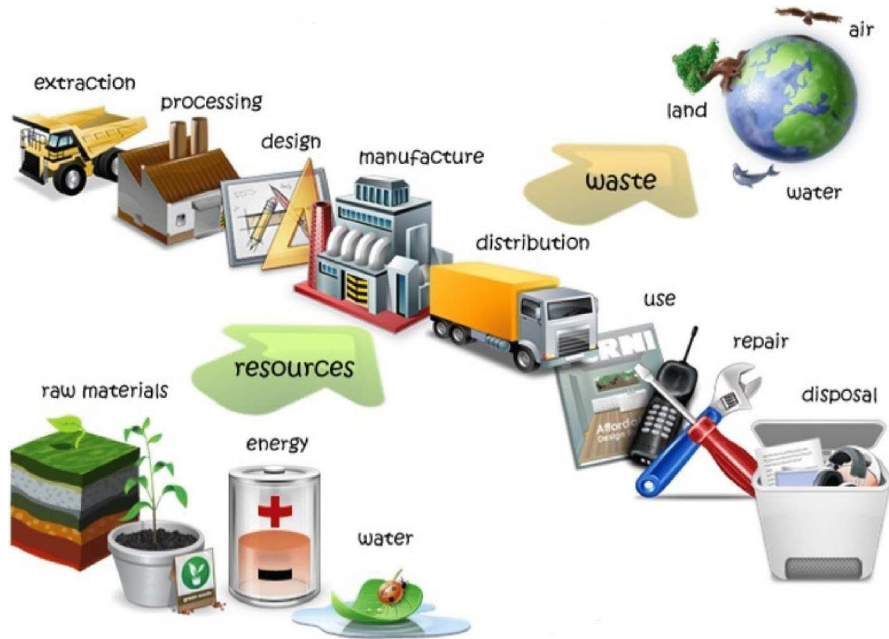


FIGURE 1 Illustration of the concept of life-cycle assessment. Figure is adapted from the sustainable graphic design blog²⁶

2 | WHAT IS LCA AND HOW IS IT IMPORTANT TO THE MATERIALS SCIENCE COMMUNITY?

As earlier highlighted, the application of functional materials has profoundly improved the quality of life across different parts of the globe. However, the products or systems upon which this improved quality of life lies also constitute huge environmental burden on the natural ecosystem. The materials and ceramics community are uniquely placed to transform the nature of such burdens. However, materials scientists and engineers lack the prerequisite skills to quantify the economic/environmental implications of their discoveries or technological breakthroughs. To lessen the environmental impact of material development, the community must be able to identify and evaluate the environmental impact of the material systems for which they are involved. To realize this, the 21st century ceramist must not only understand the technical performance of the materials but also the wider environmental impacts as well. To do this, an understanding of the technique of LCA and its application is pertinent. This assessment method is predicated upon two basic concepts. The first entails the consideration of a given product or material system of interest and mapping out all activities or processes that are associated with its fabrication, operation, and final disposal—the life cycle. The second concept is to take the list of life-cycle activities, while taking into consideration the associated environmental impact across the entire supply chain. These impacts stem from the

inflows from and outflows to the natural ecosystem that are caused by individual activities.²⁵

Consider the mobile phone's main stages of cradle-to-grave LCA and the resources that are used by the phone and the corresponding waste that resulted from it as depicted in Figure 1.²⁶ As shown, there is a huge supply chain required to manufacture the phone, starting from the raw materials mining and extraction, materials production and processing, design, manufacture, and continuing to distribution and usage. Once the phone reaches its end-of-life, some materials or components within it can be recovered for reuse, recycle, or eventual disposal. Each of the aforementioned stages of the LCA are based on a number of factors including raw material utilization, energy and water utilization, transportation, waste production, waste disposal, and its associated impact on air, water, land, and underground. The ability to track the environmental impact throughout the life span of the product (the phone in this example) is what LCA is all about.

In light of the above, for beginner materials scientists intending to employ LCA in anticipation of impact of their work, it is important to take into consideration a number of things for them to access the field of LCA with ease. For any successful LCA work to be carried out, the first most important step is to gain an understanding of the product, process, or activity for which the environmental profile is to be assessed. There are many readily available LCA software including SimaPro, Gabi, SCEnAT etc. Other LCA practitioners develop their own models based on Microsoft Excel

spreadsheets. Regardless of the software used, the LCA procedure is the same but the first most important step involves a deep understanding of the materials and energy inputs as well as other associated resources required for the fabrication of any given material system or product under consideration. This entails the construction of a bill of materials and energy inputs toward the entire fabrication process which is informed by the system boundary of the process/product under consideration. This bill of materials is derived either by primary sources where the data are supplied directly by the manufacturer or through secondary sources such as the use of Ecoinvent database and engineering heuristics. After full bill of quantity of materials have been completed, the next step is to establish how the outputs and the potential environmental impacts will be evaluated across different indicators. This requires an understanding and access to relevant database for which emissions intensity of different process or materials or products can be assessed. To gain an understanding of the LCA procedure, countless books^{27–29} and publications^{8,30–33} are available; however, in the section that follows, a detailed step-by-step procedure of the LCA procedure and key considerations is provided. It is intended that the steps will provide a guide to materials scientists who are new to LCA.

2.1 | LCA framework

2.1.1 | Key considerations in LCA

This comparative investigation of environmental impacts of products was first performed in the 1960–1970 and focused on resource consumption and emissions.²⁷ In the 1990s, the practice began to be standardized and the first journal papers on the subject were published. When considering the 21st century, the methodology was implemented throughout global policy.⁸ Guinee et al⁸ states that going forward, LCA must account for the three pillars of sustainability, namely people, planet, and profit or expressed another way societal, environmental, and economic impact.

ISO 14040:2006, Environmental management—LCA—Principles and framework describes the four phases of an LCA study as: (a) the goal and scope definition, where questions such as what, how, and why, pertaining to the LCA work are examined and where the systems boundaries and functional unit are established; (b) inventory analysis, in which input and output data of each process in the life cycle, as well as data related to impact categories, are systematically collected and integrated across the entire system; (c) impact assessment through the evaluation of the environmental effects, detailing LCA calculations, and results through classification and characterization for comparative analysis; and (d) interpretation of the inventory and impact assessment of results, from where environmental hotspots are identified.^{30,34,35} This procedure is outlined in Figure 2.

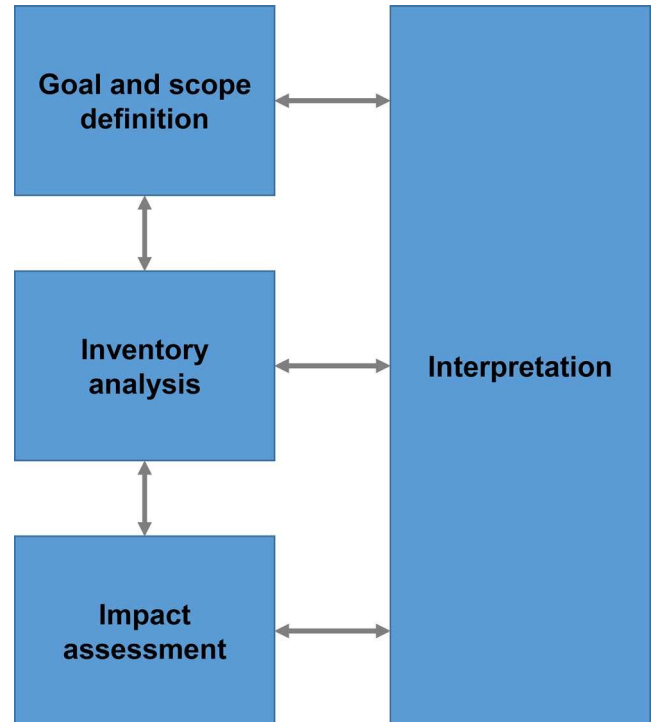


FIGURE 2 Outline of the life-cycle assessment process, adapted from ISO 14040:2006; the results of the inventory analysis and impact assessment must be assessed according to the requirements of the goal and scope definition through the interpretation phase³⁴

2.1.2 | Consideration for typical LCA of FM&D

For the specific case of LCA of FM&D, the overall assessment includes the following five main steps: (a) gaining an understanding of the materials technology under consideration in terms of raw material requirements, production, and fabrication routes processes; (b) system characterization (ie, establishing the systems boundary, functional unit, modular components, material composition, operational efficiencies etc.); (c) construction of the system inventory (eg, input requirements), supply chain information and embodied emissions, process flow, energy flow, material flow, and reference flow; (d) overall impact assessment and environmental profile evaluations across multiple environmental indicators; and (e) performance evaluation and analysis.

2.2 | Establishing the system boundary

The result of setting the goal and scope definition of the system is the establishment of a system boundary, thereby outlining the processes which are to be included in the analysis. This may include material use only or a whole device, the aim of the study must be defined through this system boundary.³⁴ An example of a system boundary is shown in Figure 3 for

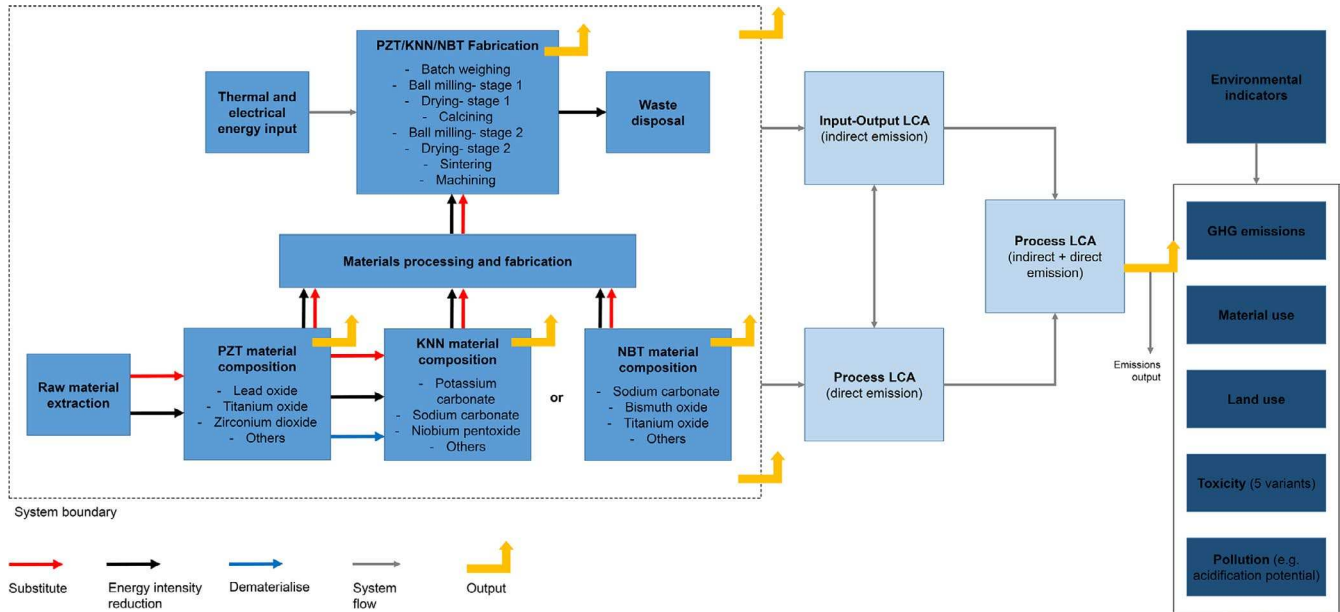


FIGURE 3 The system boundary considered in the hybrid life-cycle assessment (LCA) of lead zirconate titanate (PZT), sodium bismuth titanate (NBT), and potassium sodium niobate (KNN) materials for piezoelectric ceramic production. Substitutions, energy intensity reduction, dematerialization, and process emissions are identified through the arrows shown and major process steps for each material type are outlined^{7,36}

the production of lead zirconate titanate (PZT), sodium bismuth titanate (NBT), and potassium sodium niobate (KNN) piezoelectric ceramics.^{7,36} This system boundary models the extraction of raw materials, production and purification processes, electrical and thermal energy requirements for PZT, NBT, and KNN production, piezoelectric material fabrication, and waste disposal.^{7,36}

The system boundary can include the whole life cycle of the product or service that is cradle-to-grave/cradle, or only include specific stages of the life cycle such as the manufacturing phase that is cradle-to-gate.³⁶ This final system boundary depends on not only the goal and scope definition but also on the application, audience, and assumptions made. The system boundary can be refined based on data availability and cost constraints.³⁴

2.3 | Choice of functional unit

A functional unit is a quantified reference unit and its choice can frequently be decisive for the outcome of a specific LCA. Given that the functional unit describes and quantifies those properties of the product which must be present for the studied substitution to happen, it is therefore pertinent that the functional unit is chosen with diligence. Examples of such properties include the functionality, stability, appearance, ease of maintenance, and durability, and are in turn determined by the requirements of the market in which the product will be sold. Accordingly, a detailed procedure is chiefly important for such applications where the products or materials

for comparison differ in any of the aforementioned boundary properties.⁷ For any LCA work, the overall aim was to gain an understanding of the environmental profile of a given system of processes that deliver a defined function. The most essential quantity that defines the scope of an LCA study is, therefore, termed the functional unit.³⁰ This specifically defines the type and size of the product (or, more generally, some activity or even service), the life cycle of which is being assessed by quantitatively describing the function it delivers. A typical example of a functional unit may be the generation of “kg of material required in the production of a 100 kW-class solid oxide fuel cell (SOFC) stack at installed capacity.”

2.4 | LCA modelling techniques

Since its inception, the LCA process has been developed and is put into practice through implementation in policy throughout the world.⁸ The inventory analysis phase is known to be the most complicated, time-consuming, and expensive of the four LCA steps, consequently a wide range of techniques have been developed.³² In sections 2.4.1 to 2.4.3 three prominent LCA methodologies are outlined; the process-based LCA, input-output (IO) assessment and the hybrid LCA.

2.4.1 | Process-based LCA modelling technique

The process-based LCA modelling technique is often referred to as a bottom-up methodology, for the quantification

of energy consumption and environmental impacts, and involves adding the various energy outflows associated with the production processes of a product. When the process inputs and emissions intensities of environmental and sustainability indicators are known, the process LCA technique can be used to compute the environmental impact of the product or process under consideration. This traditional process-based methodology is labor-intensive concerning data collection, an attribute that does not lend itself well to prompt decision making. While this may produce an accurate result within the system boundary, inevitable data gaps from up and down stream in the supply chain lead to truncation errors of approximately 50%.^{32,33,37,38} The majority of reported LCAs adopts this technique for the evaluation of environmental impact of products.

2.4.2 | IO LCA modelling technique

To address the systems boundary limitations of the process-based modelling technique, the Leontief³⁹ application of environmental IO data to environmental analysis has been widely adopted, which aims to remove truncation errors by incorporating the entire supply chain into the LCA.³² IO modelling is a quantitative approach to detail how the products and services of economic sectors flow from one to another.⁴⁰ The environmental IO modelling method is performed by relating the IO tables to emission intensities. The result is the computation of the upstream, indirect emissions associated with the supply chain being incorporated into the study.^{7,41–44} While the IO methodology is faster than the process-based technique, it does not afford the same level of detail and can become quickly out of date as IO data are issued every 3–5 years.³² More importantly, the method suffers from a number of well-recognized limitations, including proportionality and homogeneity assumption, conversion of economic quantities into physical quantities and less specificity because of the aggregation of a range of activities in one sector.^{40,45–48}

2.4.3 | Hybrid LCA modelling technique

In most LCA studies, getting access to all data inputs necessary to conduct detailed analysis based on all of the areas identified in the goal and scope definition stage of the study, can be very challenging and time-consuming. For example, data including contributions from upstream processes, such as the use of imported equipment, special purpose machinery, transportation, telecommunications, research and development, and other related business services, which form part of the overall development of FM&D, may not be available. It is important not to ignore the impact of the contributions from such activities. As such, an LCA approach which combines both process-based and environmental IO LCA into

what is termed hybrid (H)LCA has been leveraged to produce LCA results that are more robust and complete. By combining the two methodologies into a HLCA approach, consistent allocation of impacts is achieved. Double counting is avoided but complex data manipulation is required.^{7,11,30,32}

In their review, Crawford et al.³¹ outline four different HLCA techniques, namely tiered, path exchange, matrix augmentation, and integrated. The tiered approach expands the system boundary by combining IO data and process coefficients. The path exchange method mathematically disaggregates an IO matrix which enables pathways to be identified and modified (the aggregation of which represents the full matrix). Matrix augmentation creates “sectors” of the economy through modification of the IO matrix and finally the integrated approach produces a single matrix of integrated process and IO data. These hybrid methodologies, while widely discussed in literature, have not yet been integrated into ISO 14040.³¹ A detailed review of work which has employed HLCA technique is provided by Crawford et al.³¹

Koh et al.¹² developed the Supply Chain Environmental Analysis Tool-*intelligence* (SCEnATi) to integrate the process and environmental IO LCA methodologies to form a consistent hybrid LCA framework through a five-step methodology. The software provides a supply chain map, carbon calculations, interventions to reduce the carbon associated with the supply chain, a performance evaluation of the supply chain compared to an industry benchmark, and finally informed decision making. Global companies have utilized the tool within their supply chains to reduce environmental impacts.¹²

Although authors such as Zamagni et al.⁴⁹ suggest caution with the use of HLCA, the augmentation of process-based LCA with environmental IO LCA ensures completeness of the analysis while taking into account the missing inputs from process-based LCA. Yang et al.⁵⁰ also argued that in certain circumstances, the hybrid LCA methodology may not produce more accurate results than the traditional process LCA technique, suggesting that the value of the hybrid process is based around whether the IO model used accurately represents the missing section of the supply chain. As the hybrid methodology involves the addition of IO models to produce sector data, to account for the missing sections of the supply chain, the final outcome will be larger than the process-based methodology. This introduces aggregation errors and the IO model must be as detailed as the process system boundary to achieve a meaningful result.⁵⁰

In their review, Crawford et al.³¹ state that, despite a 20-year research grounding, hybrid analysis can suffer from reduced uptake due to the use of inconsistent and unclear terminology and the complexity of the methodology, but its application has the ability to provide value within the LCA community. Overall, the hybrid methodology is employed

widely and has been shown to provide more accurate results when compared to a process LCA by widening the scope of the system boundary.⁷

3 | DATA COLLECTION

The increasing complexities of today's global supply chains, interacting with thousands of human activities, can rarely be gathered for individual projects due to the high cost and time restraints required for the collection of data. The foreground system, that is the process steps that are immediate to the modeller, is estimated to cover 1%-5% of the complete life cycle of a product and therefore this must be supplemented with a background system formed of generic data from available databases.⁵¹

Consequently, the remaining life-cycle inventory (LCI) data must be collated using secondary sources. The Ecoinvent database can be used to provide the background data in the form of environmental impact categories.⁵² Version 3.3 of the Ecoinvent database holds 746 environmental impacts, derived from 44 different methodologies.⁵³ The ISO standard defines “selection of impact categories and classification” and states that the impacts chosen should be of relevance to the study.³⁴ A number of different LCI methodologies are available. Dreyer et al⁵⁴ compare the methodologies of EDIP97, CML2001, and Eco-indicator 99. CML2001 and EDIP97 represent impacts at the midpoint, that is somewhere between the source and receptor, whereas Eco-indicator 99 represents impacts at the endpoint, that is the receptor. The land use impact category is represented in CML2001, but not in EDIP97, whereas EDIP97 models a waste category unlike CML2001. Due to the difference in modeling, it is not possible to directly compare all of the methodologies. As stated above, it is important that the chosen impact categories are relevant to the requirements of the LCA.⁵⁴ Currently, a universal list of impact categories does not exist but LCA professionals choose specific categories based on the scope of the study.^{7,55}

3.1 | Environmental indicators and emissions intensity

Some of the most commonly analysed environmental impacts with respect to FM&D are those from the CML 2001 methodology such as global warming potential (GWP 100a); acidification potential (AP); eutrophication potential (EP); ecotoxicity potential and human toxicity potential (HTP 100a).⁵⁶ Despite the differences in mid and endpoint impact categories, Buchgeister⁵⁷ concluded that more than one methodology (eg, eco-indicator 99, IMPACT 2002, and CML 2001) should be employed to produce a robust, high-quality

result. A sample of the different available indicators is outlined briefly below.

Global warming potential 100a quantifies climate change, that is the difference in the temperature of the earth due to the release of greenhouse gases through human activity. This model is based on the UN's Intergovernmental Panel on Climate Change (IPCC) factors with a time horizon of 100 years (other time horizons can also be assessed but this is the most common). Greenhouse gases and their effect on biodiversity, temperature, and climate phenomena are considered using this environmental impact.⁵⁸ GWP is measured in kg CO₂-equivalent (eq), which is used by the Kyoto Protocol as a means of providing a common scale on which to measure the emissions of different greenhouse gases; CO₂ has a GWP of 1 (the reference gas), whereas CH₄ has a GWP of 24.5.⁵⁹

Sulfur dioxide (SO₂) and other acidic gases form acid rain when they react with water in the atmosphere, also known as acid deposition. Usually, this rain falls far from the initial gas source causing damage to foreign ecosystems. The AP (expressed as kg SO₂-eq) assesses acidification caused by SO₂ and NO_x leading to ecosystem damage and biodiversity reduction.⁵⁸

Ecosystems are adversely affected by the build-up of nutrients which is referred to as eutrophication. It leads to the growth of plants like algae which reduces water quality and populations of animals. It is caused by the emission of ammonia, NO_x, nitrates, and phosphorus into both air and water. The EP can be measured as kg PO₄³⁻ equivalent or kg N-eq, depending on the model referenced.⁵⁸

The ecotoxicity category addresses the impact of toxic substances on marine, freshwater aquatic and terrestrial ecosystems and is given as kg 1,4-DB-eq of potentially disappeared fraction of species, depending on the model. These impact categories are: freshwater aquatic ecotoxicity potential (FAETP 100a), freshwater sediment ecotoxicity potential (FSETP 100a), marine aquatic ecotoxicity potential (MAETP 100a), marine sediment ecotoxicity potential (MSETP 100a), and terrestrial ecotoxicity potential (TAETP 100a). When certain substances, like heavy metals, are emitted they can have a negative effect on the ecosystem. The maximum tolerable concentration in water for ecosystems is used as the measurement of toxicity using the European Union's toxicity model.⁵⁸

The toxicity of a compound, and its possible dose, is used to calculate the HTP of a material. This index aims to calculate the likely harm of said material when it is released to the environment. The impact indicators used are cancer, diseases of the respiratory system, noncarcinogenic effects, and effects to ionizing radiation. As with ecotoxicity, the HTP is calculated as kg 1,4-DB-eq.⁵⁸

The Eco-indicator 99 methodology is a damage-oriented, endpoint methodology. Human health, ecosystem quality,

and resources are analysed in terms of a point (Pt) system, making it a useful model in the comparison of products.⁵⁸

A study by Genovese et al⁶⁰ used principal component analysis to assess the potential redundancies in the range of environmental indicators available to the modeller. The results showed that the climate change (GWP) indicator adequately represents the overall output of the 215 environmental indicators that were measured and therefore using any additional indicators could provide redundant information to the end user. This suggests that, within the scope of sustainability, the environmental pillar could be adequately represented by the associated GWP of the system under scrutiny. Due to the reliance of LCA to aid decision making, the quality, reliability, and robustness of the results are paramount to ensure that a reduction in environmental impact is achieved.

Overall, while the GWP indicator may be an adequate source of information to assess the environmental impacts of a product or service, it may not sufficiently address the requirements of the goal and scope and therefore the modeller must assess environmental impact categories by taking these requirements into account.

3.2 | Exemplar hybrid LCA—A MLCC

This section of the manuscript uses the four steps outlined in ISO 14040 (Figure 2) to provide a step-by-step approach to the implementation of a robust HLCA for X7R (“temperature stable” ceramics which fall into Class II of the Electronic Industries Alliance materials) MLCCs.¹

3.2.1 | Goal and scope definition

The aim of the HLCA must first be established by the modeller, for example; “to define and address the environmental hotspots within the supply chain as well as sustainability issues that are essential for the future development” of X7R MLCCs.¹ This aim provides information on what environmental impacts should be assessed during the hybrid LCA that is environmental and sustainability impacts, and considers the whole supply chain.

The functional unit of the product or service to be assessed lays the foundations for the HLCA as it determines the

scale on which all calculations will be made.³⁰ For FM&D, once the underpinning mechanisms that govern the device are known, this will likely lead the modeller to an appropriate functional unit. For this example, the functional unit of a 1 kg batch of X7R MLCCs will be applied.¹

The system boundary should align with the aim and functional unit assigned to the HLCA and can be developed in line with data and cost limitations.³⁶ With respect to the HLCA of a 1 kg batch of X7R MLCCs, this can include raw material extraction, primary material production, device production, the use phase, and end-of-life; all energy requirements throughout this supply chain must also be accounted for.

3.2.2 | Inventory analysis

To complete the bottom-up process LCA step, the material and energy inputs and outputs, relevant to the system boundary must be obtained, this is known as the LCI. An X7R MLCC requires a barium titanate dielectric, a nickel paste internal electrode, a copper paste external electrode, and nickel and tin terminations¹; the total amounts and costs of these materials should be obtained. Furthermore, the electrical and thermal energy requirements of each processing step must be calculated in kWh and MJ, respectively. For the production of an X7R MLCC, this includes (but is not limited to) milling, drying, tapecasting, pressing and sintering.¹ If the respective kWh and MJ requirements of each process step are not known, they can be simply calculated using Equations 1 and 2¹; where E represents the electrical energy requirement (kWh), P represents the power requirement of the equipment (W), and t represents time (s), Q represents the thermal energy requirement (J), C_p represents the specific heat capacity of the material in the process ($\text{J kg}^{-1} \text{K}^{-1}$), m represents the mass of the material in the process, and finally ΔT represents the change in temperature during the process (K).³⁶ An example of this calculation is shown in Table 1 relating to four processes required in the manufacture of an X7R MLCC.¹

$$E = P \cdot t \quad (1)$$

$$Q = C_p \cdot m \cdot \Delta T \quad (2)$$

TABLE 1 A selection of the process steps, performed in a laboratory, for the production of a 1 kg batch of X7R MLCCs and the associated power (W), time (s), temperature (K), and specific heat capacity of the material (J/kg K) to determine the electrical and thermal energy requirements of the production of a 1 kg batch of MLCCs according to Equations 1 and 2¹

Process	Power (W)	Time (s)	Temp (K)	Electrical energy requirement (kWh)	Specific heat capacity ($\text{J kg}^{-1} \text{K}^{-1}$)	Mass	Thermal energy requirement (kJ)
Milling	1100	3600		1.10			
Drying	1500	43 000	350	18.00	430	0.75	114
Tapecasting	4600	1800		2.30			
Sintering	270	7200	870	4.10	430	0.75	282

The necessary impact categories, aligned to the aim and system boundary identified in Section 3.1 should then be assigned. Although the GWP has been found to be the most useful environmental impact category, additional impacts should be chosen according to the requirements of the stakeholders.⁶⁰ The chosen impact categories can be attributed to each process input using the Ecoinvent database according to Equation 3; where A_p signifies the supply chain inputs (i), n denotes the total number of process inputs (i) and E_p represents the emissions intensity of the environmental indicators.⁷ The material requirements for the production of barium titanate are shown in Table 2 with the associated mass, GWP and resulting impact of each material.

$$\text{Process LCA} = \sum_{i=1}^n A_{p(i)} \cdot E_{p(i)} \quad (3)$$

Unfortunately, Ecoinvent does not hold a complete dataset, and so may not include all of the necessary data requirements to complete the process-based LCA. To overcome this, secondary sources can be accessed; mass flow calculations or stoichiometry can be used,⁶¹ published literature can be referenced and similar materials can be substituted according to their chemical characteristics and functional parallels.^{7,61}

As described in Section 2.4.3, the HLCA process allows the system boundary of a process LCA to be expanded by applying the environmental IO-LCA methodology alongside it. The SCEnATi decision support tool can be used to complete this step. SCEnATi completes the hybrid LCA calculation shown in Equation 4. The process inventory environmental extension matrix is represented by E_p and the multi-regional IO (MRIO) environmental extension matrix, for the applied environmental indicator(s) is denoted by E_{io} . A_p signifies the square

TABLE 2 Life-cycle inventory (LCI), including the mass (kg) required for chosen functional unit (1 kg batch of X7R MLCCs), global warming potential (GWP 100a) of the reference product and final impact (kg CO₂-eq) of the material according to the requirements of Equation 3¹

Material	Mass (kg)	GWP 100a (CO ₂ -eq)	Impact (kg CO ₂ -eq)
BaCO ₃	0.64	1.23	0.79
TiO ₂	0.26	7.93	2.06
Borosilicate	0.02	0.44	0.01
Solvent (methyl ethyl ketone)	0.36	1.76	0.63
Dispersant (Hypermer KD1)	0.02	3.70	0.07
Plasticiser (PEG 400)	0.05	1.88	0.09
Binder (Butvar)	0.10	2.07	0.21
Dy ₂ O ₃	0.02	16.61	0.33

Abbreviations: GWP, global warming potential; MLCC, multilayer ceramic capacitor; PEG, polyethylene glycol.

matrix representation for process LCA inventory; A_{io} represents the IO technology coefficient matrix; I is the identity matrix, and finally, the $\begin{bmatrix} y \\ 0 \end{bmatrix}$ functional unit column matrix.

$$\text{Hybrid LCA} = \begin{bmatrix} E_p & 0 \\ 0 & E_{io} \end{bmatrix} \begin{bmatrix} A_p & -C_d \\ -C_u & I - A_{io} \end{bmatrix}^{-1} \begin{bmatrix} y \\ 0 \end{bmatrix} \quad (4)$$

Ecoinvent holds a dataset for the cumulative energy demand which is also known as the material embodied energy. This impact category describes the primary energy demand required for the extraction of embodied energy of natural resources which are yet to be changed into practical energy such as gas or electricity.^{7,9} The measure is expressed in MJ-eq, and is equal to the summation of the untransformed energy sources such as fossil fuels, nuclear, solar, wind, and geothermal energy as shown in Table 3.⁶²

3.2.3 | Impact assessment

The results provided by the process and HLCA can be assessed in a number of ways. To assess the impact of each of the chosen environmental impact categories, the results can be normalized to provide an absolute indicator of 100% for each impact category.³⁶ The relative impact of each component can then be addressed, this is shown in Figure 4.

If the production steps are broken down according to Table 1, using Equations 1 and 2, the overall impact of the individual processing steps can be evaluated. An example of this is shown in Figure 5 for the thermal energy distribution of a 1kg batch of X7R MLCC. It can be seen that the drying, sintering, and calcination phases of the manufacturing process have the highest impact on the total thermal energy requirement. Mitigation strategies that may be employed in industry to reduce this impact is the use of sintering aids and low-temperature processing technologies, such as cold sintering.¹ This process can be repeated for the electrical energy distribution and the impact of each materials material embedded energy distribution can also be broken down to this level for analysis.

Finally, the primary energy demand, that is the electrical, thermal, and material embedded energy, can be compared (as described in Table 3). This allows the modeller to assess the potential mitigation strategies to reduce the impact of processing steps during component manufacture. The toxicological impacts can also be compared due to their similar unit measurement (kg 1,4-DB-eq). This information can be supported by the use of additional LCI methodologies, for example the Eco-Indicator 99 or ReCiPe 2008 datasets.^{1,62} The analysis of two LCI methodologies allows for further assessment of the impacts though they

TABLE 3 Equivalent energy demand for both electricity and gas in MJ-eq based on data from Ecoinvent.⁶² So for the case of electrical energy consumption, this implies that 1 kWh is equivalent to 11.84 MJ-eq and 1 MJ of thermal energy is equivalent to 0.44 MJ-eq

Untransformed energy sources	Cumulative energy demand (CED) as a function of electrical energy (MJ-eq)	Cumulative energy demand as a function of Gas (thermal energy) (MJ-eq)
Biomass	0.51	0.0002
Fossil	7.71	0.44
Geothermal	0.00	0.000
Nuclear	3.25	0.001
Primary forest	0.001	1.34E-06
Solar	0.02	1.30E-07
Water	0.10	0.001
Wind	0.24	5.40E-05
Total (CED)	11.84	0.44

cannot be directly compared.⁵⁷ Finally, the results of the environmental IO analysis, provided by the SCEnATi decision support tool, can be analysed which provides information to the modeller regarding the impact of the product in the expanded system boundary through HLCA. The data relating to this exemplar case for these four additional analysis styles outlined here are shown and discussed in more detail in Section 4.3; Figure 10.

3.2.4 | Interpretation

ISO 14040:2006 defines the interpretation phase of the LCA as the process of evaluating the findings of the inventory analysis and impact assessment in accordance with the goal and scope definition.³⁴ In practice this provides the discussion and ultimate conclusion to an investigation through which the overall impact of a material, process, or product can be determined.

With respect to the environmental impacts of a 1 kg batch of X7R MLCCs, Figure 4 clearly shows that it is the

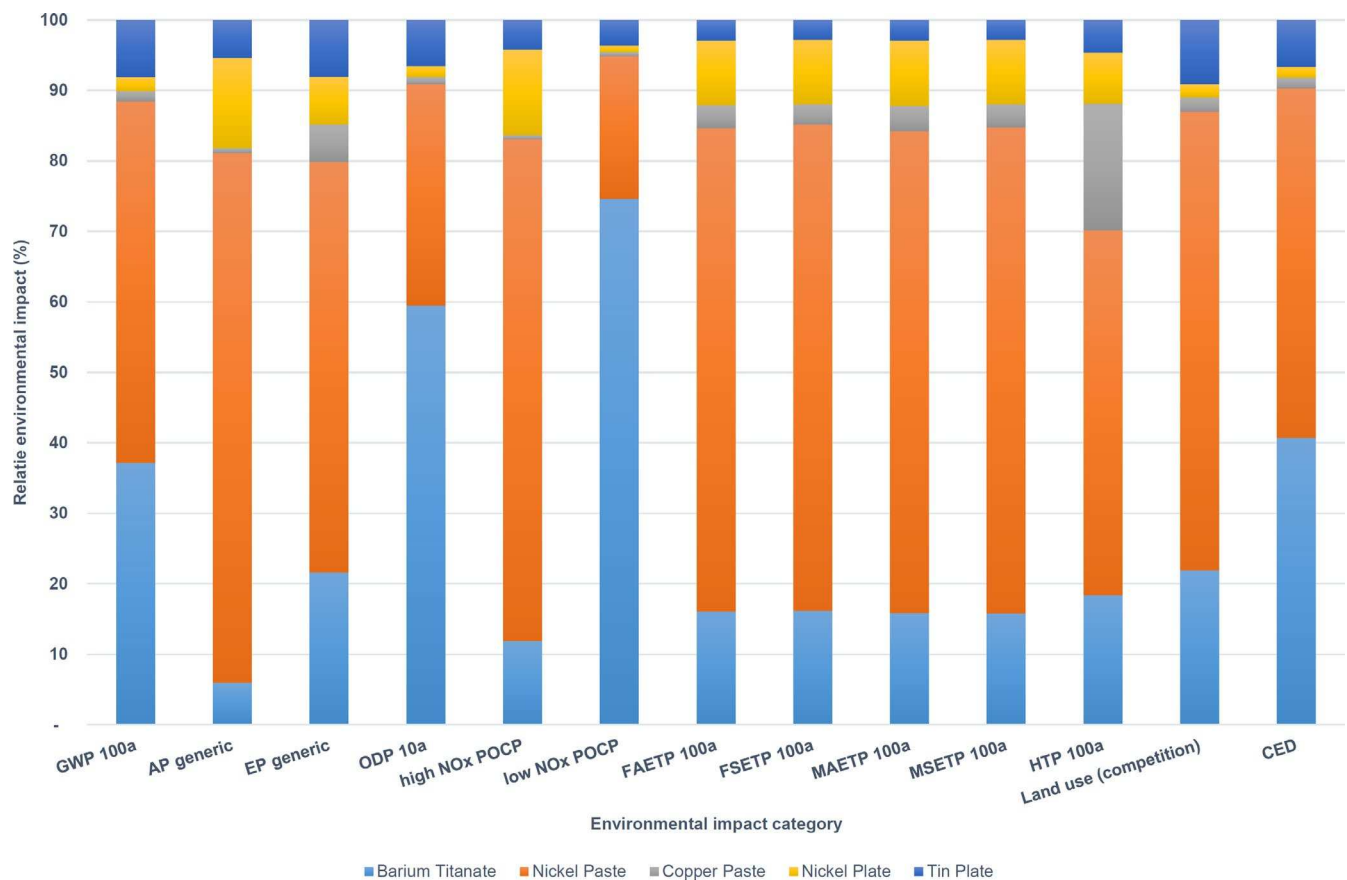


FIGURE 4 The percentage contribution of each X7R multilayer ceramic capacitor manufacturing component of the environmental impact categories investigated; global warming potential (GWP 100a); acidification potential (AP generic); eutrophication potential (EP generic); ozone depletion potential (ODP 10a); high NO_x photochemical ozone creation potential (POCP); low NO_x POCP; freshwater aquatic ecotoxicity (FAETP 100a); freshwater sediment ecotoxicity (FSETP 100a); marine aquatic ecotoxicity (MAETP 100a); marine sediment ecotoxicity (MSETP100a); human toxicity potential (HTP 100a); land use (competition) and cumulative energy demand (CED)¹

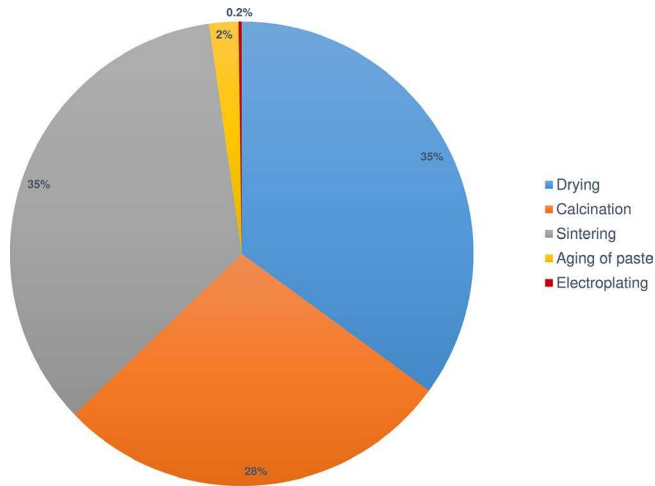


FIGURE 5 Thermal energy distribution of the production of a 1 kg batch of X7R multilayer ceramic capacitors (MLCCs); all production steps requiring thermal energy input are included: drying, calcination, sintering, aging, and electroplating¹

use of nickel paste in the structure that results in the highest impact, consequently it can be determined that research into reducing this specific impact should be explored. Furthermore, as it is the drying, sintering, and calcining steps in the production process that leads to the highest impact, effort should be directed at these processes to make the largest savings when reducing the environmental impact of the product.¹

4 | APPLICATION OF LCA TO FUNCTIONAL CERAMICS AND RELATED DEVICES

The available published literature relating to the LCA of FM&D is widespread for components such as photovoltaic (PV) solar cells and batteries.^{63–68} This section reviews recently published literature pertaining to lesser studied areas, to highlight their importance for future industrial operations. The component level LCAs of piezoelectric materials, third-generation solar cells, capacitors, SOFCs, TENGs, and solid-state batteries (SSBs) are outlined; a material level LCA relating to the use of lead-based piezoelectric materials is discussed and finally the use of critical materials in functional devices is touched on.

4.1 | Piezoelectric ceramics

Worldwide policy initiatives and legislation, such as the EU directives on Waste Electrical and Electronic Equipment (WEEE) and Restriction of Hazardous Substance (RoHS), have called for the prohibition of lead in many electronic

components and devices due to its toxicity.³⁶ For the particular case of piezoelectric ceramics, this call has reinvigorated the race to develop substitutes for lead PZT based mainly on KNN and NBT. Although criteria for exemption with RoHS recognizes the consideration of life-cycle impacts of alternative materials, little thought was given to the importance of tracking the overall environmental impact of these new materials. Such importance was demonstrated by Ibn-Mohammed et al,^{7,36} who generated debate and discussion among ceramists regarding the overall environmental viability of lead-free materials, given the surprising conclusion that KNN is not intrinsically greener than PZT.

The study established that KNN is environmentally worse than PZT with respect to climate change and ecotoxicity due to the presence of the niobium pentoxide. The mining and milling, through hydro- and pyro-metallurgical processing, to refining niobium has significant adverse impacts on air quality, surface and groundwater quality, and the land.^{7,69} During the mining and production of niobium (which is detailed in Figure 6), heavy metals and radioactive metals leak into water bodies as there is a need to dig through several types of radioactive rock to reach the niobium deposit.^{7,69} Essentially, the damage is already done at the beginning of its life cycle.

Given the above findings through LCA, there is a tendency to investigate NBT as the solution to achieving an environmentally green lead-free piezoelectric material. This prompted further LCA work by Ibn-Mohammed et al,³⁶ where it was concluded that the lower energy consumed by NBT during synthesis results in a lower overall environmental profile, with respect to the primary energy consumption and toxicological impact, when compared to both PZT and KNN. This information is shown in Figure 7A which provides a comparison of the primary energy requirements of NBT, PZT, and KNN with respect to the thermal energy, electrical energy and material embedded energy of each material type. It can clearly be seen that the energy requirements of KNN are much higher than the NBT and PZT alternatives in line with the applied functional unit.³⁶

Figure 7B compares the toxicological footprint of each material type with respect to the HTP (100a), FAETP (100a), FSETP (100a), MAETP (100a), and marine sediment ecotoxicity (MSETP 100a); all of which are explained in more detail in Section 3.1. Again, KNN clearly demonstrates a much higher toxicological impact when compared to NBT and PZT. While the toxicological impacts of the NBT component materials are higher than those of PZT, there is a higher toxicological impact relating to the electrical energy consumption in PZT manufacturing that leads to an overall higher PZT result.³⁶

However, bismuth and its oxide are mainly the by-product of lead smelting, and the comparison of NBT and PZT indicates that the environmental profile of bismuth oxide surpasses that of lead oxide across several key indicators, especially climate change, due to additional processing and

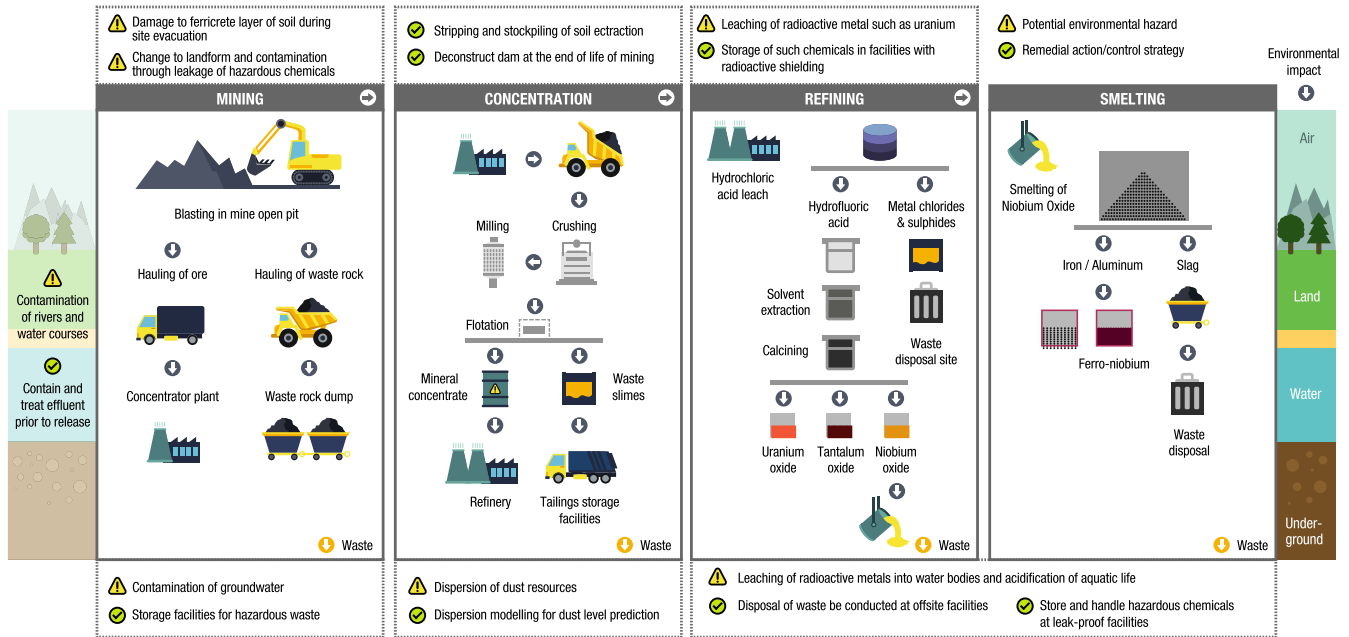


FIGURE 6 Schematic of the extraction of niobium from its ore, the most important hazards are indicated by the danger icon, causing significant adverse effect on air quality, water quality and the land. Potential remedial action/strategies for their control are highlighted by the solution icon⁶⁹

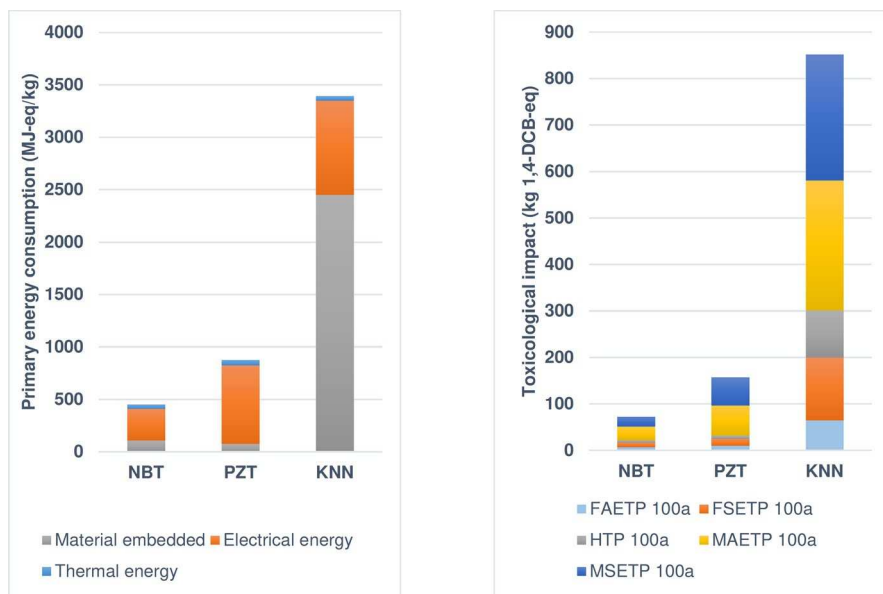


FIGURE 7 Comparison of overall environmental profile of lead-based (lead zirconate titanate [PZT]) and lead-free (potassium sodium niobate [KNN] and sodium bismuth titanate [NBT]) piezoelectric functional ceramics. A, Primary energy demand, (B) toxicological footprint: human toxicity potential (HTP 100a); freshwater aquatic ecotoxicity potential (FAETP 100a); freshwater sediment ecotoxicity potential (FSETP 100a); marine aquatic ecotoxicity potential (MAETP 100a); marine sediment ecotoxicity (MSETP 100a)³⁶

refining steps which pose extra challenges in metallurgical recovery. Furthermore, bismuth compares unfavorably with lead due to its higher energy cost for recycling. The fact that roughly 90%-95% of bismuth is derived as a by-product of lead smelting constitutes a major concern for future upscaling.

These findings have posed several important questions including: (a) should lead-free piezo research continue considering the great deal of research efforts, heavy funding, and investment that have already been put in? (b) How will LCA

shape the decision-making mechanism of policymakers and regulators? (c) How will the outcomes of research efforts and policy initiatives be received by the society (ie, end users) given the strategic importance of piezoelectric materials in different technologies? (d) What is the overall future of lead-free piezoelectric research? The latest study concluded that the context in which a piezoelectric material is used must constitute a major consideration when its potential risks and challenges are reviewed.

4.2 | Solar cells

Organic solar cells (OSC), utilize materials of low cost in the active layer and substrate production, require a low level of energy input and provide the potential to easily scale up for industry manufacturing but have been hindered by reduced stability, low limits of efficiency, and poor electron-hole pair and charge carrier transport.⁶⁶ A study by García-Valverde et al⁶⁶ compared the LCA result of an OSC manufactured in a laboratory to existing PV technologies produced in an industrial setting. In total, the embedded energy of the OSC was found to be 2800.79 MJ/m², compared to a range of industrially available technologies as high as 7771.95 MJ/m² for a thin film-based technology and as low as 720 MJ/m² for a dye synthesized PV technology. The embedded energy use in relation to the manufacturing process of the OSC was predominantly affected by the maintenance of the N₂ atmosphere. The highest percentage contribution of the materials to embedded energy is attributed the use of indium tin oxide.⁶⁶

TiO₂ semiconductors are utilized in dye-sensitized solar cells (DSSCs) along with fluorine-doped tin oxide (FTO) substrates; this technology functions through the capture of photons by a photosensitizer which is absorbed on the anode.⁷⁰ Parisi et al⁷¹ published a cradle-to-grate LCA of DSSCs across the component synthesis, module fabrication and roof-top operation using three different dyes. The results of the analysis relating to module fabrication show that the FTO substrate provides a high-percentage contribution to each of the 17 environmental impact categories studied, regardless of dye type. The authors conclude that the energy consumption relating to the module support (ie, FTO) could be reduced by 35% if the material was changed to a polymeric substance.⁷¹

Novel perovskite solar cells (PSCs) have been tipped to be the “third-generation solar cells” in the race to produce economically viable and environmentally friendly renewable energy technologies.⁷⁰ With commercialization on the horizon, the environmental impacts of these materials are under scrutiny.

An LCA study by Gong et al⁶⁷ presented the environmental impacts of two PSC types over 16 impact categories. This comparative evaluation of a TiO₂ module with a ZnO module found that, over the two predominant impact categories (primary energy consumption and carbon footprint), the TiO₂ module presented the highest impact. Predominantly, this was affected by the use of gold in the structure and the sintering process. The impact of ZnO module was mainly affected by the use of the indium tin oxide-coated glass in the structure and the cathode evaporation process.⁶⁷ Indium has been identified by the EU as a critical raw material, and therefore its continued use in a

number of these solar cell structures may hinder the technology's development.⁷²

Zhang et al⁷³ compared the environmental impacts of five different material structures and work by Ibn-Mohammed et al⁷⁰ details the comparison of two of these structures using the HLCA methodology. Ibn-Mohammed et al⁷⁰ outline a methodologically robust life-cycle supply chain assessment for a MAPbX₃-based module (A) and a CsFAPbX₃-based module (B) which is compared to that of current (PV) technologies. Their results found that, not only are the novel PSC structures more environmentally sound, but they also have a shorter energy payback period (EPBP) when compared to available PV technologies. This is shown in Figure 8.

This reduction in the EPBP was found to be due to a reduction in the energy intensive processes required for PSC manufacturing as silicon and rare earth element processing is eliminated.⁷⁰

The comparative assessments made by Zhang et al⁷³ show that the MAPbI₃ and FAPbI₃ PSC structures have higher environmental impacts when compared to the remaining structures that were analyzed, namely MASnI_{3-x}Br_x, CsPbBr₃, and MAPbI₂Cl. This difference was attributed to the organic solvent requirements for each device. Overall, it was found that the use of gold leads to the highest environmental impact; aluminum or silver substitution in this case was found to reduce the environmental impact further.⁷³

To conclude, the movement to PSC technologies for the third-generation solar cell will increase the sustainability of the devices as both environmental and cost savings are made when compared to commercially available PV alternatives. In the case of PSCs, the use of precious metals in their structure has been found to relate to the highest environmental impact. With respect to other solar cell technologies, the use of oxides such as indium tin oxide and FTO have been found to cause the highest environmental impacts.

4.3 | High-volumetric efficiency capacitors

A wide range of capacitor types, for example, electrolytic capacitors (ECs), super capacitors, and multilayer capacitors are used in modern technologies such as communication devices, energy generation, and healthcare; and while the technical features of such devices are well documented in published literature, there is a shortage of work pertaining to their environmental impacts.¹ Alaviitala et al⁷⁴ explored the impact of using engineered nanomaterials for power capacitors in place of conventional materials as nanomaterial popularity increases due to increased functionality, size, cost, transport, and maintenance reduction. The work found that the use of the nano SiO₂ reduces the overall environmental impacts by approximately 20% for the most pertinent impact categories, although ozone depletion and terrestrial ecotoxicity were found to increase.

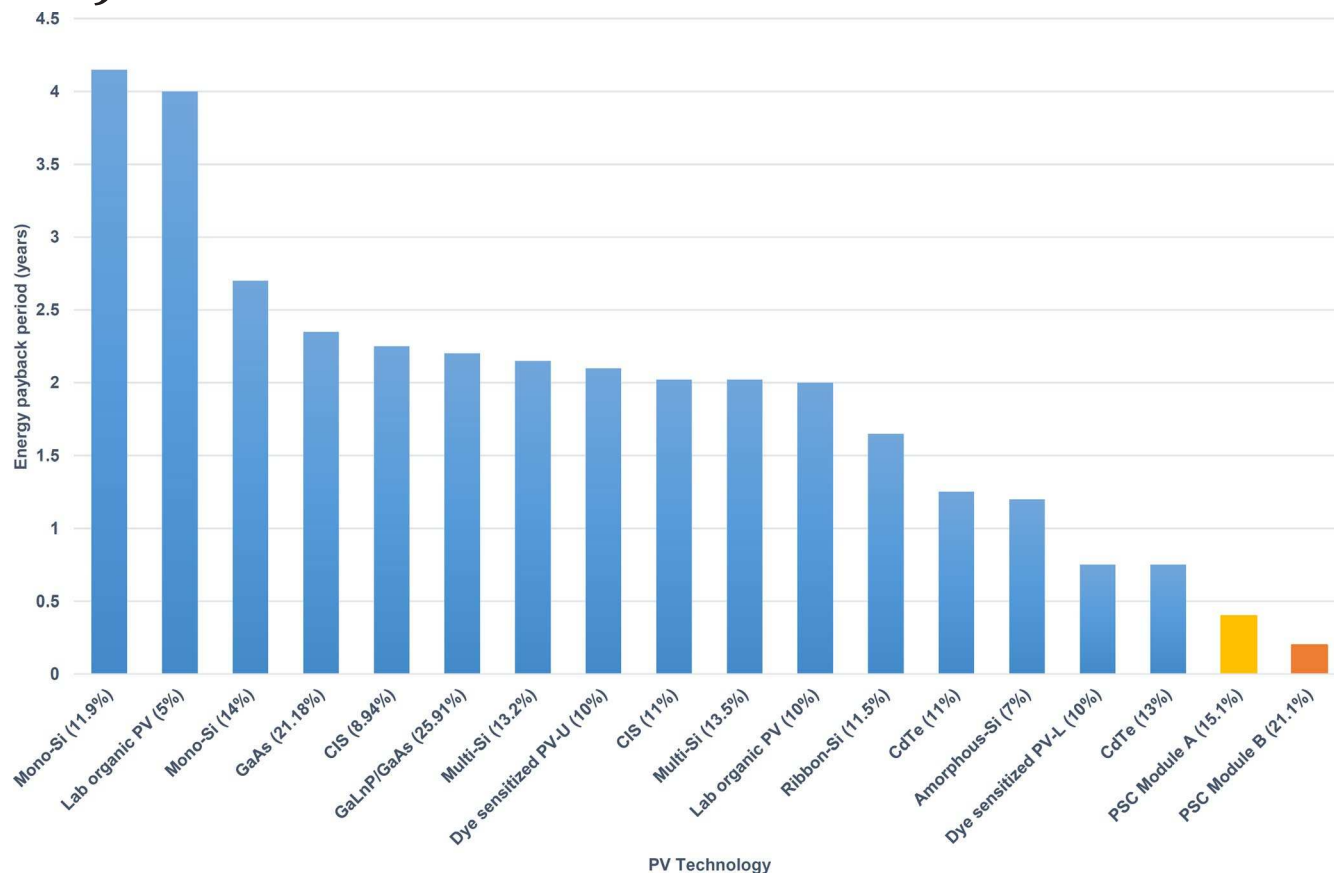


FIGURE 8 Comparison of the energy payback period, in years, of available photovoltaic (PV) technologies with two perovskite solar cell (PSC) modules⁷⁰

Work presented by Smith et al¹ is the first comparative hybrid LCA to determine whether or not the industrial trend in moving away from the use of Tantalum ECs (TECs) to functionally similar MLCCs is environmentally sound. Figure 9 describes the different properties of these and similar capacitor types to demonstrate the trend in moving toward MLCCs for current and future applications.

The development of large capacitance MLCCs, as shown in Figure 9A,^{75–81} aids the replacement of ECs, along with the higher voltage range of MLCCs when compared to ECs (Figure 9B,^{77–79,81–85}). The lower the equivalent series resistance (ESR), as shown in Figure 9C,^{77,79,86,87} the better the ripple voltage can be maintained at lower levels which also improves the properties of MLCCs over other capacitor types.

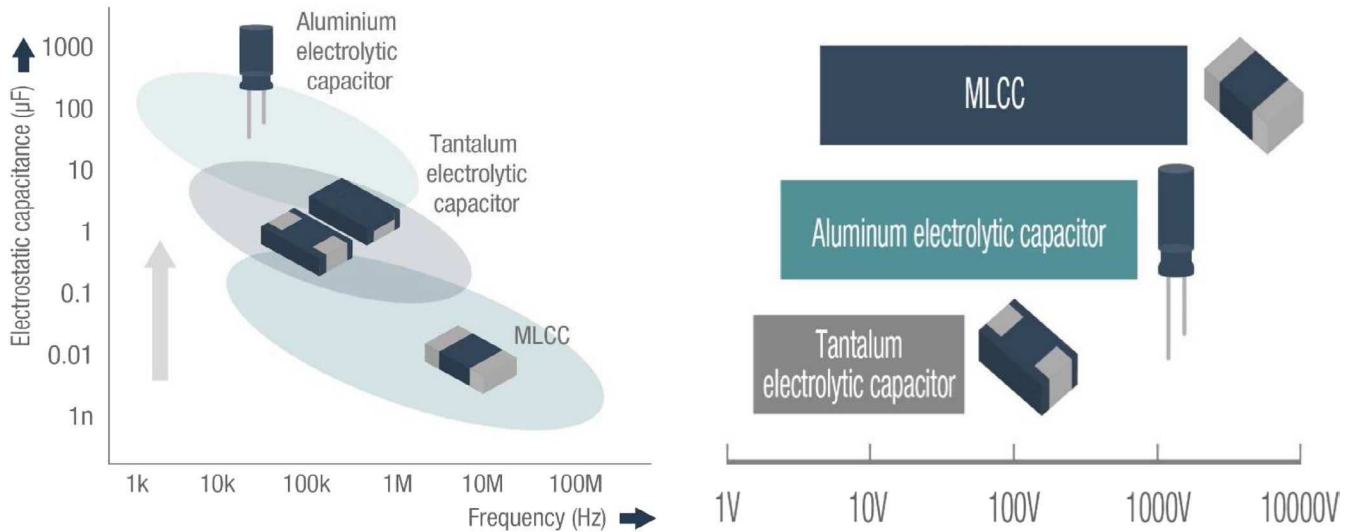
The system boundary incorporates the full life cycle of the capacitor and the chosen functional unit is based on the production of a 1 kg batch of each capacitor type. For all of the 13 environmental impacts measured, over 85% of the environmental impact for TECs can be attributed to the use of tantalum. The mining process for the extraction of tantalum is very energy-intensive requiring blasting, crushing, smelting, and also separation from other ores such as niobium. This analysis clearly points to the need to improve the

energy efficiency of tantalum mining and extraction, if the environmental profile of TECs is to be reduced.

The highest environmental impact within the MLCC manufacturing process is caused by the use of the nickel paste electrode and efforts should be made to reduce or replace the use of nickel. This, however, may not be technologically feasible since there are few alternative electrode types which have an intrinsically low-environmental profile. A comparison of the primary energy consumption for each capacitor type is shown in Figure 10. The largest difference can be seen in the material-embedded energy impact where the impact for TECs (4192 MJ-eq) is almost 20 times that of MLCCs (214 MJ-eq). Comparatively, the higher electrical energy requirements for the fabrication of MLCCs (5353 MJ-eq compared to only 2666 MJ-eq for TECs), does not outweigh the total primary energy demand of TECs at 6862 MJ-eq (compared to 5567 MJ-eq for MLCCs).¹

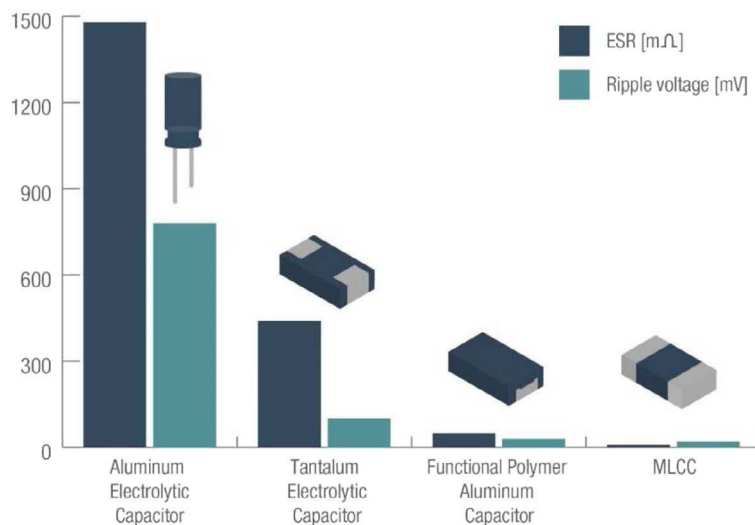
4.4 | Solid oxide fuel cells

Solid oxide fuel cells use electrochemical reactions to convert a fuel to energy. Energy generation through SOFCs is more efficient than the long-established combustion process as their efficiency is not constrained by the confines of the



(A) Frequency band and range of ECs and MLCCs

(B) Rated voltage range of ECs and MLCCs



(c) Relationship between the equivalent series resistance (ESR) and ripple voltage of ECs, polymer capacitors and MLCCs

FIGURE 9 Comparison of the frequency band and capacitance range of aluminum electrolytic capacitors (ECs), tantalum ECs, and MLCCs^{75–81}; (B) The rated voltage range of aluminum ECs, tantalum ECs and multilayer ceramic capacitors (MLCCs)^{77–79,81–85}; (C) the relationship between the equivalent series resistance (ESR) and ripple voltages of ECs, polymer capacitors, and MLCCs^{77,79,86,87}

Carnot cycle of a heat engine.⁸⁸ Furthermore, SOFCs can lead to reductions in environmental impacts when compared to conventional methods; they are efficient and can eliminate NO_x and SO_x emission entirely.^{89,90} With potential efficiencies in excess of 85% (lower heating value) available in combined heat and power application, they are one of the most clean energy generation technologies available.⁶²

Figure 11 shows a schematic of a SOFC⁸⁸ to demonstrate the energy generation process. This requires a permeable anode and cathode, separated by an impermeable electrolyte. Oxygen, which is supplied to the cathode, reacts with electrons from an external circuit, forming oxide ions. These oxide ions move to the anode, through the ion conducting impermeable electrolyte, where they combine with

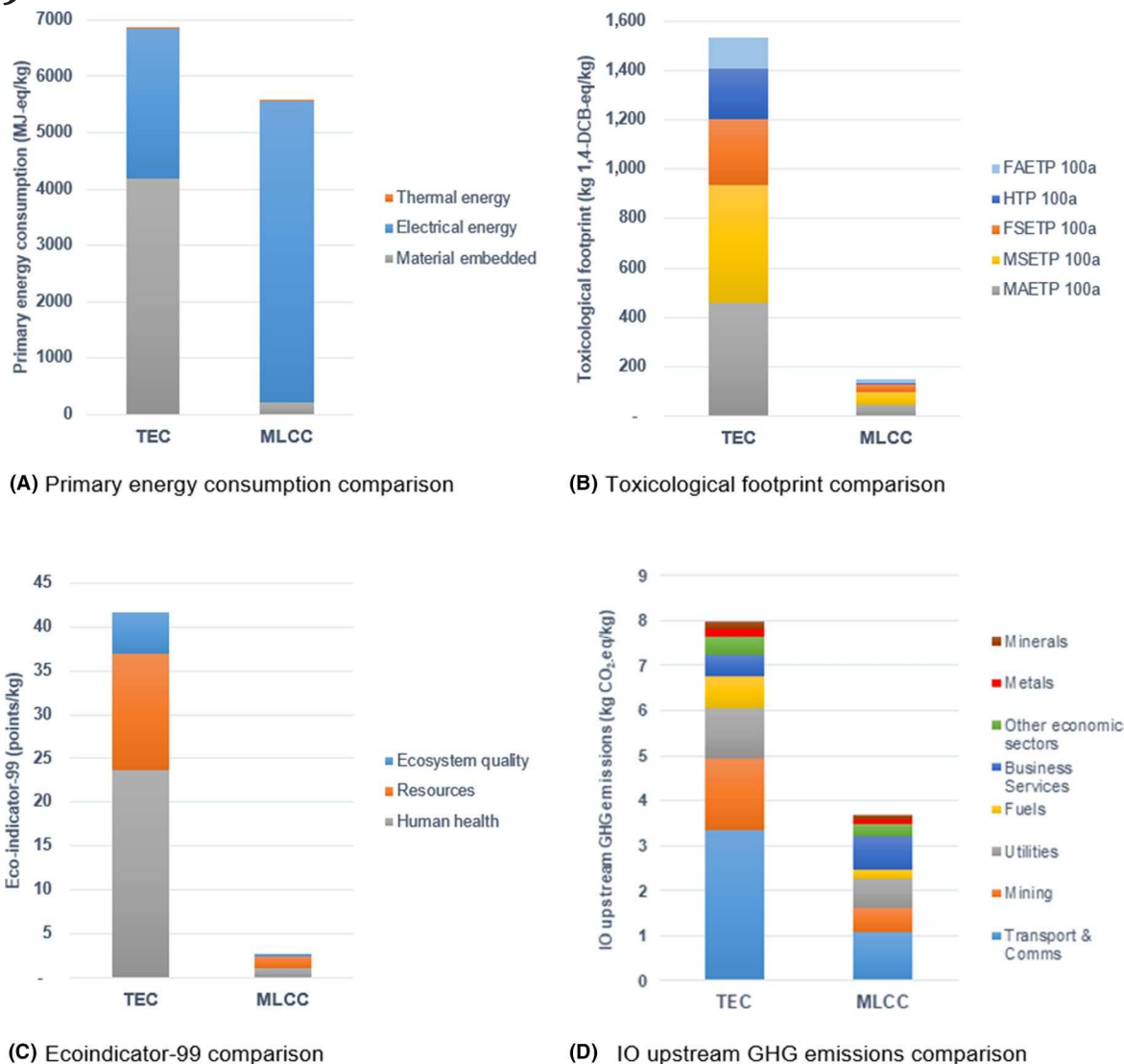


FIGURE 10 Comparison of the (A) primary energy demand, (B) toxicological footprint: human toxicity potential (HTP 100a); freshwater aquatic ecotoxicity potential (FAETP 100a); freshwater sediment ecotoxicity potential (FSETP 100a); marine aquatic ecotoxicity potential (MAETP 100a); marine sediment ecotoxicity (MSETP 100a) (C) eco-indicator-99, and (D) input-output (IO) upstream greenhouse gas (GHG) requirements for the production of a 1 kg batch of tantalum electrolytic capacitors and a 1 kg batch of multilayer ceramic capacitors (MLCCs)¹

hydrogen and/or carbon monoxide to form water and/or carbon dioxide, thereby liberating electrons. Electricity is then able to flow through the external circuit from the anode to the cathode.⁸⁸

The priority of currently published work, regarding the LCA of SOFCs, relates to the impacts of energy sources, processing, and material choice.⁵⁶ Work performed by Strazza et al⁹¹ analyzed the following environmental impacts with regard to fuel production, fuel storage, and SOFC manufacturing, operation and maintenance of SOFCs: GWP 100a, ozone depleting potential (ODP, given as kg CFC 11-eq), AP, photochemical ozone creation potential (POCP, expressed as kg C₂H₄-eq) and EP. A further two impact categories describing the use of nonrenewable and renewable

resources with energy content (given in MJ-eq) were used and finally an impact category giving the use of nonrenewable resources without the energy content (expressed as kg) was investigated.⁹¹

The fuels investigated were methanol, bio-methanol, natural gas, biogas, and hydrogen. Due to the different SOFC configurations required for each fuel type, the work shows that the configuration required for natural gas and biogas fuels have the lowest environmental impact over all of the categories investigated, except for the ODP. This high-ODP impact was attributed to the required transportation of methanator.

Research is now underway to develop SOFCs that can operate at lower temperatures (as low as approximately

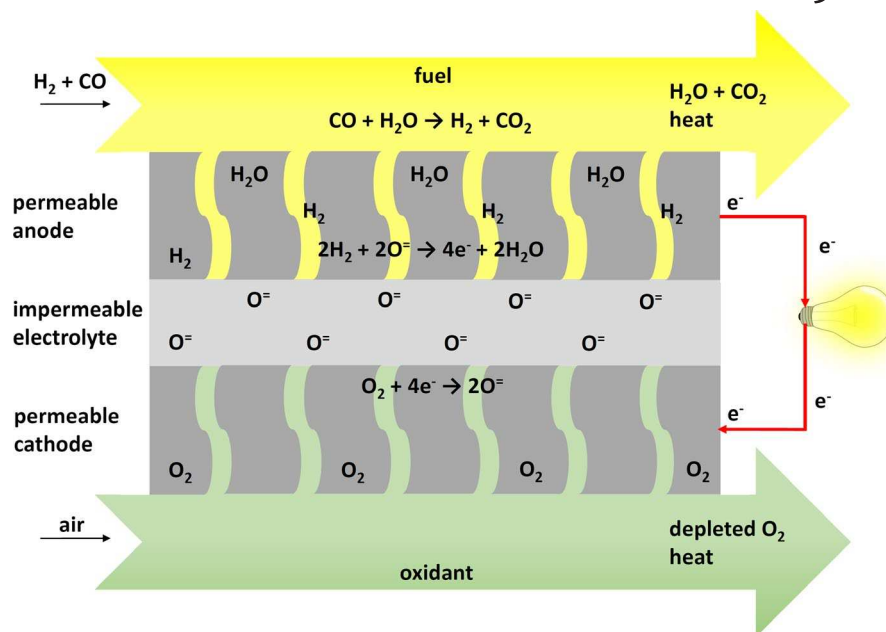


FIGURE 11 Operating principle of a solid oxide fuel cell, adapted from Ref. [88]

350°C in some cases) to enable higher operating efficiencies, lower costs, and reduced risk of failure due to thermal cycling.⁹² Work performed by Smith et al⁶² compares the material architectures of three SOFCs, namely a commercially available, high-temperature structure utilizing an yttrium stabilized zirconia electrolyte; an intermediate temperature structure with an erbia-stabilized bismuth (ESB) electrolyte; and a second intermediate temperature structure with a NBT electrolyte. The results show that the intermediate temperature structures lead to a reduced environmental impact over all categories studied. This is clearly shown in Figure 12 (which outlines the same environmental impacts as those presented in Figure 10 relating to the LCA of a 1 kg batch of MLCCs) highlighting the primary energy consumption and toxicological footprints of all three SOFC structures.

Figure 12A shows that the primary energy consumption for the commercial SOFC is much higher than that of both the ESB and NBT intermediate temperature SOFCs and that, in all three cases, the material-embedded energy has the highest contribution to the overall total. When the toxicological footprints of each SOFC were compared in Figure 12B, it was again found that the commercial high temperature SOFC has a higher impact over the five categories than the ESB and NBT intermediate temperature structures. This pattern is also observed when comparing the ReCiPe Endpoint and IO upstream greenhouse gas emissions (Figure 12C,D).

This reduction in environmental impacts, paired with the savings made in the operational phase due to the reduction in temperature, leads to a positive overall picture with regard

to the development of new and novel material structures for intermediate temperature SOFCs.⁶²

4.5 | Triboelectric nanogenerators

The aim of harvesting energy from day-to-day activities like breathing, talking, and walking was conceived through the use of nanogenerators based on piezoelectricity and triboelectricity; TENGs offer the potential to generate energy in self-powered devices at low cost but their environmental impact is relatively unknown.⁹³ To fill this gap Ahmed et al⁹³ considered the LCA and technoeconomic analysis of two TENG modules. Module A, a thin film-based micro-grating TENG, with its electrode arrays arranged linearly and generates enough energy to power standard electronics and Module B, which uses a planar structure that is based on electrodes generating periodically charged triboelectric potential and yields energy from water and air flow and bodily movement. An overview of the parameters of each module is provided in Table 4.

The team showed that the material embedded energy of the raw materials leads to around 90% of the primary energy demand for each module type. The use of acrylic in both structures leads to the highest impact over the climate change (74%), carcinogens (82%), respiratory organics (85%), and inorganics (73%), fossil fuels (81%), and eutrophication/acidification (76%) impact categories. In the manufacturing stage, it is the copper coating of each module that leads to the highest energy demand.⁹³

Overall, the results show that Module A has a better environmental profile, lower production costs, lower CO₂

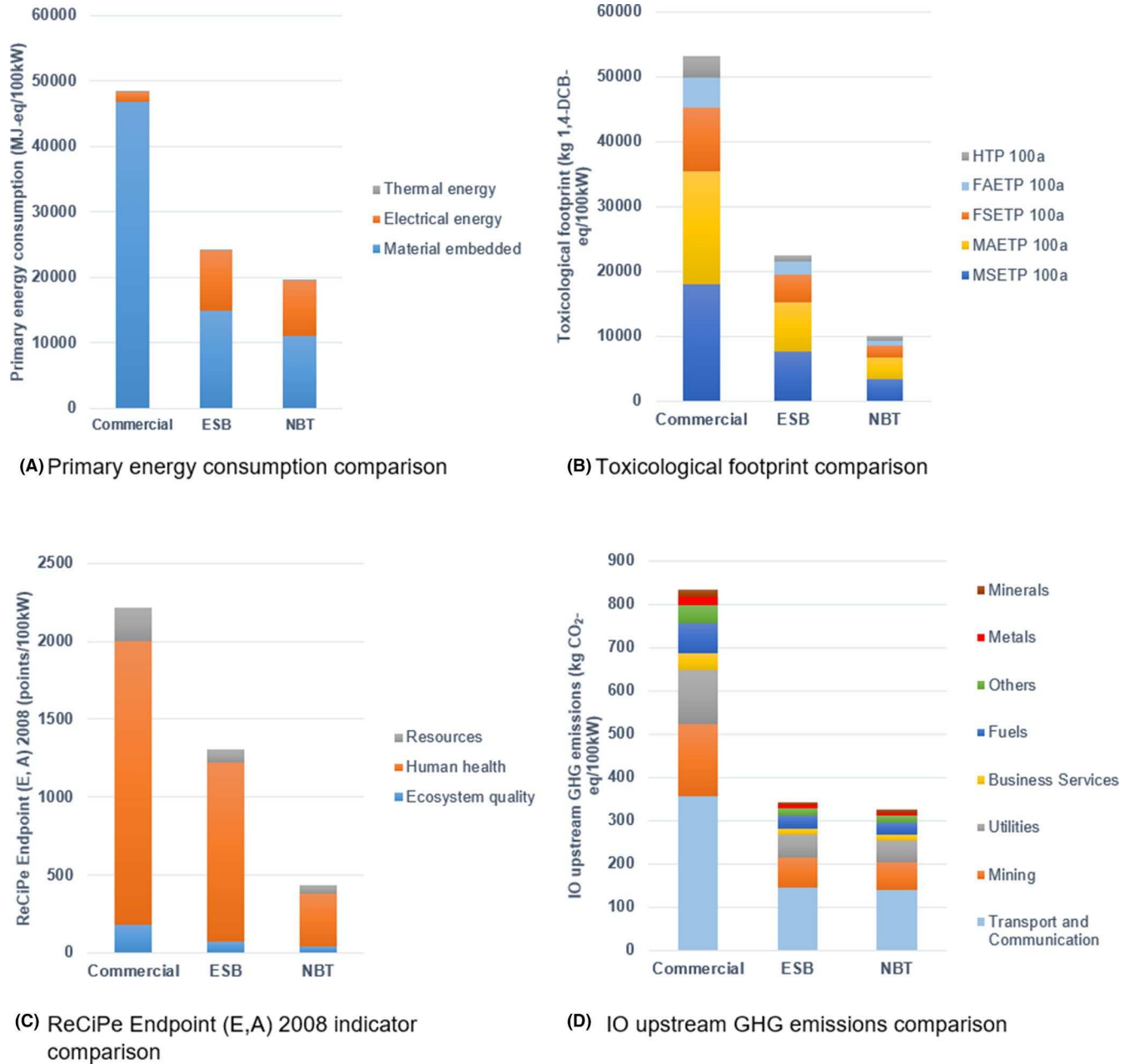


FIGURE 12 The comparison of the commercial, erbia-stabilized bismuth (ESB), and sodium bismuth titanate (NBT) solid oxide fuel cell material structures for (A) primary energy demand, (B) toxicological footprint: human toxicity potential (HTP 100a); freshwater aquatic ecotoxicity potential (FAETP 100a); freshwater sediment ecotoxicity potential (FSETP 100a); marine aquatic ecotoxicity potential (MAETP 100a); marine sediment ecotoxicity (MSETP 100a), (C) ReCiPe endpoint (E,A), and (D) input-output (IO) upstream greenhouse gas (GHG) emissions⁶²

emissions, and shorter EPBP when compared to Module B. Module B's environmental profile is affected by the higher content of acrylic in the structure and higher electrical energy requirements during fabrication. Although acrylic leads to a high impact within this architecture, it can be recycled or reused at the end-of-life stage and no toxic gases are emitted in the event of combustion. The environmental profile of 1 m² of the Module B TENG is shown in Figure 13. All the environmental metrics are normalized, ensuring that the absolute indicator of each category of impact is 100%.

$$\text{Energy payback period} = \frac{\text{Embodied energy (kWh m}^{-2}\text{)}}{\text{Energy output (kWh m}^{-2}\text{year}^{-1}\text{)}} \quad (5)$$

The EPBPs of both TENG modules were compared to that of existing PV technologies using Equation 5. This determined that TENG modules have a shorter EPBP when compared to available PV technologies,⁹³ but the payback period of Module B is marginally higher than that of a PV technology based

TABLE 4 Overview of the parameters of each TENG module examined⁹³

Module parameter	Unit	Module A	Module B
Size	cm ²	60	78.95
Distance between TENG unit	cm	1	1
Efficiency	%	50	24
Power output of one piece of module	W	3	1.5
Power output of one piece of TENG	W/m ²	500	190

Abbreviation: TENG, triboelectric nanogenerator.

on perovskite structured methyl ammonium lead iodide. The group concludes that future development of TENGs must relate to lifetime and efficiency improvements rather than the identification of cheaper materials and manufacturing processes.⁹³

4.6 | Solid-state batteries

Batteries are prevalent in modern society from their use in laptops, mobile phones, and other small portable devices up to those used on the electrical distribution grid with capacities in the megawatt scale.⁹⁴ At present, lithium ion batteries dominate the research and development in industry but safety issues surround their use due to the possibility of the flammable electrolyte leaking and igniting^{95,96} which has driven research into new battery structures.

Solid-state batteries (SSBs) utilize a solid electrolyte and therefore are less hazardous when compared to the current generation of lithium ion batteries. SSBs are also more vibration and shock resistant, operate over a wider temperature range, have higher storage capacities, and undergo less operation stress and consequently last longer than their predecessors.⁹⁵

Troy et al⁹⁶ published the environmental impacts of a pouch bag house SSB, manufactured in a laboratory, using a LiCoO₂/Li₇La₃Zr₂O₁₂ cathode and a Li₇La₃Zr₂O₁₂ solid-state electrolyte. The results show that the production of the electrolyte leads to the highest percentage GWP (kg CO₂-eq) impact of the manufacturing process, followed by the cathode production. When assessed in further detail, the electricity required for the lithium lanthanum zirconate production and tapecasting in both the cathode and electrolyte manufacturing leads to the highest GWP (kg CO₂-eq) impact.⁹⁶

Furthermore, the group's study assessed these environmental impacts at a laboratory level, under ideal laboratory conditions and industrial scale production. The ideal laboratory conditions were assumed to be conducted with the use

of as little material and energy loss as possible. The authors state that precisely translating the laboratory process up to the industry level is not possible due to the complexities involved and therefore, only assumptions can be made with regard to process improvements. Figure 14 shows the results of this analysis; the laboratory results are shown as 100% and then compared to the ideal laboratory and industrial conditions. It can be seen that improving the processing condition leads to environmental impact savings across all of the studied categories.⁹⁶

The environmental impacts of two separate SSB manufacturing processes are compared by Lastoskie and Dai,⁹⁷ specifically thin-film vapour deposition and lamination. With respect to the lamination process, lithium cobalt oxide, lithium manganese oxide, and lithium nickel-cobalt-manganese oxide cathodes were investigated. Additional materials such as lithium vanadium oxide and silver vanadium oxide were also studied with respect to the thin-film vapour deposition process. The results found that the lowest environmental impact, across the eight mid-point impact categories that were tested, could be attributed to the lithium vanadium oxide SSB.⁹⁷

Future work in this arena may continue to tackle all aspects of the environmental impacts of SSBs. Specifically, a comparison of the environmental impacts of conventional LIBs and SSBs that performs in the same function space, is underway.

4.7 | Use of critical materials

Many of the devices in this review, including SOFCs, MLCCs and third-generation solar cells, utilize critical materials in their structures materials.^{1,92} In total, the EU has classified 27 critical materials in their 2017 report,⁹⁸ examples include tantalum, bismuth, and rare earth elements. Criticality, in this report, is determined according to supply risk and the importance of its use, although other methodologies have been developed which take in additional factors to the calculation.⁹⁸

Taking rare earth oxides as an example; the challenge arises as they are classed as critical materials, but their addition to functional devices, such as MLCCs and antennas, has been found to enhance their properties. MLCCs utilize 2-3 wt% of either dysprosium, holmium, or erbium oxide¹; The US Department of Energy has determined that dysprosium is the most critical element available.⁹⁹ Demanding and environmentally damaging separation and refining processes, combined with uneconomic concentrations in the earth's crust and a Chinese monopoly on the market, have led rare earth elements to be labeled as critical.^{100,101} Although the use of rare earth oxides continues to rise,^{102,103} their recovery from devices during the recycling phase is not well-documented. Work by Rocchetti et al¹⁰⁴ described the precipitation of yttrium-using oxalic acid but the environmental impact of the

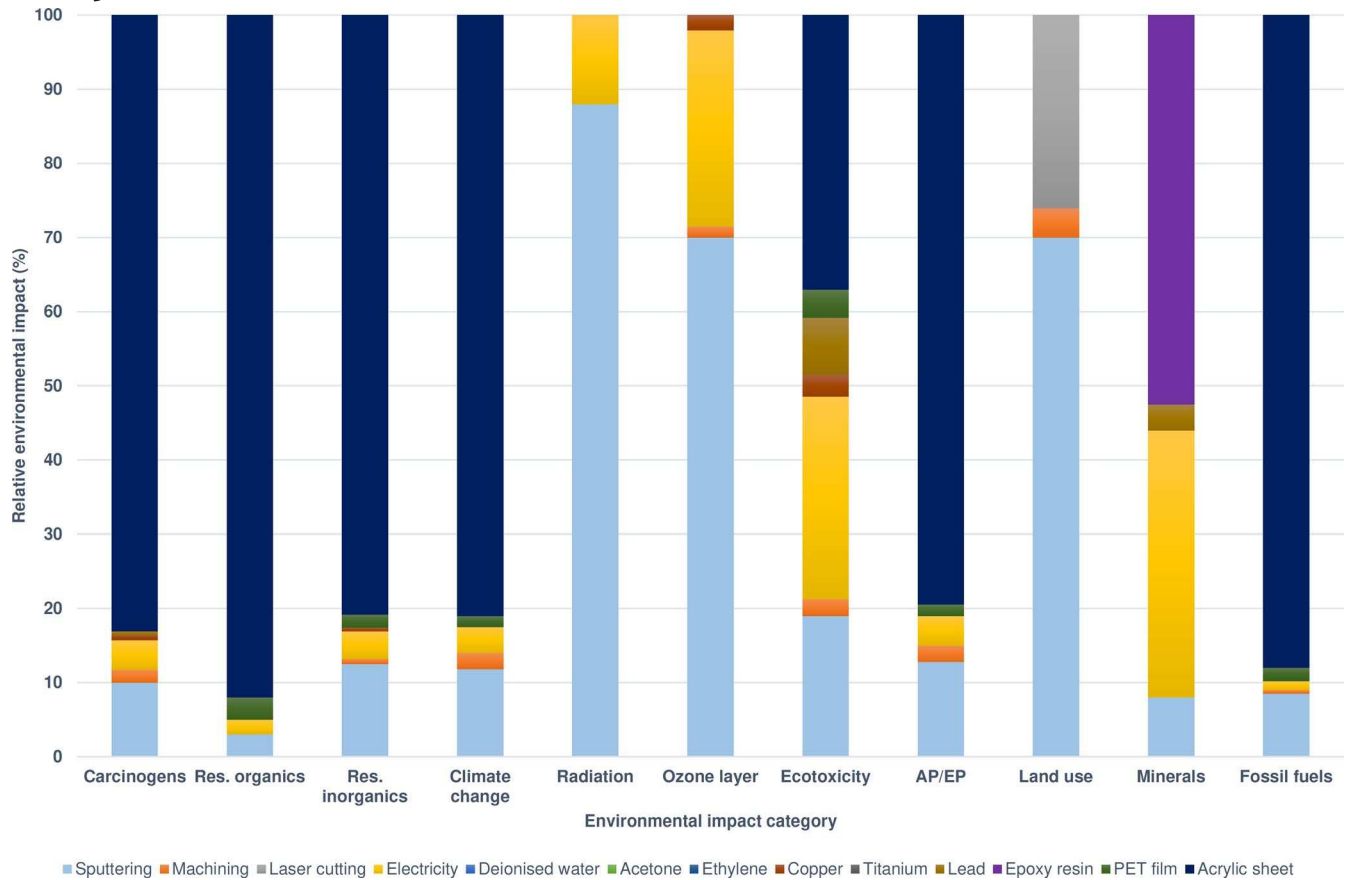


FIGURE 13 The environmental profile of 1 m² of the Module B triboelectric nanogenerator (adapted from Ref. [93]). Each environmental impact category has been normalized to provide an absolute indicator of 100% for each impact category. NB. “Res.” refers to respiratory, AP denotes acidification potential, and EP denotes eutrophication potential

manufacturing process of oxalic is known to be high which could outweigh the benefits of yttrium recovery.

Despite their importance as a critical material and use within many modern devices, it can be seen from the work by Smith et al¹ that the concentration of dysprosium in a MLCC is so low that it does not lead to an environmental hot spot using the hybrid LCA methodology.

5 | SUSTAINABILITY OF FUNCTIONAL CERAMICS AND RELATED DEVICES

While the environmental impacts of FM&D are of high importance, the sustainable supply chain management of materials and components is becoming more prevalent with regard to the triple-bottom line; economy, society, and environment.¹⁰⁵

The BS 8905:2011 standard¹⁰⁶ deals specifically with the sustainability of materials and states that sustainability decision making should be made with a balance of social, economic, and environmental aspects. The standard outlines three phases to the sustainability assessment process;

scoping, data collection and assessment, and reporting. The environment, economy, and society are deemed symbiotic; a change to one aspect may have an effect on another. Therefore, a life-cycle sustainability assessment (LCSA) requires the calculation of each of the three aspects for example using the Global Reporting Initiative (GRI) G3 Guidelines for the social LCA (SLCA), LCA for the environmental examination and life-cycle costing (LCC) for the economic calculation, followed by an amalgamation of the results.¹⁰⁶ LCC is a process that was developed to determine the cost (and/or gain) impacts of an investment (or in this case product or service) throughout its life cycle; the economic “hot spots” from cradle-to-grave (or cradle) can be determined to aid the decision-making process.¹⁰⁷ The social impacts of a product can be determined using SLCA though, in comparison to the LCA and LCC processes, there is less published research relating to the social impact categories required to provide robust data for decision making.^{108,109}

Life-cycle sustainability assessment is a framework that is still evolving within the scientific community and aims to broaden and deepen the existing LCA methodology.¹¹⁰ By extending the reach of the LCA methodology, through the

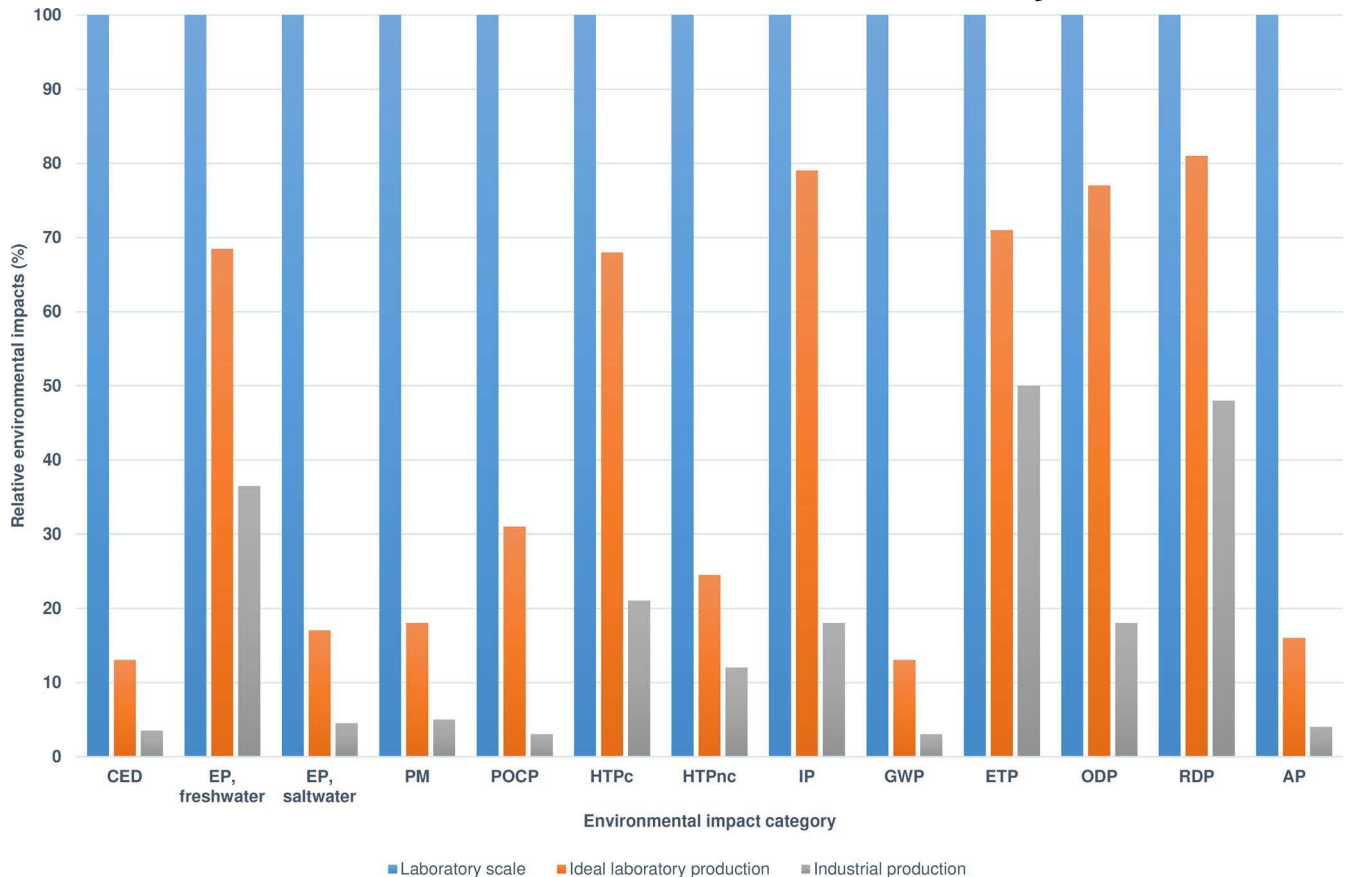


FIGURE 14 Comparison of the life-cycle assessment result of a 43.75 mAh capacity solid-state battery at the laboratory scale (100%), under ideal laboratory conditions and using industrial production methods. Adapted from Ref. [96]. All acronyms are included in the Abbreviations section at the start of this manuscript

inclusion of social and economic impacts, and expanding the system boundary from a process-based methodology to reach across the economic spectrum, the scope of the methodology will be widened. To deepen the framework of the LCSA the shifting and interdependent nature of the three pillars of sustainability must be addressed and their governing mechanics must be understood in more detail.¹¹⁰

Publications relating to SLCA date back to 2006 but despite this, the social impacts relating to materials and components are regularly ignored. It has been argued that social impacts may not be, or are only slightly, related to technical processes but to the management of the company in which those process are performed. Consequently, the same product may be manufactured in multiple companies, leading to differing social impacts.¹⁰⁹ Further research in the area of social impacts will enable future research into material and component analysis.¹⁰⁵

The LCC is a tool used to determine the cost and/or benefit impacts during the life cycle of an investment, importantly, as in LCA, the “hot spots” within a system can be identified that is those influences which have the largest effect on the whole life cycle. Overall, the methodology provides important economic information for decision makers.¹⁰⁷ Onat et

al¹¹⁰ stated that the current disadvantages of LCSA are the simple approach of assessing the three pillars (through environmental LCA, SLCA, and LCC) separately and the lack of understanding of the interconnected nature of the concept.¹¹⁰ In contrast to this, Kloepffer¹¹¹ supported this approach under the constraint that consistent system boundaries between the three assessment methodologies are set.

Kolotzek et al¹⁰⁵ present a quantitative corporate-oriented raw material assessment model that focusses on supply risk assessment, environmental impact assessment, and social assessment. The model uses a total of 11 supply risk indicators, 15 environmental indicators, and 18 social indicators, and finally provides three scores between 0 and 100 which determine how critical a material is (where 0 relates to the least critical score and 100 relates to the most critical score), one for each assessment. Using a capacitor supplier as a case study, the team presents the measurements for aluminum, niobium, and tantalum with respect to capacitor production. The results, detailed in Table 5, show that aluminum has the lowest supply and environmental risk but socially, niobium provides the best result.¹⁰⁵

While this methodology goes one step further in the attempt to quantify sustainability, one overall “sustainability”

	Al assessment	Nb assessment	Ta assessment
Social risk	52	40	50
Environmental risk	4	11	28
Supply risk	47	56	65

TABLE 5 Overview of the result of the sustainability assessment given by Kolotzek et al for the use of aluminum, niobium, and tantalum in capacitors, scores range from 0-100, where 0 relates to the least critical score and 100 relates to the most critical score¹⁰⁵

measure is not provided but three individual scores, leaving the decision maker to make a final assessment on which of the three measures is of overriding importance. Furthermore, while the triple bottom line is cited within the paper as the economy, society, and environment, the economy is not addressed within the model presented.¹⁰⁵ Moving forward, the “holy grail” of sustainability measurements must be an efficient, reliable tool that assesses the triple-bottom line,¹¹² preferably in a single simple metric. A comprehensive “Materials Sustainability Index” is a long-term goal of the work of Koh and co-workers but premature publication of such an index is potentially damaging and due diligence is required to cross reference the acquired data/methodology against detailed HLCA. We particularly note how an oversimplification of environmental issues by Rödel et al¹¹³ in PbO free piezoelectrics has led to a striking misrepresentation of their “green” credentials.

6 | THE ROLE OF LCA IN POLICYMAKING AND ENVIRONMENTAL REGULATION

As mentioned in the introduction of this manuscript, LCA is used in policy implementation worldwide. This section therefore discusses relevant legislation in Europe and the United States.⁸ One prominent example of this is the European RoHSs Directive (2002/95/EC) which was passed in 2003 and restricted the use of lead, mercury, cadmium, hexavalent chromium, polybrominated biphenyls, and polybrominated diphenyl ethers in electrical and electronic components.¹¹⁴ Thirty-six exemptions for the specific use of these materials were issued with an expiry date. When the second round of RoHS (2011/65/EU) was issued in 2011, this included over 100 exemptions.¹¹⁴

An application for a RoHS exemption under the second round of the directive requires a LCA to be issued exploring the impacts of the exemption. The LCA must compare the environmental impacts relating to the use of the restricted substance, for which the exemption is requested, and its substitutes throughout the lifecycle of a product.¹¹⁵ Exemption No. 7c-1 of the directive currently allows the use of “lead in a glass or ceramic other than dielectric ceramic in capacitors, for example piezoelectronic devices.”¹¹⁶ For the electroceramic industry to continue using lead in these devices future exemptions using LCA must be obtained. Therefore,

the work outlined in Section 4.1 of this document stands as evidence that the use of lead in piezoelectric devices has a lower impact on both the environment and human, than potential substitutes.

The Environmental Design of Electrical Equipment Act was introduced to the United States House of Representatives in 2009 but was not enacted. This act was similar to RoHS in that it restricted the use of the same materials listed above for manufacturing in the electronics industry.¹¹⁷ The Registration, Evaluation, Authorisation and Restriction of Chemicals (REACH) Directive was launched in the EU at the end of 2006. It involves the registration of chemicals (substances and mixtures) produced or imported into the EU to the EU's Chemicals Agency. The human and environmental exposure potential must be registered along with recommendations for safe usage.¹¹⁸

Askham¹¹⁸ concludes that while REACH and LCA are different in scope and framework, they assess the same issues and may be complementary in some cases while causing contradictions in others. The gathering of toxicity data through REACH can greatly aid the results of a LCA, while the functional approach adopted by LCA modellers would be beneficial in the completion of a REACH assessment. The combination of LCA into the REACH analysis can provide a competitive edge to a company and provide societal benefits.

The supply chains of electroceramic devices depend on a wide range of materials including naturally occurring minerals, metals and, in some cases, polymers. The contribution of such devices toward a low-carbon economy can only be fully appreciated when a holistic approach is used which takes into consideration the complete lifecycle of the final product across its lifespan. Such holistic approach within a LCA framework must consider all pertinent environmental indicators including water use, ecological, and human toxicity as well as biodiversity. This will ensure the responsible promotion of functional ceramics produced with concerns for the environment in mind as against those imported from countries with less stringent environmental policy and regulations. Policymakers must therefore embrace the use of LCA in their overall decision making.

7 | CHALLENGES OF LCA OF FM&D

The challenges of an LCA may vary from study to study, though the data collection phase is often the most difficult

of the required stages to complete. In the absence of industry data, the use of primary laboratory data, for example in⁷ and¹ can be used. When measurements are taken from high-tech, accurately calibrated pieces of equipment, any associated experimental errors are minimized.⁷ Uncertainty can arise if laboratory scale manufacturing routes are being used to represent industrial scale processing since production may lead to a lower impact on an industrial scale due to more efficient methods. Sensitivity analysis to understand how the input measures affect the final result is not possible due to the lack of primary industrial data. Despite this, the laboratory scale results provided by Smith et al¹ relating to the environmental impacts of MLCCs and TEC were corroborated by engineers in Murata Manufacturing Co., Ltd. (a leading global capacitor manufacturer) on an industrial scale.

Work by Troy et al⁹⁶ states that products at a low-technology readiness level must be managed cautiously with respect to the result of their associated LCAs, especially when comparing with high-technology readiness or commercialized products. This is due to the incomparable nature of laboratory processes with industrial production against which low-technology readiness level products cannot be assessed. Despite this, a timely comparative environmental analysis such as that performed on PZT and KNN⁷ can lead to early intervention in industry¹¹⁶ to avoid future negative environmental impacts.

The criticality of materials is now widely assessed^{99,101,119} and rare earth elements are consistently identified as critical, independent of the methodology used for the assessment. As demonstrated by Smith et al,¹ the results of the LCA did not highlight the use of dysprosium in the structure of MLCCs as an environmental hotspot. This is due to the relatively low concentration of dysprosium within the MLCC structure, despite this, with the growth rate of use of such devices estimated as high as 4.8% per annum,⁵ the total use of dysprosium (which is not currently recycled¹²⁰) will be high. Therefore, this indicates that the use of LCA may not be substantial enough to aid the decision-making process on a standalone basis, and should be used in conjunction with other metrics such as criticality assessment.¹

In some circumstances, the LCI of the materials under consideration within the system boundary may not exist and therefore additional secondary sources must be consulted. LCI data can be calculated using mass flows or stoichiometry,⁶¹ published literature can be consulted and similar materials can be used based on chemical characteristics and functional parallels.^{7,61}

The application of the HLCA methodology requires the modeller to apply subjectively additional impacts to the modelled supply chain in order to expand the reach of the system boundary, without double counting. This requires in-depth

knowledge of the supply chain and could result in conservative or even excessive results.^{7,61}

8 | CONCLUSIONS AND FUTURE WORK

This manuscript introduces the application of LCA with specific reference to FM&D, to which there are few applied studies despite their importance in modern society. Overall, there is a vast array of published material relating to the applied LCAs of many different product and service types, a scopus search of “LCA” currently provides over 20 000 results. Where there is an abundance of information relating to batteries for example, there is a dearth of that for newer technologies such as TENGs. This could be attributed to the popularity of such devices which would lead to an increase in published information as the use of such devices continues to grow.

Many “best practice” guides are available to help the modeller to implement LCA, specifically the “BS EN ISO 14040:2006 Environmental management. LCA. Principles and framework” standard document provides a plethora of information relating to the process LCA methodology.³⁴ Highly cited work by Rebitzer et al³⁰ and Pennington et al¹²¹ discuss the process of assessing a product's life cycle and how different indicators have been developed to aid the life-cycle impact assessment process. More general information relating to the development of LCA can be found in works by Guinée et al⁸ and finally, important work specifically relating to the LCAs of FM&D can be found in work by Ibn-Mohammed et al.^{7,36,69}

The importance of LCA in the research and development of ceramics technologies is highlighted specifically in the work completed by Smith et al⁶² and Ibn-Mohammed et al⁷; application of the LCA methodology prior to making a change to the design of a device is critical. It is clear that some materials present a conundrum when faced with the assumptions of how “green” they are. By applying the LCA methodology in the design phase, time and costs can be saved in the long term.⁷

While LCA has been in use for almost 50 years, the methodology is not applied consistently throughout academia. Many different LCI methodologies are available to the modeller and so (as required by the international standard) one is chosen based on the requirements of the output. The application of HLCA, despite its clear ability to quantify the environmental impacts of the wider supply chain, is not yet fully implemented in all analysis. Furthermore, when HLCA is used, it is not always made fully clear which of the four different methodologies are utilized.

This document outlines the two basic LCA methodologies, namely process and environmental IO LCA, and the

four HLCA methodologies that have been developed to amalgamate the two approaches. Although HLCA is backed up by over 20 years of research, it is a complex method which uses varying terminology which has led to fewer modellers employing the technique.³¹ Opinions differ with regard to whether or not the use of the hybrid methodology provides a more accurate result than the basic process LCA method.^{7,49,50} Despite this, when the most appropriate IO model is employed, the relevant missing inputs from the supply chain can be captured by HLCA to provide completeness in the assessment.⁵⁰

Looking into the future, LCA will continue to evolve as it has from its first implementation in the 1960s. Though the original aim of understanding the environmental impacts of a product or service will continue, extensive research is required to achieve a robust methodology to assess sustainability.⁸

Despite this, as shown by Smith et al¹ the impact of materials may be overlooked by the LCA process if they are present in small amounts when compared to other materials. Therefore, developers of FM&D intending to make use of critical materials such as rare earth elements should consider a secondary criticality assessment to understand the impact of using those materials on a wide scale.¹

It has been suggested that LCSA, discussed in Section 5, is the future of LCA. This requires the scope of an LCA to be broadened to incorporate the economic and social aspects of sustainability⁸ and further work into the standardization of social impacts to be developed.¹⁰⁵

With respect to the implementation of LCA at a laboratory and industrial level, as shown by Ibn-Mohammed et al,⁷ the implementation of this established and system based methodology is a critical tool to be implemented alongside innovation and new product development.⁷ As it has been found over the years that the main environmental impacts of a product are established in the production, disposal, or transportation phase (rather than the use phase) it is key for both researchers and industry to implement the LCA methodology as a decision-making tool in the early phases of development to avoid any retrospective costs required to reduce the environmental impact of a new product or service.^{7,8}

Future work in the area of LCA of FM&D must continue to compare existing technologies with novel, low technology readiness level opportunities to ensure that technological progress does not come at the price of the environment. In addition to this, the environment should not be assessed as an individual concept, but integrated into sustainability alongside the economy and society.

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