Sustainability-informed materials selection, design, discovery, and development

Julie M. Schoenung,* Oladele A. Ogunseitan, and Lauren G. Heine

Performance criteria and economic considerations remain potent but increasingly insufficient drivers of innovation in the discovery and selection of materials. Global-scale challenges associated with resource depletion, climate change, intractable waste, and toxicity have highlighted the urgent need for a new paradigm, named here as sustainability-informed materials selection, design, discovery, and development (SIMS-D^3). The SIMS-D^3 approach demands intentional application and transparent coordination of methods for identifying and ranking a broad set of criteria that contribute to the situation of specific materials and their prospective uses on a sustainability continuum. This article covers strengths, weaknesses, and gaps in existing methods, tools, resources, and databases necessary for advancing SIMS-D^3, with emphasis on safer chemicals, energy, and implementation of circularity in materials utilization. Case studies on leaded materials, flame retardants, and compositionally complex inorganic materials are described to illustrate the complexity of the challenges with conventional approaches, and the opportunities presented by adopting SIMS-D^3.

Introduction

The imperative for sustainability-informed materials selection

Human communities have probably always grappled with the concept of sustainability of materials—and suffered through adverse consequences of depletion and use of dangerous materials at local levels—for example, inadequate supply and safe use of firewood for warmth and for cooking during winter seasons. However, there has been no time in recorded history until now when sustainability of materials is imbued with a connotation of global scale and the recognition that the pace at which essential materials are being used (e.g., fossil fuels), coupled with the generation and accumulation of dangerous waste (e.g., greenhouse gases) are already impacting human communities worldwide with concomitant threats to the survival of other species and to the integrity of ecosystems that sustain life on Earth. Increase in global demand for materials is driven by population growth, urbanization, and economic development. The surge in demand is exerting unprecedented pressure on natural resources and ecosystems, exacerbating environmental degradation and social inequalities. Consequently, the need for materials that can meet this demand while minimizing adverse impacts has never been more pressing.

The contemporary concept of sustainability continues to be refined and may be summarized by reference to the practice of meeting the needs of the present without compromising the ability of future generations to meet their own needs.[1] Sustainability science is an interdisciplinary field of study that focuses on the dynamic interactions between natural and social systems, with the goal of understanding and promoting sustainable development. It integrates knowledge from various disciplines, including natural sciences, social sciences, engineering, and humanities, to address sustainability challenges, including improved understanding of complex systems of interactions between human needs, desires, and the natural environment; addressing global issues such as climate change, biodiversity loss, and resource depletion with solutions that are both effective and equitable; and influencing regulatory policies and institutional practices.[2,3] We argue here that all aspects of sustainability rely on the choice of materials used across a wide range of societies for various indispensable products or

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processes. Consequently, materials that support the goals of sustainability are those that are produced, used, and discarded in ways that have no or minimal adverse impacts on the quality of environmental systems upon which human health and well-being rely.

The traditional paradigm of materials selection has focused primarily on technical performance and cost-effectiveness, often overlooking the broader environmental and social impacts.[4] However, escalating environmental crises, such as climate change, global environmental pollution, and biodiversity loss, have underscored the necessity for a different approach that encourages systems thinking and intentionality in the consideration of projected long-term fates of materials to reduce or eliminate projected adverse impacts on environmental quality and human health. Therefore, assessments of long-term fates of materials are expected to be captured in a latent construct of sustainability, which is calculated to inform established protocols for the discovery, design, and development of materials, and to transform decision-making strategies for evaluating alternative options and selecting the best materials for specific uses. As an approach, sustainability-informed materials selection through discovery, design, and development (SIMS-D^3), as illustrated schematically in **Figure** 1, adapted from Schoenung and Olivetti,[5] aligns with increasingly important initiatives such as the United Nations Sustainable Development Goals (SDGs) that emphasize the importance of sustainable consumption and production patterns, and prioritize a shift toward materials that minimize environmental footprints and promote social equity in response to the triple planetary crisis: climate change, biodiversity loss, and pollution.[6]

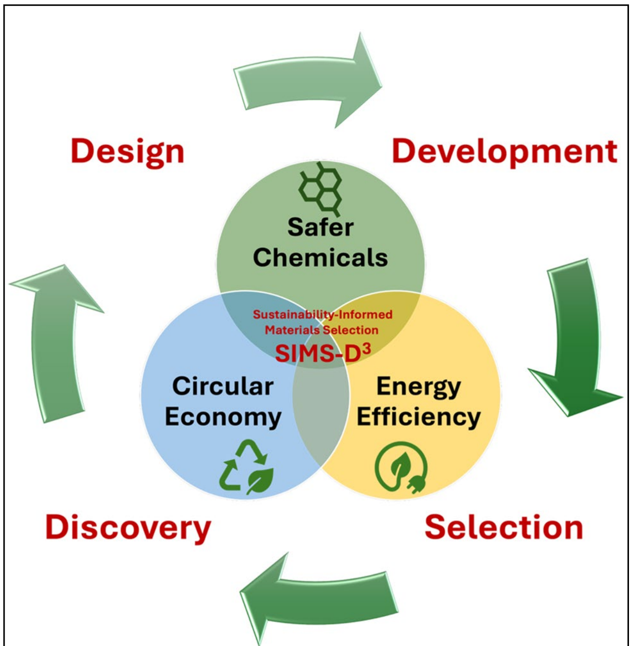


Figure 1. Intrinsic and interactive properties of materials are central to the emergence of threats to sustainability of life on Earth, summarized as the triple planetary crisis of climate change, biodiversity loss, and pollution. Sustainability-informed materials selection is supported by prioritized consideration of sustainability attributes in the discovery, design, and development of materials (adapted with permission from Reference 5 © Springer Nature 2023).

For more than half a century, researchers have identified differential characteristics of materials that align with the sustainability paradigm, including derivation from renewable or abundantly available sources; requirement of low energy for production; processing associated with low carbon footprint; relatively nontoxic and safe for human health; and can be easily recycled, reused, or biodegraded in the context of a circular economy.[7–13] Information on sustainability characteristics should influence both the active selection of specific materials among a variety of options, and the design of products such that materials can be reused. Where there are no suitable sustainable material options, research should be incentivized to support the discovery, development, and adoption of alternatives. Based on the platform of sustainability science, SIMS-D^3 enables the prioritization of materials for products, processes, or systems that consider environmental, social, and economic factors throughout the materials' life cycle. The approach demands multidisciplinary research and the development of quantitative and qualitative methods that are suitable for use within clearly articulated system boundaries and reasonable assumptions. Inevitably, the global and international scope of material life cycles means that there are gaps in data sets, and the methods and results must meaningfully characterize uncertainties and provide guidance for the decision-making in the process of selecting a specific material from a set of alternatives. One of the most challenging ambitions of SIMS-D^3 is the establishment of guidance regarding tradeoffs among materials characteristics in a continuum of desirable sustainability parameters beyond traditional performance characteristics of materials to include resource depletion potential, energy consumption, noxious emissions and waste generation, recyclability and biodegradability, toxicity and health impacts, social and ethical considerations, and economic feasibility.[14–16]

Due to methodological limitations, data gaps, and regional differences in regulatory policies, outcomes of SIMS-D^3 applications are inherently incomplete and subject to updates as investigators learn more about potential impacts of materials in rapidly changing and variable environmental and societal conditions that influence materials usage and their interactions with physical and chemical circumstances and biological entities. Therefore, it is necessary to articulate the contexts in which the SIMS-D^3 approach can continuously advance the stages of including sustainability in the process of selecting materials and examples regarding their potential contributions to sustainability. In materials discovery, emphasis is placed on exploration of new materials that meet preestablished sustainability criteria, including innovations in biomaterials, recycled materials, and materials derived from renewable sources. For example, the discovery of new bioplastics that can replace conventional plastics can help reduce dependence on fossil fuels and mitigate plastic pollution.[17] In materials design, emphasis is placed on designing for end-of-life scenarios such as recycling or biodegradation, and designing products with fewer components or using modular designs can facilitate repair and recycling, extending the lifespan of materials. In materials development, emphasis is placed on refining and scaling up the production of materials that have been vetted for sustainability to ensure they are economically viable and can be integrated into industrial processes. This involves optimizing manufacturing techniques, improving materials properties, and ensuring that such materials can compete with traditional materials in terms of economic cost and engineering performance.

Advances in SIMS-D^3 implementation

Since the 1990s, there has been a growing emphasis on incorporating sustainability considerations into materials selection processes. The existing methods and tools have helped establish the conceptual foundation and databases that are essential for enabling the various dimensions of SIMS-D^3. Collectively, these methods are defined by eco-design principles that encourage product designers to consider environmental factors from the earliest stages of product design and development.[18] Life-cycle assessment (LCA) methods were developed to evaluate the environmental impacts of materials across their entire life cycle—from raw material extraction to disposal or recycling.[19] Additional emerging methods and tools include material flow analysis (MFA), multi-criteria decision analysis (MCDA), chemical hazard assessment (CHA), and alternatives analysis (AA) to evaluate the benefits and risks of proposed replacements in order to avoid regrettable substitutions. Descriptions of some of these methods and additional tools are provided in designated sections of this article. Still, we note that full implementation of SIMS-D^3 across the manufacturing sector will require the refinement of existing methods and development of increasingly integrative, sensitive, and accurate analytical tools with fewer assumptions, particularly regarding composite sustainability parameters such as embodied energy, recyclability, and toxicity.[20,21]

Methodological innovation to support comparative evaluation of materials is advancing in parallel to other advances in the conceptual framework for implementing SIMS-D^3. For example, it is important to improve the understanding of drivers of technological innovations, regulatory pressures, and consumer demand for products that are perceived to be sustainable in part because of their material composition. The development of biomaterials derived from renewable resources, such as bioplastics and bio-based composites, has gained momentum among manufacturers. These materials offer the potential to reduce dependence on fossil fuels and mitigate environmental impacts.[22] Successful implementation of SIMS-D^3 will also benefit from advances in manufacturing techniques, including additive manufacturing, and less fragmentation and better integration of overlapping research and implementation frameworks such as industrial ecology, circular economy, and planetary health.[23–25]

Despite the progress made in SIMS-D^3 implementation, several challenges remain. These include the need for more comprehensive and standardized sustainability metrics, the integration of sustainability criteria into existing industrial processes, and the development of scalable and economically viable sustainable materials. For instance, the lack of standardized metrics for assessing the sustainability of materials can make it difficult to compare different options and make informed decisions. Future R&D should focus on addressing these challenges and exploring new frontiers. This may involve advancing the understanding of the environmental and social impacts of materials, developing innovative materials and manufacturing techniques, and fostering collaboration between academia, industry, and policymakers to drive the adoption of sustainable practices. For example, research into new biomaterials and advanced manufacturing techniques can help overcome the challenges of scalability and economic viability.

This article provides a comprehensive overview, highlighting the rationale and significance of integrating sustainability information and materials science and technology. By understanding the opportunities and challenges of SIMS-D^3, researchers, industrialists, and policymakers can make informed decisions that contribute to a more sustainable and resilient future. The transition to materials that support sustainability—as opposed to contributing to global-scale problems—is not just a necessity, but also an economic opportunity, offering the potential for impactful innovation that benefits environmental quality and human health and well-being everywhere.

SIMS-D^3 methods, tools, resources, and databases

Safer chemicals

In order to move to safer chemicals in line with SIMS-D^3, we must understand the concepts of hazard, toxicity, and risk. Hazard refers to the intrinsic property of a substance that can cause harm and includes physical hazards such as flammability, toxicity to humans and other species, and environmental hazards such as ozone depletion. Toxicity is a key consideration in any sustainability-informed materials selection process. The use of highly toxic and otherwise hazardous chemicals in commercial and consumer products and processes is undesirable and often avoidable. Green chemistry has emerged to directly address the need for inherently safer chemicals that can perform as desired.

Green chemistry is "the design of products and processes that reduce or eliminate the use or generation of hazardous substances."[26] Risk is a function of hazard and exposure. A key strategy underlying the practice of green chemistry is to reduce risk by reducing the inherent hazard of chemicals. This can be done by designing, creating, and using molecules that are inherently benign. Reducing hazard is a more failsafe method for reducing risk than controlling exposure because exposure controls can, and will, fail.

Chemical hazard assessment (CHA)[27] is a key methodology for assessing and communicating information about the hazards associated with a substance. Substances are evaluated for a suite of hazard classes that are classified for severity. The hazard classes may be human hazards (e.g., carcinogenicity, acute mammalian toxicity), environmental hazards (e.g., aquatic toxicity, hazardous to the ozone layer), or physical hazards (e.g., flammability, explosives). The results may be presented in a summary hazard table using color codes and symbols to indicate what is known and unknown about a substance's hazard profile including hazard classification levels (severity), data gaps, and exposure routes. An example is included later in this article. Most CHA methods assign an overall chemical rating based on the individual hazard class assignments.

To understand CHA, it is important that we first understand the Globally Harmonized System of Classification and Labeling of Chemicals (GHS).[28] The GHS was born out of the 1992 United Nations Conference on Environment and Development (The Earth Summit).[29] The United Nations developed the GHS to promote a worldwide standard for hazard classification and communication. Prior to the implementation of GHS, each country had its own hazard classification and communication system, including different pictograms, labels, and safety data sheets, which created complexity and confusion (and lots of paperwork). The first edition of GHS (also known as "The Purple Book") was published in 2003, and it is updated every two years. GHS Revision 10 was published in 2023.[30] GHS is designed to be adopted by individual countries worldwide. As of November 2023, more than 90 countries have adopted GHS either in part or as a whole.[31]

GHS is not a regulation or a scoring system. Rather, it is a framework with guidance for (1) classifying the severity of individual hazard classes by assigning category levels, and (2) labeling hazardous chemicals in a way that can be consistently understood worldwide using hazard (H)-statement codes and phrases. **Table** I shows the hazard classes included in the GHS Revision 10. H-statement codes that begin with 200 are assigned to physical hazards, those that begin with 300 are assigned to human health hazards, and those that begin with 400 are assigned to environmental hazards.

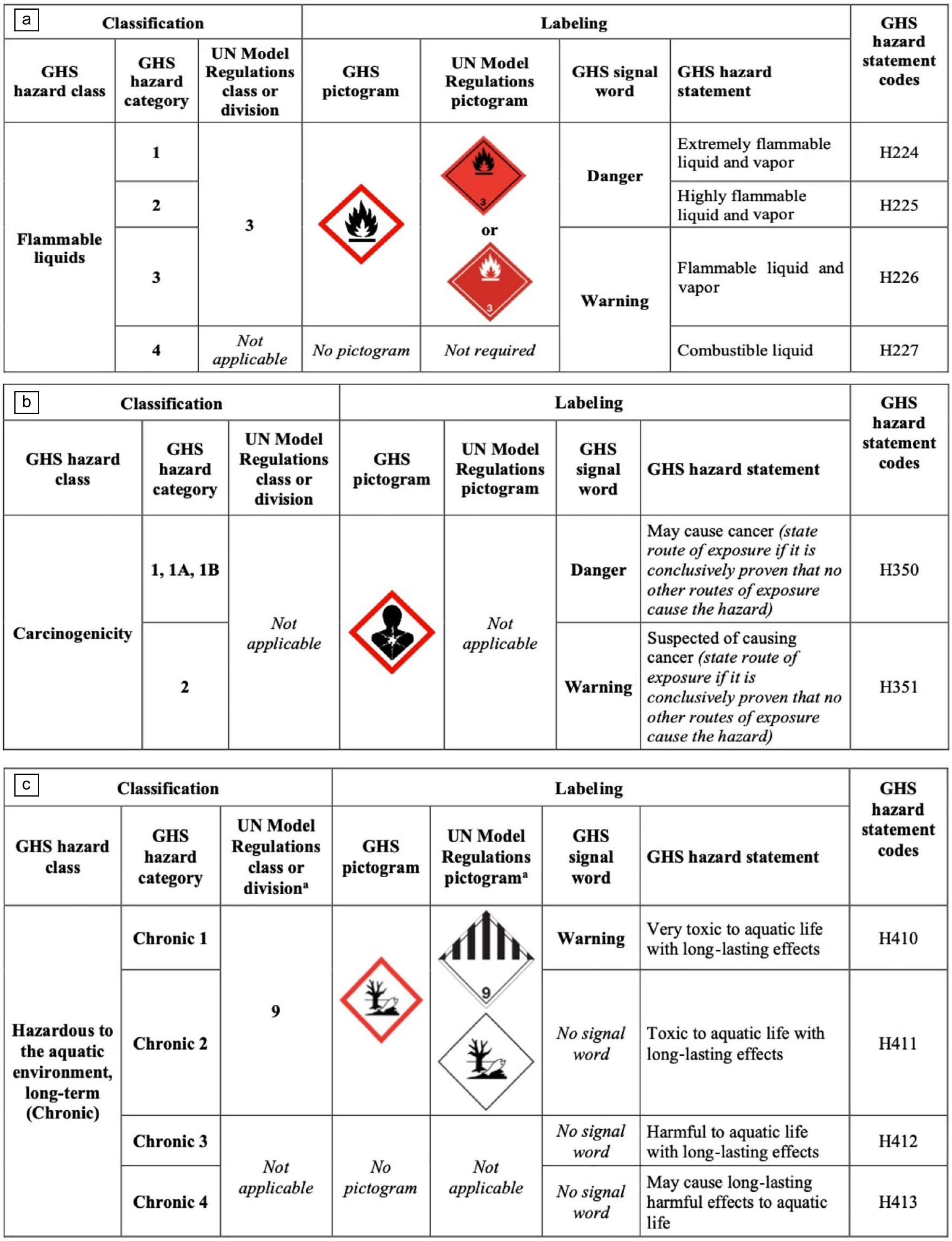
With respect to severity, Category 1 hazards are the most severe. If a chemical is "Not Classified," it means that the chemical is not hazardous enough to be assigned a category level. If data are insufficient to classify a hazard class, then "Classification is Not Possible." Some hazard classes have multiple category levels (e.g., Acute Toxicity has five), while others have only one (e.g., Aspiration). In **Figure** 2, taken from GHS Revision 10, we provide examples of how GHS classifies and labels hazards for physical, human health, and environmental hazards. Also included are the pictograms and GHS signal words used for labeling. Note that a Category 1 Flammable Liquid carries the H-statement code H224 and the accompanying H-statement phrase, "Extremely Flammable Liquid and Vapor;" a substance that is a Category 1 Carcinogen carries the H350 H-statement code and the accompanying H-statement phrase, "May Cause Cancer;" a substance that is a Category 1 for Aquatic Toxicity Chronic (long-term) carries the H410 H-statement code and the accompanying H-statement phrase, "Very Toxic to Aquatic Life with Long Lasting Effects."

Several methods for CHA have emerged to guide decision-making toward the use of safer chemicals. These CHA methods include the GreenScreen® for Safer Chemicals,[32] Cradle to Cradle Certification® Material Health Assessment,[33] and ChemFORWARD.[34] While these methods are all based primarily on GHS, they include additional hazard classes that are NOT currently in the GHS (i.e., endocrine disruption, persistence, and bioaccumulation potential). Each CHA method has an algorithm that integrates the hazard classification results, prioritizes them based on national and international regulatory and public health concerns, and assigns simple overall chemical ratings intended to help non-toxicologists choose safer chemicals and materials (and to avoid those that are highly

Table I. Hazard classes in the GHS Revision 10.[30]

Physical Hazards (H200 Series)	Human Health Hazards (H300 Series)	Environmental Hazards (H400 Series)

• Explosives
• Flammable gases
• Flammable aerosols
• Oxidizing gases
• Gases under pressure
• Flammable liquids
• Flammable solids
• Self-reactive substances
• Pyrophoric liquids/solids
• Self-heating substances and mixtures
• Substances and mixtures in contact with water, emit flammable gases
• Oxidizing liquids/solids
• Organic peroxides
• Corrosive to metals
	• Acute toxicity:
	  • Oral
	  • Dermal
	  • Inhalation
	• Skin corrosion/irritation
	• Serious eye damage/irritation
	• Respiratory sensitization
	• Skin sensitization
	• Germ cell mutagenicity
	• Carcinogenicity
	• Reproductive toxicity (includes developmental toxicity)
	• Specific target organ toxicity (STOT) single exposure
	• Specific target organ toxicity (STOT) repeated exposure
	• Aspiration hazard
		• Hazardous to aquatic environment (acute)
		• Hazardous to aquatic environment (chronic)
		• Harms public health/environment by destroying the ozone layer



a

Classification			Labeling				GHS hazard statement codes
GHS hazard class	GHS hazard category	UN Model Regulations class or division	GHS pictogram	UN Model Regulations pictogram	GHS signal word	GHS hazard statement	
Flammable liquids	1	3		or	Danger	Extremely flammable liquid and vapor	H224
	2					Highly flammable liquid and vapor	H225
	3				Warning	Flammable liquid and vapor	H226
	4	*Not applicable*	*No pictogram*	*Not required*		Combustible liquid	H227

b

Classification			Labeling				GHS hazard statement codes
GHS hazard class	GHS hazard category	UN Model Regulations class or division	GHS pictogram	UN Model Regulations pictogram	GHS signal word	GHS hazard statement	
Carcinogenicity	1, 1A, 1B	*Not applicable*		*Not applicable*	Danger	May cause cancer *(state route of exposure if it is conclusively proven that no other routes of exposure cause the hazard)*	H350
	2				Warning	Suspected of causing cancer *(state route of exposure if it is conclusively proven that no other routes of exposure cause the hazard)*	H351

c

Classification			Labeling				GHS hazard statement codes
GHS hazard class	GHS hazard category	UN Model Regulations class or division[a]	GHS pictogram	UN Model Regulations pictogram[a]	GHS signal word	GHS hazard statement	
Hazardous to the aquatic environment, long-term (Chronic)	Chronic 1	9			Warning	Very toxic to aquatic life with long-lasting effects	H410
	Chronic 2				*No signal word*	Toxic to aquatic life with long-lasting effects	H411
	Chronic 3	*Not applicable*	*No pictogram*	*Not applicable*	*No signal word*	Harmful to aquatic life with long-lasting effects	H412
	Chronic 4				*No signal word*	May cause long-lasting harmful effects to aquatic life	H413

Figure 2. GHS classification and labeling summary for (a) flammable liquids, (b) carcinogenicity, and (c) chronic aquatic toxicity.[30]

hazardous). The frameworks use different scoring nomenclature. For example, GreenScreen® uses Benchmarks 1–4, where 4 is least hazardous and ChemFORWARD uses Hazard Bands A–F, where A is least hazardous. Because these CHA methods are based on GHS and are designed to align with national and international hazard priorities, the scoring results are generally in agreement, even if communicated differently.

It can be overwhelming to gather and interpret comprehensive toxicological data. CHAs provide insight into the hazard profile of an existing chemical or material and readily communicate that information in a simplified way to help chemists and engineers make informed decisions. One source of CHAs is freely available at the website of the Interstate Chemicals Clearinghouse (IC2), a collaboration of state government entities.[35] The IC2 hosts a website called Knowledge-base, where users have a variety of search options.[36] In the Chemical Hazard Assessment Database (CHAD), users can search for existing GreenScreen® CHAs by chemical name or Chemical Abstract Services (CAS) registry number and directly link to the associated CHA report[37]

The IC2 Knowledge-base also links to ChemFORWARD resources including freely available CHAs.[38]

In ChemFORWARD, chemicals can be rapidly searched by name, numerical identifiers, or function and organized by industry sectors such as beauty and personal care, electronics, or packaging. The platform allows for a single, current CHA results per chemical to be displayed, and alternatives to be compared.[34] Another source of CHAs based on GHS is the for-profit entity Enhesa, which supports a subscription-based database called SciveraLENS®.[39]

If a CHA is not available for a chemical of interest, start by reviewing the Safety Data Sheets (SDSs),[40] which are required by law. They contain 16 sections and include requirements for composition information and hazard identification using the GHS system. While SDSs can be highly informative, they can also be incomplete and erroneous.

Table II contains key governmental databases that are helpful in evaluating substances based on hazard, and regulatory status. In the case of the US Environmental Protection Agency (EPA) Safer Chemical Ingredients List (SCIL),[41] the database supports finding safer alternatives for chemical functions tied to products certified via the Safer Choice Program. The data sources in **Table** II include information on GHS classifications, specific hazard classes such as carcinogenicity, occupational exposure limits designed to protect workers, and community exposure to industrial releases. Hazard list searching has been automated via a platform called Pharos.[42] Pharos allows users to search for a substance and summarizes all of the human and environmental hazard lists on which that substance is found. This "List Translator" is a useful step toward full CHAs and is also incorporated into ChemFORWARD and SciveraLENS®.

These governmental databases can be searched to identify the H-statement codes and hazards associated with some example substances listed in **Table** III.

CHA continues to evolve in response to advances in toxicology regarding (1) data sources, (2) new hazard classes, and (3) integration into various design and assessment schemes.

Data for CHAs have traditionally come from the scientific literature and standardized test results. Today, they are increasingly informed by new approach methods (NAMs), which are ways of evaluating hazard without the use of traditional animal testing. NAMs generate data using *in vitro* assays, *in silico* models, and machine learning.[49] Besides the benefit of avoiding harm to animals, NAMs are also relatively fast and inexpensive. The use of NAMs requires experts to

Table II. Key government databases for identifying substance hazards and GHS classifications.

Source and Link	Description
US EPA CompTox Chemicals Dashboard[43]	This database includes extensive information on more than 1.2 million chemicals. You can access GHS classifications by looking up a chemical and selecting from the Safety > GHS option on the left-hand menu.
European Chemicals Agency (ECHA) website[44]	Select the Search for Chemicals tab and search by name or CAS number. The initial Substance Info card identifies properties for concern. Select Brief Profile to see Substance Description and Scientific Properties. At the top of the Substance Description is a summary of GHS hazard classification and labeling results. Those classifications with a check mark are "harmonized" while the others are assigned by submitters but not considered harmonized.
International Agency for Research on Cancer (IARC)[45]	IARC is a specialized cancer agency of the World Health Organization (WHO). IARC classifies chemicals and other agents based on their potential to cause cancer in humans (Group 1 Carcinogenic to humans, Group 2A Probably carcinogenic to humans, Group 2B Possibly carcinogenic to humans, and Group 3 Not classifiable as to its carcinogenicity to humans). Information and classifications are found in the IARC Monographs via a searchable database.
NIOSH Pocket Guide—[46]	The NIOSH Pocket Guide to Chemical Hazards (NPG) is a concise reference published by the National Institute for Occupational Safety and Health (NIOSH), which is part of the US Centers for Disease Control and Prevention (CDC). It provides essential information on workplace chemical hazards, including exposure limits, safety precautions, and health effects.
US EPA Toxics Release Inventory (TRI)[47]	The TRI includes a public database managed by the US EPA that tracks the release and management of about 760 toxic chemicals by industrial facilities across the United States. The TRI Toxic Tracker—Reference 48—shows which toxic chemicals are released by facility and by location. Users can compare trends over time and monitor their community for chemical impacts.
US EPA Safer Chemical Ingredients List[41]	The Safer Chemical Ingredients List (SCIL) is a list of chemical ingredients, arranged by functional-use class, that the Safer Choice Program has evaluated and determined to be safer than traditional chemical ingredients. This list is designed to help manufacturers find safer chemical alternatives that meet the criteria of the Safer Choice Program.

Table III. Search databases for CHAs and GHS classifications for the following substances.

Chemical Name	CAS Number	Function
Benzene	71-43-2	Multiple
Hexabromocyclododecane (HBCD)	25637-99-4	Halogenated flame retardant
Polyphosphoric acids, ammonium salts	68333-79-9	Nonhalogenated flame retardant
Lead	7439-92-1	Multiple; see case study

integrate and weigh all of the toxicological evidence available (some of which may be conflicting) and to make expert judgments. Because NAMs are used to predict toxicity, they are increasingly being used to inform molecular and materials discovery and design. They allow us to evaluate hazards associated with chemicals and materials before they are even made.

New hazard classes and the associated hazard classification criteria that define them are also emerging. The EU uses GHS as part of their regulatory infrastructure but includes additional classifications and stricter criteria to address specific regulatory needs within the EU under their Classification, Labeling, and Packaging (CLP) Regulation ((EC) No. 1272/2008).[50] The key CLP hazard classes not (yet) in the GHS include substances as follows:

- Endocrine disruptors to human health and/or the environment,
- Persistent, bioaccumulative, and toxic (PBT)/very persistent very bioaccumulative (vPvB), and
- Persistent, mobile, and toxic (PMT)/very persistent very mobile (vPvM).[51]

The combined hazard classes (i.e., PBTs, PMTs) are important because they identify chemicals with inherent properties that result in increased exposure; thus, increasing risk.

CHAs are used in design and assessment schemes for both regulatory and nonregulatory purposes. Alternatives assessment has emerged as a science policy framework that is being used in support of regulations that seek to restrict chemicals of high concern as used in specific products or processes. It extends CHA by also considering exposure, cost and availability, performance, life-cycle impacts, circularity, and more. The goal of alternatives assessment is to determine whether there are viable alternatives to highly hazardous chemicals or materials, and to guide people toward the use of inherently safer alternatives, while avoiding unacceptable tradeoffs that may not be toxicity related.[52–55]

The EU Safe and Sustainable by Design (SSbD) Initiative[56] aims to benefit the development of chemicals and materials that are safe for human health and the environment, while promoting sustainability throughout their life cycle. SSbD integrates hazard reduction, resource efficiency, and circularity from the design phase to minimize risks and environmental impact. Similar to SIMS-D^3, SSbD emphasizes early-stage safety assessment and uses an iterative approach, fostering innovation in green chemistry.

One could argue that small amounts of hazardous substances do not pose an unacceptable risk to human health or the environment. For some hazards, that is true. However, not all hazards are of equal concern to the public and to regulatory experts. For example, many people are familiar and comfortable working with flammable substances such as fuels, but it can be difficult to explain to the average consumer why it is acceptable for a consumer product to contain even small amounts of chemicals that have been experimentally shown in various mammalian models to cause cancer or to disrupt the endocrine system in ways that may adversely affect children. Arguments about acceptable levels of cancer or risks to normal child development can fall on deaf ears for those whose primary concern is the health and well-being of their families. Engineers who must wear personal protective equipment (PPE) to safely work with certain substances in a laboratory should question the use of those substances in consumer products. Colleagues at the erstwhile US EPA Design for the Environment Program used to say, “if it’s not in your product, you don’t have to worry about it.” It is important to always ask: “Might alternatives be available that will perform adequately without having to worry about them in the laboratory, in the workplace, or for the public?”

Energy

When we think about materials and energy, we often consider the energy that can be saved by making more efficient products. Examples include increasing the fuel efficiency of aircraft through light-weighting or through improvements in engine efficiency (such as by operating at higher temperatures),[57] or increasing the energy-conversion efficiency of solar panels.[58] We could also think about advances in materials that enable renewable energy sources such as wind turbines and energy-storage systems as alternatives to fossil-fuel-based energy sources.[59] These material-enabled improvements in energy production and use scenarios are of course important to overall sustainability goals. In the context of SIMS-D^3, however, there is another important aspect of the intersection between materials and energy, and we generally refer to this as embodied energy; which is “the energy that must be committed to create 1 kg of usable materials, measured in MJ/kg.”[12] We can also refer to the embodied energy per unit weight (or volume) of a product, which then also

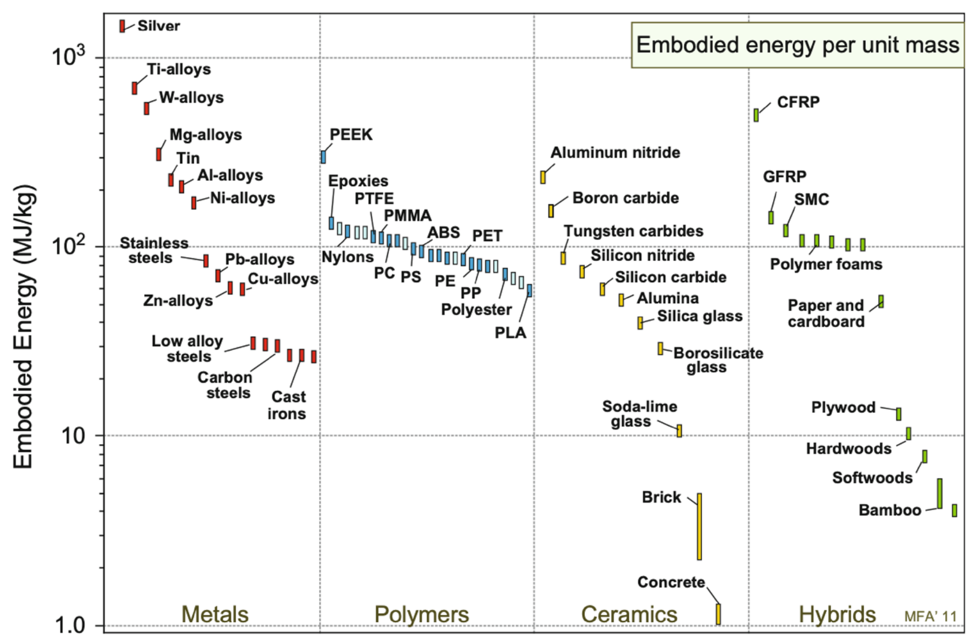


Figure 3. Embodied energy values for primary materials per unit mass; gold, not included in the chart, has a value of 240,000–265,000 MJ/kg. Reprinted with permission from Reference 12. © 2020 Elsevier.

considers the energy required to manufacture the bottle, not just produce the material. The importance of the concept of embodied energy is that materials themselves, and the products into which they are fabricated, require energy for processing and manufacturing, as well as for transport, and therefore impose a burden on the environment and human health due to the energy resources required ("embodied"), which lead to undesirable emissions of pollutants such as carbon dioxide, NO_x, and SO_x. The magnitude of the energy embodied in raw materials is captured, for instance, in a study by Cullen and Allwood,[60] which highlights that the embodied energy associated with materials production is approximately 30% of the total global energy flow. The primary sources for this energy, which include oil, coal, and gas, are known to produce negative impacts on the environment and on human health. Thus, for every kilogram of material produced, the associated embodied energy corresponds to negative human health and ecological impacts. These impacts can be avoided if (1) the energy required to produce the material is reduced, (2) the amount of material produced is reduced, (3) the primary energy sources used to produce the materials become "cleaner," or (4) materials with lower embodied energy values are selected for use. From a SIMS-D^3 perspective, we can focus on (4), and utilize data such as those illustrated in **Figure** 3,[12] to include embodied energy in our multi-attribute decision.

Another approach to considering energy in the context of SIMS-D^3 is through LCA. LCA is an analytical method by which the entire life cycle of a part, including raw materials production, product manufacturing, product use/reuse, and end-of-life management (recycling, landfilling, etc.) are considered and quantitatively evaluated from the perspective of the environmental and human health impact due to resource use (raw materials and energy) throughout the defined life cycle, as shown in **Figure** 4.[61] Outputs including atmospheric emissions, waterborne wastes, solid wastes, coproducts, and other releases are also quantitatively evaluated. The method is quantitative, relying on a detailed life-cycle inventory (LCI) of inputs and outputs, and builds on established (and evolving) environmental chemistry models that quantify environmental fate, exposure, and effects of chemicals, allowing us to conduct what is referred to as a life-cycle impact assessment (LCIA). The LCI step measures things we can quantify. The LCIA step converts these into things that we value, such as human health and the burden of disease, environmental and ecological health, and depletion of natural resources. Ultimately, an LCA should facilitate the selection of materials, manufacturing methods, use scenarios, and/or end-of-life management strategies that minimize negative impact, damage, or burden.

The earliest application of LCA was reported in the 1960s, with a focus on accounting for energy consumed in the use stage, not just in the manufacturing stage, given the energy crisis of that era. While early years led to the development of a variety of approaches and methodologies, the US Environmental Protection Agency formally defined LCA in 1993.[61] In 1997, the International Organization for Standardization (ISO) published ISO Standard 14,000, providing further definition to standardize the LCA approach, consisting of the following four steps: (1) definition of goal and scope, (2) inventory analysis (LCI), (3) impact assessment (LCIA), and (4) interpretation.[62] In 2002, the Life Cycle Initiative was initiated by the United Nations Environment Programme (UNEP) and the Society for Environmental Toxicology and Chemistry (SETAC), developing broadly applicable and standardized LCI databases and promoting harmonized methods for LCIA.[63] Although the effort required to

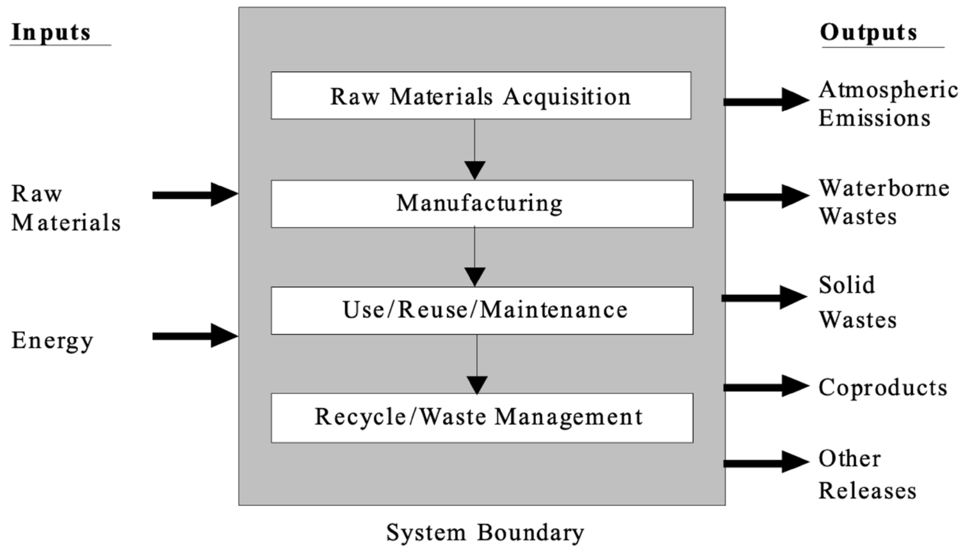


Figure 4. Life-cycle stages and system boundary defined in life-cycle assessment.[61]

complete an LCA is still extensive, existing resources allow for increased comparability across studies. Software platforms such as SimaPro and Sphera (formerly GaBi),[64,65] as well as open-source platforms such as openLCA,[66] are now widely used within the community, both in industry and in academia. Commonly used databases for LCI include Ecoinvent,[67] and ReCiPe and USEtox are commonly used to conduct the LCIA portion of the studies.[68,69] The literature on LCA studies, in general, has dramatically increased since the mid-2000s, as described in the study by Moutik et al.,[70] but the fraction focused specifically on materials is very small. There is an opportunity here to increase the application of LCA to support SIMS-D^3 decisions.

Circularity

Historically, the production, use, end-of-life cycle for goods have followed a linear path, similar to that depicted in Figure 4. In parallel with efforts to promote life-cycle thinking, as utilized in LCA, which lead to the reduction in resource inputs and emission outputs, significant efforts have been made in the last 15–20 years to promote what is now commonly referred to as a circular economy. This concept builds on the idea of avoiding the linear paradigm and instead motivating product reuse, remanufacturing, recycling, as well as materials recovery. Positive outcomes of this approach include reduced material waste (which leads to reduced energy waste, considering the concept of embodied energy noted above), reduced product waste, and overall reduced emissions and negative impacts on human health and the ecosystem. While this concept is broadly promoted by government (e.g., US EPA, National Institute of Standards and Technology (NIST), National Renewable Energy Laboratory (NREL), the EU, the United Nations, and the Organization for Economic Co-operation and Development (OECD)[71–77]), the Ellen MacArthur Foundation has aggressively endorsed this strategy,[78] as have numerous other nongovernment and industry organizations (e.g., the Cradle to Cradle Products Innovation Institute, and the REMADE Institute, which is funded by the US Department of Energy[79,80]). The economic benefits alone are fairly easy to conceptualize, thus providing incentives across sectors.

Another analytical tool in our SIMS-D^3 toolbox, material flow analysis (MFA), allows us to quantitatively track how specific materials are used, reused, recycled, recovered, or discarded. Graedel notes in his perspective article on MFA published in 2019[81] that the concept of MFA was first developed in the late 1980s to early 1990s, as part of the expansion of the field of industrial ecology, providing an important complement to LCA methodologies. Since that time, the methodology has expanded and become more refined, extending to more and more materials and mineral categories, developing appropriate and standardized software tools, extending material flow cycle details, expanding the boundary of analysis, and, of most relevance to the topic of circular economy, deriving recycling rates and recycled content. MFA results are commonly illustrated in Sankey diagrams, such as the one shown in **Figure** 5,[82] allowing for quick interpretation of current recycling activities. Because, as noted previously, materials represent embodied energy due to energy needed for primary production, product manufacturing, and end-of-life options such as materials recovery, an MFA can provide an important foundation for evaluating energy, both from the perspective of embodied energy and through LCA.

There are challenges with implementing a circular economy. A primary concern is the presence of toxic substances in products. Keeping these toxins circulating into new products is not beneficial to society, despite the potential reductions in waste. Note, for instance the recent example of plastic materials from electronic waste (e-waste, aka electronic scrap) being recycled into black cooking utensils and food storage containers.[83] While the avoidance of landfilling e-waste is a positive outcome, the continued presence of flame retardants (added to the plastics to prevent explosions and fires in their initial application) in these black plastics should preclude the material's use in cooking utensils, where direct exposure to humans in their food becomes problematic. Thus, designing products without toxic chemicals, which will

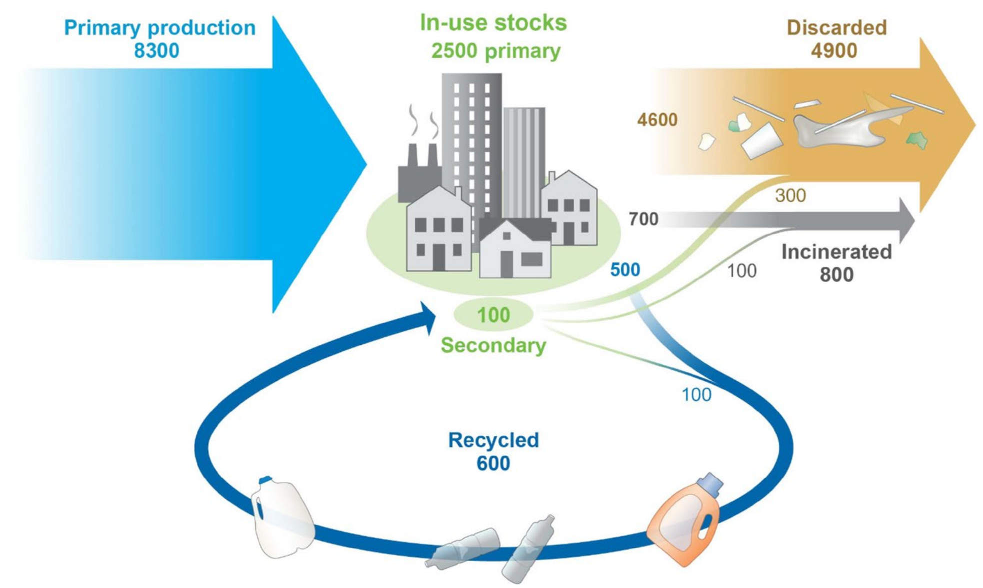


Figure 5. Global production, use, and fate of polymer resins, synthetic fibers, additives (1950 to 2015; in million metric tons).[82]

avoid the creation and recycling of toxic waste products must be the first step.

We must also recognize that every loop in the circular economy requires some resources. Reuse likely requires packing and/or transportation. Remanufacturing, recycling, and materials recovery require energy (thermal or mechanical) and/or chemicals (e.g., etchants and solvents). These additional resource (and waste/emission) profiles can and should be evaluated using tools such as CHA, LCA, and MFA to ensure a net benefit.

SIMS-D^3 case studies

Leaded materials

The malleable nature and low melting point of metallic lead (Pb) have made it an attractive material for various applications throughout history. Archeological evidence indicates that ancient Egyptians (ca. 1550–1070 BCE) used lead sulfide (galena) for manufacturing kohl, an eye cosmetic. The Romans expanded lead's use significantly, employing it in water pipes, cookware, and even as a sweetener for wine. They mined and smelted lead extensively, leading to widespread environmental contamination and adverse human population health effects, including cognitive decline.[84] During the Middle Ages, lead continued to be used in construction, particularly for roofing and windows in churches and cathedrals. The invention of the printing press in the fifteenth century led to widespread use of lead type for printing. The Industrial Revolution saw a surge in lead usage in paints, bullets, gasoline additives, energy-storage batteries, electronic products, and solar panels. Lead pipes remained common in plumbing systems well into the 20th Century. In the United States, lead-containing water distribution pipes remain a major public health problem, affecting up to 10% of homes or 22 million people.[85,86] The metal's ability to block radiation made it useful in the nuclear and medical industries, and ubiquitous cathode-ray tubes used in television sets contained leaded glass consisting of up to 40% lead oxide in some component parts.[87,88] As the understanding of lead's pervasive toxicity increased in the mid-20th century, regulations began to restrict its use. Lead was phased out of gasoline, paints, and plumbing in many countries. Despite these restrictions, lead remains in use today in certain applications such as car batteries and radiation shielding. Initiatives to phase-out lead from consumer electronic products was a protracted endeavor driven in part by regulatory policies, and challenged with uncertainties regarding safer alternatives to ensure performance expectations and economic feasibility.[89,90] Despite claims of high levels of recyclability, the continuing use of lead in automobile batteries remains a major source of environmental health risk for many polluted communities worldwide, and has implications for understanding the potential long-term risks posed by a new generation of energy-storage batteries and technologies being developed to address global climate change.[91–94] Unlike mercury, the only element for which a United Nations convention was established to curb its use,[95] it remains difficult to cultivate international regulatory and industrial agreement on the use of lead in various products. Examples of the wide range of commercial products manufactured with lead and its compounds are presented in **Table** IV. In many cases, epidemiological evidence of damage caused by lead to human health and well-being was necessary to stimulate regulatory policies banning or phasing out the use of lead in products and processes, and motivating the selection of sustainable alternatives. In other cases, innovative design strategies were essential for making the use of leaded materials irrelevant.[96,97] The history of lead usage reflects humanity's evolving understanding of materials science and sustainability. Lead's unique properties made it valuable for millennia; its toxic effects have led to a significant reduction in its use in recent decades, but more research is needed to find suitable safer alternatives and strategies for implementing SIMS-D^3 for leaded materials.

Table IV. Examples of products manufactured with lead (Pb) and its compounds, and the slow process of alternatives assessments that generated piecemeal replacement with sometimes equally or more hazardous chemicals and materials. In some cases, complete redesign of a product or process has been the sustainable strategy that avoids lead usage.

Commercial Product	Usage and Performance	Metallic Lead (Pb) and Compounds	Regrettable and Unsustainable Chemical Substitutions	Selected Potentially Safer Chemical Alternatives	Discovery, Design, and Development Solutions
Petrochemical gasoline	Octane booster	Tetraethyl lead	Methyl tert-butyl ether (MTBE) Methylcyclopentadienyl manganese tricarbonyl (MMT)	Ethanol	Contemporary automobile engines are designed to operate on lower-octane fuel without knocking, reducing the need for high-octane additives
Energy-storage batteries	*Electrodes:* Lead and lead dioxide are used for the negative and positive electrodes, respectively *Battery grid:* A lead alloy forms the supporting grid for the active material *Battery Casing:* Sometimes made of hard rubber or plastic, but may contain lead in older models	Metallic lead Lead oxide	Lithium-ion (Li-ion) batteries Nickel-metal hydride (NIMH) batteries	Sodium-ion Aluminum-air Solid-state *Flow batteries:* Vanadium redox Zinc-bromine Iron-chromium: Organic flow (e.g., quinones) Polysulfide-bromine Zinc-cerium Hydrogen-bromine All-iron Lithium-sulfur	Ultracapacitors made with activated carbon electrodes, but may contain risky acetonitrile-based electrolytes and halogenated binders
Surface-Coating Paints	Paint durability, corrosion resistance, color brilliance, and drying agent	Lead carbonate Lead chromate Lead tetroxide Lead sulfate Lead naphthenate Lead octoate	Chromium oxides Zinc chromate Cobalt-based driers Acrylic resins	Titanium dioxide Zinc oxide Barium sulfate Iron oxides Zinc phosphate Calcium phosphosilicate Zirconium-based driers Polyurethane resins	Modern building materials and design techniques have largely eliminated the need for lead paint. The Benefits of Paint-Free Design include: Reduced maintenance costs Elimination of VOCs associated with paint Potentially longer lifespan for building envelope More sustainable approach (less frequent repainting) Unique aesthetic possibilities
Electronic Printed Wiring (Circuit) Boards	Strong, reliable joining of electronic components; good electrical conductivity and excellent wetting and flow characteristics	Tin–lead solder (63% tin, 37% lead—eutectic composition)	Tin–antimony Tin–bismuth Tin–copper–nickel Indium-based alloys	Tin–silver–copper Nonmetallic Adhesives, consisting typically of polymer resins filled with carbon Anisotropic and Isotropic Conductive Adhesives	Innovation in solderless or mechanical electronic component connections, including "Press-fit Technology," "Magnetic Connections," and "Interlocking Printed Circuit Board Design"
Cathode-Ray Tubes	Radiation (x-ray) Shield	Leaded Glass (18–35% Lead Oxide)	Quantum dot light-emitting diode (QLED) displays due to toxic metal content	Liquid-Crystal Displays (LCDs) Light-Emitting Diode (LED) Displays Organic Light-Emitting Diode (OLED)	Laser projection, although the use of rare earth elements, and some potentially hazardous chemicals remain concerning for resource recovery and waste management

Table IV. (continued)

Commercial Product	Usage and Performance	Metallic Lead (Pb) and Compounds	Regrettable and Unsustainable Chemical Substitutions	Selected Potentially Safer Chemical Alternatives	Discovery, Design, and Development Solutions
Perovskite solar cells	Light-absorbing layers	Methylammonium lead iodide	Cadmium telluride (CdTe) cells III–V semiconductor cells: gallium arsenide (GaAs) Quantum dot solar cells: CdSe, PbS	Tin-based perovskites: $FASnI_3$ or $MASnI_3$ FA = formamidinium, MA = methylammonium	There are several alternative designs and technologies to capture and utilize the sun's energy without solar panels. These approaches vary in their level of development efficiency and applications. Examples are: Artificial Photosynthesis Solar Thermal Collectors
Pottery glazes	Glassiness Colorant and pigmentation	Lead oxide Red lead (Pb_3O_4) White lead ($2PbCO_3{\cdot}Pb(OH)_2$) Lead silicate ($PbSiO_3$) Lead bisilicate ($PbO{\cdot}2SiO_2$) Lead antimonate ($Pb_2Sb_2O_7$) Lead chromate ($PbCrO_4$) Lead tin oxide ($PbSnO_3$)	Lithium oxide (Li_2O)	Zinc oxide (ZnO) Calcium oxide (CaO) Feldspar ($KAlSi_3O_8$, $NaAlSi_3O_8$, or $CaAl_2Si_2O_8$)	Several design strategies and techniques have been developed to create functional pottery without using chemical glazes, including Unglazed high-fire ceramics Terra Sigillata Salt or soda firing
Water distribution pipes	Malleability Durability Joint sealing Low economic cost	Elemental lead Lead–antimony Tin–lead alloy	PVC (polyvinyl chloride) pipes can leach phthalates Cross-linked Polyethylene (PEX) Pipes may leach volatile organic compounds and methyl tertiary-butyl ether (MTBE) Epoxy linings may leach bisphenol-A	Copper Glass Ceramic	Rainwater harvesting systems Atmospheric water generators Decentralized water treatment Modular water systems Biological water purification
Projectile bullets	High density Ballistic performance Barrel wear tolerance Efficient energy transfer	Elemental lead Lead–antimony alloy Lead–tin alloy Lead–arsenic Lead styphnate ($C_6HN_3O_8Pb$) Lead azide ($Pb(N_3)_2$) Lead oxide (PbO)	Tungsten Polymer–metal composites	Copper Bismuth	Tranquilizer darts or projectiles Technologies for improved communication in tense situations Wildlife conservation strategies Directed energy weapons Electromagnetic pulse (EMP) devices Nets and entanglement systems Acoustic weapons Foam-based systems

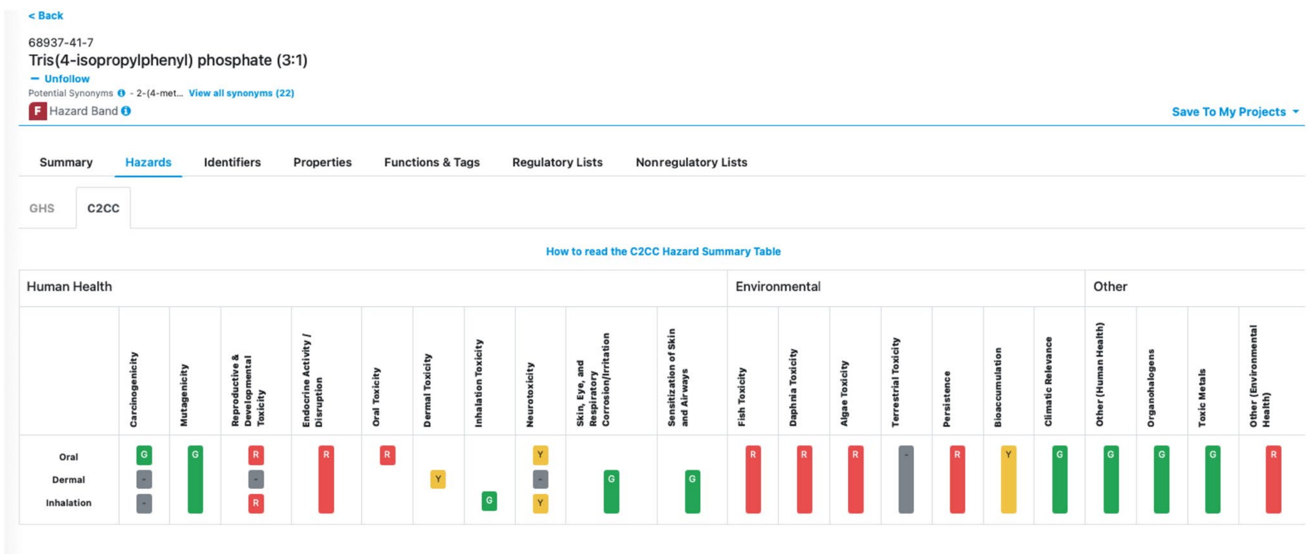


Figure 6. Summary hazard table from ChemFORWARD for tris(4-isopropylphenyl) phosphate (3:1) (PIP 3:1) (Cradle to Cradle Certified Material Health View). Reprinted with permission from Reference 34. © 2025 ChemFORWARD.

Flame retardants

Flame retardants are used in products worldwide to improve fire safety in many sectors, including buildings, automobiles, and electrical and electronic products. In some cases, manufacturers are required to perform standardized tests on materials and products to ensure that they meet minimum fire safety requirements. Materials that are not inherently fire retardant may need the addition of substances that reduce flammability to meet these requirements. Different flame retardants work by different chemical or physical mechanisms such as cooling, char formation, or gas phase inhibition.[98] Information has emerged that raises concern about the toxicity of some flame retardants, particularly those that are organohalogens or organophosphate esters.[99] These chemicals are added to plastics and other materials. Some of the chemicals slowly migrate out of the materials and are found in the surrounding environments, including air and dust.[99] The remaining flame retardant stays in the plastic or other material. If that plastic is recycled, then the flame retardant is recycled with it. This is especially unfortunate when the recycled plastic is then used in products that lead to direct exposure such as in cooking utensils and food storage containers, as previously noted.[83] The only way to ensure that hazardous additives do not leach out of products is to avoid the use of hazardous additives in the first place.

All companies must comply with regulations that restrict specific chemicals in products. Developing regulatory restrictions is usually a slow but predictable process because it is based on scientific evidence, concern for certain hazard classes, and likely exposure scenarios. By proactively avoiding chemicals that are likely to be regulated, we can avoid the enormous cost and difficulty of eliminating a chemical from a product or process after the fact. Proactive companies such as Apple and Google first screen chemicals used in their products[100,101] to avoid the use of those that are highly hazardous, reducing both health and business risks. The scientifically based hazard criteria that result in regulations are the same as the hazard criteria that result in high hazard scores in the CHA methods previously described. The following case study illustrates the wisdom of using CHA to avoid the selection of flame retardants that are highly hazardous, even if they are not (yet) regulated.

In 2021, the US EPA took expedited action and finalized rules restricting phenol, isopropylated phosphate (3:1) (also known as PIP 3:1, CAS No. 68937-41-7) from certain products and articles including those in electronics, aerospace, and manufacturing. The expedited action resulted in a mad scramble by industry to determine (1) if the flame retardant was in fact used in products, (2) if so, where and (3) what to replace it with. The EPA had to extend the deadline to October 2024 due to the inability of industry to comply on the expedited timeline.[102]

Had companies first evaluated these flame retardants (and other material additives) used in their products using comprehensive CHAs, they could have seen this coming. **Figure** 6 is a screenshot of the CHA for PIP 3:1 taken with permission from ChemFORWARD (using the Cradle to Cradle Material Health view). PIP 3:1 was scored as an "F" because it is endocrine disrupting, systemically toxic, persistent, and it has reproductive and developmental toxicity. These are hazards that define a substance of very high concern. In the ECHA database, it is currently being evaluated as a PBT,[103] which would officially classify it as a substance of very high concern.

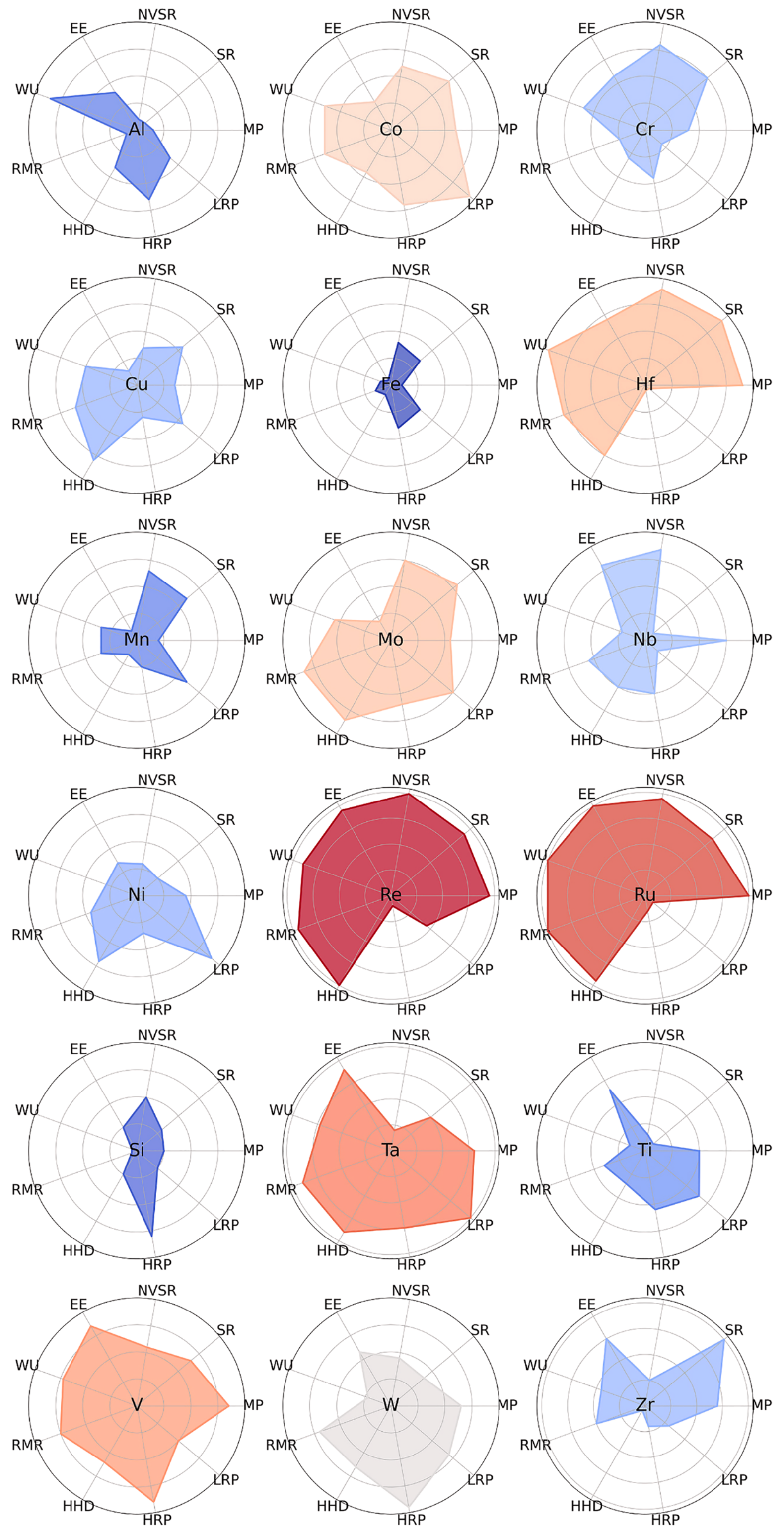


Figure 7. Radial plots—"footprints"—across 9 indicators for 18 elements. The further the distance from the center, the greater the (negative) impact. MP—material prices, SR—supply risk, NVSR—normalized vulnerability to supply risk, EE—embodied energy, WU—water usage, RMR—rock-to-metal ratio, HHD—human health damage, HRP—human rights pressure, LRP—labor rights pressure.[13]

The challenge to materials scientists and engineers is to consider chemical and material hazards early in the materials selection, discovery, and design process. To the extent that highly hazardous substances can be avoided, there will be benefits throughout the value chain. Future direction should include more education for engineers about how to find hazard information in support of SIMS-D^3 decision-making and to incorporate chemical hazard assessment early in the material discovery process.

Compositionally complex inorganic materials

The historical development of inorganic materials—metallic alloys and ceramics—for the wide range of applications in commerce has focused on fine-tuning chemistry and microstructure to enhance properties and performance. There are rare applications of pure metallic or even ceramic substances. Gold, for instance, is sometimes used in its pure form, but even gold is more commonly alloyed, due to its high price and the need to make the gold more resistant to deformation (i.e., less soft). Thus, gold is commonly alloyed with silver, copper, and/or zinc, as well as platinum, palladium, iron, cadmium, aluminum, and/or nickel. As another example, high-purity silicon is used for electronic applications, but even silicon wafers ultimately are doped with other elements (e.g., boron and phosphorus, as well as aluminum, gallium, indium, arsenic, and antimony) to produce integrated circuits. More commonly, metals are highly alloyed, traditionally with one principal element (e.g., aluminum, copper, iron in steel, nickel in superalloys) corresponding to at least 50% and commonly more than 90% of the alloy composition. Recently, however, significant materials research, discovery, and development have focused on "multi-principal element alloys" (MPEAs), also known as "complex concentrated alloys" (CCAs), which consist of three or more metallic elements in nearly equal concentrations. Much of the literature refers to these materials as "high-entropy alloys" (HEAs), as some of the compositions appear to be stabilized by entropy when equiatomic ratios of three or more elements are included in the alloy. Similarly, in the ceramics domain, compositionally complex (also known as high entropy or "entropy stabilized") oxides, carbides, borides, silicides, etc., are also an area of active research.

While the discovery of these materials has led to the potential for enhanced performance in many performance domains, their increased complexity presents challenges from the perspective of SIMS-D^3. Many of the elements/oxides being included in the compositions are toxic, in short supply, and/or complex to source/refine. These issues already exist for traditional alloys, but with the increasing concentration of each element in these new alloys, the consequences increase proportionally. Moreover, from a circular economy perspective, the concern over recycling materials that contain toxins continues, and moreover, the complexity to separate and reuse any of the alloying elements has become consequentially much more difficult. Fortunately, there have been a few recent studies on the sustainability issues related to these materials, as briefly discussed below, but clearly more work is needed to promote SIMS-D^3 strategies early in the materials discovery and design stage, to avoid regrettable choices.

One of the first studies on the "sustainability-related issues" associated with the complex compositional space of HEAs was published by Fu et al. in 2017.[104] They first performed elemental screening based on material price, price volatility, and resource availability (using the Herfindahl–Hirschman index, HHI). Their additional analysis of these metrics for the multicomponent alloys assumed compositionally weighted average values, as is commonly done in the literature, leading them to conclude that for some alloy compositions, dilution leads to benefits, but many alloying elements, such as precious metals, platinum group metals, scandium, germanium, tellurium, tantalum, cobalt, vanadium, and zirconium should be avoided. From a circularity perspective, the potential to recycle these novel alloy compositions in existing metal recovery streams is evaluated, indicating limited positive paths forward.

Two additional recent studies on HEAs explored a broader range of sustainability attributes.[13,105] The study by Wang et al.[105] evaluated resource availability (using data from the US Geological Survey, USGS), material price (assuming alloy price is determined by compositionally weighted average values), and CHA (using GreenScreen® for Safer Chemicals). Their study concludes that chromium and vanadium should be avoided due to their carcinogenicity, rhenium should be limited in use due to price, and hafnium and vanadium present scarcity and cost issues. The need to develop recycling technology to recapture these scarce elements is also noted. Gorsse et al.[13] evaluated 340 HEAs as potential substitutes for steels and/or high-temperature nickel-based superalloys using nine sustainability attributes, grouped into three topical areas: economic viability, environmental impact, and human well-being. The results for the 18 metallic elements studied are shown in **Figure** 7; for these charts, low values are preferred and therefore larger colored areas are less desirable. They conclude by recommending that complex HEAs (and novel superalloy compositions) avoid the use of rhenium, ruthenium, tantalum, vanadium, molybdenum, hafnium, cobalt, and tungsten.

For ceramic materials, the evaluations can be more complex, because the established databases for pricing data, resource availability, or chemical hazard end points either do not exist or are far less robust than those for elemental metals (which are already limited in scope). Consequently, there are no known studies using a sustainability perspective to screen, select, or design compositionally complex ceramics.

There are two recent publications that apply machine learning/artificial intelligence to screen hypothetical compositions for magnets.[106,107] Vishina et al.[106] used a high-throughput screening technique to evaluate approximately one million not-yet-synthesized crystal structures to identify promising novel rare earth-free permanent magnetic materials. As part of the screening step, the authors applied the following sustainability-based screening criteria: excluding "all the materials with rare earth elements, as well as the elements that are expensive, difficult to work with experimentally, and radioactive." While this is a very limited screening protocol, at least some acknowledgment of the need to screen for sustainability at these early materials discovery stages is a step in the right direction. Zeni et al.[107] used a new generative artificial intelligence model, called MatterGen, to design "low-supply-chain-risk magnets." Here, the authors include the HHI score used previously by Fu et al.[104] as one of the property constraints. While adding supply risk to the performance criteria is again a step forward, it is unclear how the authors of this study applied this method to oxide compositions, as all available HHI data are uniquely for elements; it appears that they utilized HHI values for the cations, and for oxygen, and applied a compositionally weighted average approach.

While these limited publications indicate a growing appreciation for including sustainability attributes when designing these compositionally complex inorganic materials, the primary focus is on economic attributes, which are easier to measure and compare, with limited efforts to robustly address toxicity, circularity, or embodied energy.

Concluding remarks

Sustainability is now a ubiquitous reference target toward which corporations, individuals, and academics strive to make credible advances. We can make the most impact by incorporating sustainability metrics into the materials selection, discovery, design, and development process as early in the design stage as possible—this includes at the fundamental research stage. In addition to the sustainability metrics described in this paper (toxicity, energy, circularity), corporate responsibility and environmental justice concerns should also be carefully considered, as well as supply risks and material criticality. Advances in data science, informatics, machine learning, and artificial intelligence, in combination with computational materials science, will enhance our ability to make these SIMS-D^3 decisions early in the design stage. Challenges remain for properly assessing alloys, mixtures, and products, which are becoming increasingly complex. Innovative strategies and increased engagement are needed to advance these critical areas.

Author contributions

J.M.S. had the original idea for the article and developed the content scope. J.M.S., O.A.O., and L.G.H. contributed equally to performing the literature review and writing the manuscript. All authors contributed to refining the manuscript draft and reviewing the final version.

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Conflict of interest

J.M.S. is a member of the Green Ribbon Science Panel (GRSP) associated with the Department of Toxic Substances Control (DTSC) at the California Environmental Protection Agency (Cal EPA). O.A.O. and L.G.H. are co-chairs of the Green Chemistry Advisory Board for Apple Inc. L.G.H. is co-founder and Strategic Advisor, ChemFORWARD.

References

1. J.E. Moore, A. Mascarenhas, J. Bain, S.E. Straus, *Implement. Sci.* **12**, 110 (2017). https://doi.org/10.1186/s13012-017-0637-1
2. R.W. Kates, W.C. Clark, R. Corell, J.M. Hall, C.C. Jaeger, I. Lowe, J.J. McCarthy, H.J. Schellnhuber, B. Bolin, N.M. Dickson, S. Faucheux, *Science* **292**(5517), 641 (2001). https://doi.org/10.1126/science.1059386
3. W.C. Clark, *Proc. Natl Acad. Sci. U.S.A.* **104**(6), 1737 (2007). https://doi.org/10.1073/pnas.0611291104
4. G.E. Dieter (ed.), *ASM Handbook*, *Vol. 20: Materials Selection and Design* (ASM International, Materials Park, 1997)
5. J.M. Schoenung, E.A. Olivetti, *MRS Bull.* **48**(4), 362 (2023). https://doi.org/10.1557/s43577-023-00521-8
6. United Nations Environment Programme, International Resource Panel, *Global Resources Outlook 2024: Bend the Trend—Pathways to a Liveable Planet as Resource Use Spikes* (United Nations Environment Programme, Nairobi, 2024). https://wedocs.unep.org/20.500.11822/44901
7. J.R. Mihelcic, J.C. Crittenden, M.J. Small, D.R. Shonnard, D.R. Hokanson, Q. Zhang, H. Chen, S.A. Sorby, V.U. James, J.W. Sutherland, J.L. Schnoor, *Environ. Sci. Technol.* **37**(23), 5314 (2003). https://doi.org/10.1021/es034605h
8. D.C.A. Pigosso, H. Rozenfeld, P. Ferrao, *J. Clean. Prod.* **18**(15), 1464 (2010)
9. M.D. Bovea, J.M. Pérez-Bella, *J. Clean. Prod.* **28**, 1 (2012)
10. S. Kara, M. Işık, *J. Clean. Prod.* **142**, 1757 (2017)
11. E.A. Olivetti, J.M. Cullen, *Science* **360**(6396), 1396 (2018). https://doi.org/10.1126/science.aat6821
12. M.F. Ashby, *Materials and the Environment: Eco-Informed Material Choice*, 3rd edn. (Elsevier, 2020)
13. S. Gorsse, T. Langlois, M.R. Barnett, *Sustain. Mater. Technol.* **40**, e00938 (2024). https://doi.org/10.1016/j.susmat.2024.e00938
14. B. Ness, E. Urbel-Piirsalu, S. Anderberg, L. Olsson, *Ecol. Econ.* **60**(3), 498 (2007). https://doi.org/10.1016/j.ecolecon.2006.07.023
15. O.A. Ogunseitan, J.M. Schoenung, *MRS Bull.* **37**(4), 356 (2012). https://doi.org/10.1557/mrs/2012.8
16. O.A. Ogunseitan, *MRS Bull.* **48**(4), 368 (2023). https://doi.org/10.1557/s43577-023-00518-3
17. N. Singh, O.A. Ogunseitan, M.H. Wong, Y. Tang, *Sustain. Horiz.* **2**, 100016 (2022). https://doi.org/10.1016/j.horiz.2022.100016
18. G. Wernet, C. Bauer, B. Steubing, J. Reinhard, E. Moreno-Ruiz, B. Weidema, *Int. J. Life Cycle Assess.* **21**(9), 1218 (2016). https://doi.org/10.1007/s11367-016-1087-8
19. M.Z. Hauschild, R.K. Rosenbaum, S.I. Olsen (eds.), *Life Cycle Assessment: Theory and Practice* (Springer, Cham, 2018). https://doi.org/10.1007/978-3-319-56475-3
20. O.A. Ogunseitan, J.M. Allgood, S.C. Hammel, J.M. Schoenung, *Environ. Sci. Technol.* **47**(22), 12625 (2013). https://doi.org/10.1021/es4040864
21. M.G. Ibrahim, H. He, J.M. Schoenung, O.A. Ogunseitan, *JOM* **75**(12), 5021 (2023). https://doi.org/10.1007/s11837-023-06267-7
22. O.A. Ogunseitan, J.M. Schoenung, J. Lincoln, B.H. Nguyen, K. Strauss, K. Frost, E. Schwartz, H. He, M. Ibrahim, *Nat. Rev. Mater.* **7**(10), 749 (2022). https://doi.org/10.1038/s41578-022-00485-2
23. H. Weisz, S. Suh, T.E. Graedel, *Proc. Natl. Acad. Sci. U.S.A.,* **112**(20), 6260 (2015). https://doi.org/10.1073/pnas.1506532112
24. X. Zeng, O.A. Ogunseitan, S. Nakamura, S. Suh, U. Kral, J. Li, Y. Geng, *Circ. Econ.* **1**(1), 100003 (2022). https://doi.org/10.1016/j.cec.2022.100003
25. O.A. Ogunseitan, *One Earth* **5**(11), 1189 (2022). https://doi.org/10.1016/j.oneear.2022.10.016
26. P.T. Anastas, J.C. Warner, *Green Chemistry: Theory and Practice* (Oxford University Press, New York, 1998), p. 30
27. M.H. Whittaker, L. Heine, *Patty's Toxicology: Chemical Alternatives Assessment,* 7th edn. (Wiley, Hoboken, 2023). https://doi.org/10.1002/0471125474.tox172
28. United Nations Economic Commission for Europe (UNECE), About the GHS (UNECE, 2025). https://unece.org/about-ghs. Accessed 15 Feb 2025
29. United Nations Commission on Sustainable Development, Agenda 21, Chapter 19, Environmentally Sound Management of Toxic Chemicals, Including Prevention of Illegal International Traffic in Toxic and Dangerous Products, *United Nations Conference on Environment & Development* (Rio de Janeiro, June 3–14, 1992). https://sustainabledevelopment.un.org/content/documents/Agenda21.pdf. Accessed 15 Feb 2025
30. United Nations Economic Commission for Europe (UNECE), Globally Harmonized System of Classification and Labelling of Chemicals (GHS Rev. 10) (UNECE, 2023). https://unece.org/transport/dangerous-goods/ghs-rev10-2023. Accessed 15 Feb 2025
31. United Nations Economic Commission for Europe (UNECE), GHS Implementation by country (UNECE, 2023). https://unece.org/sites/default/files/2023-11/GHS%20implementation%20by%20country_2023-11.pdf (link to https://unece.org/ghs-implementation-0). Accessed 15 Feb 2025
32. About GreenScreen® for Safer Chemicals (n.d.). https://www.greenscreenchemicals.org/assess/about-greenscreen-for-safer-chemicals. Accessed 15 Feb 2025
33. Cradle to Cradle Certified® Material Health Assessment Methodology (2025). https://c2ccertified.org/the-standard. Accessed 15 Feb 2025
34. ChemFORWARD, Turning Chemical Data into Positive Impact (n.d.). https://www.chemforward.org/. Accessed 15 Feb 2025
35. The Interstate Chemicals Clearinghouse (n.d.). https://www.theic2.org/. Accessed 15 Feb 2025
36. The Interstate Chemicals Clearinghouse Knowledgebase (n.d.). https://www.theic2.org/knowledgebase/. Accessed 15 Feb 2025
37. The Interstate Chemicals Clearinghouse, Chemical Hazard Assessments Database (CHAD) (2025). https://www.theic2.org/hazard-assessment-database/. Accessed 15 Feb 2025
38. The Interstate Chemicals Clearinghouse, ChemFORWARD Resources (2025). https://www.theic2.org/chemforward-resources/. Accessed 15 Feb 2025
39. Enhesa. SciveraLENS® (n.d.). https://www.enhesa.com/sustainablechemistry/support/user-guide-sciveralens/welcome-to-sciveralens/. Accessed Feb 2025
40. Occupational Safety and Health Administration (OSHA), OSHA Brief. Hazard Communication Standard: Safety Data Sheets (n.d.). https://www.osha.gov/sites/

default/files/publications/OSHA3514.pdf#:~:text=The%20information%20contained%20in%20the,the%20contents%20of%20the%20SDSs. Accessed 15 Feb 2025
41. US Environmental Protection Agency, Safer Chemical Ingredients List (SCIL) (n.d.). https://www.epa.gov/saferchoice/safer-ingredients#scil. Accessed 15 Feb 2025
42. Pharos, Search Pharos (2025). https://pharos.habitablefuture.org. Accessed 15 Feb 2025
43. US Environmental Protection Agency, CompTox Chemicals Dashboard (n.d.). https://comptox.epa.gov/dashboard/. Accessed 15 Feb 2025
44. European Chemicals Agency (ECHA) website, https://echa.europa.eu/information-on-chemicals. Accessed 15 Feb 2025
45. The International Agency for Research on Cancer (IARC), Classifications (n.d.). https://monographs.iarc.who.int/agents-classified-by-the-iarc/. Accessed 15 Feb 2025
46. National Institute for Occupational Safety and Health (NIOSH), *NIOSH Pocket Guide to Chemical Hazards* (n.d.). https://www.cdc.gov/niosh/npg/default.html. Accessed 15 Feb 2025
47. U.S. Environmental Protection Agency, Toxics Release Inventory (TRI) Program (n.d.). https://www.epa.gov/toxics-release-inventory-tri-program. Accessed 15 Feb 2025
48. US Environmental Protection Agency, Toxics Release Inventory Toxics Tracker (n.d.). https://edap.epa.gov/public/extensions/TRIToxicsTracker/TRIToxicsTracker.html. Accessed 15 Feb 2025
49. J. Abedini, B. Cook, S. Bell, X. Chang, N. Choksi, A.B. Daniel, D. Hines, A.L. Karmaus, K. Mansouri, E. McAfee, J. Phillips, J. Rooney, C. Sprankle, D. Allen, W. Casey, N. Kleinstreuer, *Comput. Toxicol.* **20**, 100184 (2021). https://doi.org/10.1016/j.comtox.2021.100184
50. European Chemicals Agency, Understanding CLP (n.d.). https://echa.europa.eu/regulations/clp/understanding-clp. Accessed 15 Feb 2025
51. European Chemicals Agency, New Hazard Classes 2023. https://echa.europa.eu/new-hazard-classes-2023. Accessed 15 Feb 2025
52. California Department of Toxic Substances Control (DTSC), Safer Consumer Products, Alternatives Analysis (n.d.). https://dtsc.ca.gov/scp/alternatives-analysis/. Accessed 15 Feb 2025
53. Washington Department of Ecology, Safer Chemicals for Manufacturers (n.d.). https://ecology.wa.gov/regulations-permits/guidance-technical-assistance/safer-alternatives/safer-chemicals-for-manufacturers. Accessed 15 Feb 2025
54. Interstate Chemicals Clearinghouse (IC2), *Alternatives Assessment Guide* (v1.2) (2017). https://www.theic2.org/alternatives-assessment-guide/. Accessed 15 Feb 2025
55. National Research Council, *A Framework to Guide Selection of Chemical Alternatives* (National Academies Press, Washington, DC, 2014). https://nap.nationalacademies.org/catalog/18872/a-framework-to-guide-selection-of-chemical-alternatives. Accessed 15 Feb 2025
56. E. Abbate, I. Garemendia Aguirre, G. Bracalente, L. Mancini, D. Tosches, K. Rasmussen, M.J. Bennett, H. Rauscher, S. Sala, *Safe and Sustainable by Design Chemicals and Materials—Methodological Guidance* (Publications Office of the European Union, Luxembourg, 2024). https://doi.org/10.2760/28450
57. X.S. Zheng, D. Rutherford, *Fuel Burn of New Commercial Jet Aircraft: 1960–2019*, White Paper (International Council on Clean Transportation, 2020). https://theicct.org/sites/default/files/publications/Aircraft-fuel-burn-trends-sept2020.pdf. Accessed 15 Feb 2025
58. National Research Energy Laboratory (NREL), Best Research-Cell Efficiencies (2025). https://www.nrel.gov/pv/assets/pdfs/best-research-cell-efficiencies.pdf. Accessed 15 Feb 2025
59. P. Moriarty, P. Veers, Land-Based Wind Research (National Energy Research Laboratory (NREL), 2025). https://www.nrel.gov/wind/land-based-wind.html. Accessed 15 Feb 2025
60. J.M. Cullen, J.M. Allwood, *Energy Policy* **38**(1), 75 (2010). https://doi.org/10.1016/j.enpol.2009.08.054
61. US Environmental Protection Agency (EPA), Life-Cycle Assessment: Inventory Guidelines and Principles (EPA/600/SR-92/245) (EPA, Washington, DC, 1993)
62. ISO 14000 Family, Environmental Management (n.d.). https://www.iso.org/standards/popular/iso-14000-family. Accessed 15 Feb 2025
63. United Nations Environment Programme, Life Cycle Initiative (n.d.). https://www.lifecycleinitiative.org. Accessed 15 Feb 2025
64. Pre Sustainability, SimaPro, LCA Software for Informed Changemakers (n.d.). https://simapro.com. Accessed 15 Feb 2025
65. LCA Software Directory, Sphera (GaBi) (February 23, 2024). https://lca-software.org/sphera-gabi/. Accessed 15 Feb 2025
66. GreenDelta GmbH, openLCA, Leading the Future of LCA Software (n.d.). https://www.openlca.org. Accessed 15 Feb 2025
67. ecoinvent, The Worlds' Most Transparent Life Cycle Inventory Database (n.d.). https://ecoinvent.org. Accessed 15 Feb 2025
68. National Institute for Public Health and the Environment, Ministry of Health, Welfare and Sport, LCIA: The ReCiPe Model (October 29, 2024). https://www.rivm.nl/en/life-cycle-assessment-lca/recipe. Accessed 15 Feb 2025
69. USEtox Team, USEtox Scientific Consensus Model (n.d.). https://usetox.org. Accessed 15 Feb 2025
70. B. Moutik, J. Summerscales, J. Graham-Jones, R. Pemberton, *Sustainability* **15**(18), 13408 (2023). https://doi.org/10.3390/su151813408
71. US Environmental Protection Agency, What is a Circular Economy? (n.d.). https://www.epa.gov/circulareconomy/what-circular-economy. Accessed 15 Feb 2025.
72. K. Schumacher, M. Seitz, N. Last, Circular Economy (National Institute of Standards and Technology (NIST), US Department of Commerce, Gaithersburg, 2025). https://www.nist.gov/circular-economy. Accessed 15 Feb 2025
73. G. Heath, Circular Economy Modeling and Analysis (National Renewable Energy Laboratory (NREL), 2025). https://www.nrel.gov/analysis/circular-economy-modeling-analysis.html. Accessed 15 Feb 2025
74. European Parliament, Circular Economy: Definition, Importance and Benefits (May 24, 2023). https://www.europarl.europa.eu/topics/en/article/20151201STO05603/circular-economy-definition-importance-and-benefits. Accessed 15 Feb 2025
75. United Nations Development Programme (UNDP), What Is Circular Economy and Why Does It Matter? (UNDP, April 24, 2023). https://climatepromise.undp.org/news-and-stories/what-is-circular-economy-and-how-it-helps-fight-climate-change. Accessed 15 Feb 2025
76. United Nations Environment Programme (UNEP), Understanding Circularity (UNEP, 2025). https://buildingcircularity.org. Accessed 15 Feb 2025
77. O. Romano, Circular Economy in Cities and Regions (Organisation for Economic Co-operation and Development (OECD), n.d.). https://www.oecd.org/en/topics/circular-economy-in-cities-and-regions.html. Accessed 15 Feb 2025
78. Ellen MacArthur Foundation, Circular Economy Introduction (n.d.). https://www.ellenmacarthurfoundation.org/topics/circular-economy-introduction/overview. Accessed 15 Feb 2025
79. Cradle to Cradle Products Innovation Institute, Product Circularity, Verified (n.d.). https://c2ccertified.org/. Accessed 15 Feb 2025
80. Sustainable Manufacturing Innovation Alliance Corp., REMADE Institute, A Division of the Sustainability Manufacturing Innovation Alliance Corp. https://remadeinstitute.org. Accessed 15 Feb 2025
81. T.E. Graedel, *Environ. Sci. Technol.* **53**, 12188 (2019). https://doi.org/10.1021/acs.est.9b03413
82. R. Geyer, J.R. Jambeck, K. Lavender Law, *Sci. Adv.* **3**(7), e1700782 (2017). https://doi.org/10.1126/sciadv.1700782
83. M. Liu, S.H. Brandsma, E. Schreder, *Chemosphere* **365**, 143319 (2024). https://doi.org/10.1016/j.chemosphere.2024.143319
84. J.R. McConnell, N.J. Chellman, A. Plach, S.M. Wensman, G. Plunkett, A. Stohl, N.K. Smith, B. Møllesøe Vinther, D. Dahl-Jensen, J.P. Steffensen, D. Fritzsche, *Proc. Natl. Acad. Sci. U.S.A.* **122**(3), e2419630121 (2025). https://doi.org/10.1073/pnas.2419630121
85. M. Hanna-Attisha, J. LaChance, R.C. Sadler, A. Champney Schnepp, *Am. J. Public Health* **106**(2), 283 (2016). https://doi.org/10.2105/AJPH.2015.303003
86. R.J. Santucci Jr., J.R. Scully, *Proc. Natl. Acad. Sci. U.S.A.* **117**(38), 23211 (2020). https://doi.org/10.1073/pnas.1913749117
87. S.E. Musson, Y.-C. Jang, T.G. Townsend, I.-H. Chung, *Environ. Sci. Technol.* **34**(20), 4376 (2000). https://doi.org/10.1021/es0009020
88. S. Shams, "Solution and Challenges in Recycling Waste Cathode-Ray Tube," in *E-waste Recycling and Management: Present Scenarios and Environmental Issues,* Environmental Chemistry for a Sustainable World Series, vol. 33, ed. by A. Khan, Inamuddin, A.M. Asiri (Springer, Cham, 2020), pp. 1–17. https://doi.org/10.1007/978-3-030-14184-4_1
89. J.M. Schoenung, O.A. Ogunseitan, J.D.M. Saphores, A.A. Shapiro, *J. Ind. Ecol.* **8**(4), 59 (2004). https://doi.org/10.1162/1088198043630496
90. O.A. Ogunseitan, *JOM* **59**(7), 12 (2007). https://doi.org/10.1007/s11837-007-0082-8
91. O.A. Ogunseitan, *Environ. Sci. Technol.* **50**(16), 8401 (2016). https://doi.org/10.1021/acs.est.6b03174
92. B. Tarroja, J.M. Schoenung, O. Ogunseitan, A. Kendall, Y. Qiu, T. Malloy, J. Peters, J.M. Cha, D. Mulvaney, O. Heidrich, M. Baumann, *iScience* **27**(6), 109898 (2024). https://doi.org/10.1016/j.isci.2024.109898
93. G. Schileo, G. Grancini, *J. Mater. Chem. C* **9**(1), 67 (2021). https://doi.org/10.1039/D0TC04552G
94. A. Babayigit, H.G. Boyen, B. Conings, *MRS Energy Sustain.* **5**, E1 (2018). https://doi.org/10.1557/mre.2017.17

95. O.A. Ogunseitan, *Environ. Sci. Policy Sustain. Dev.* **59**(4), 4 (2017). https://doi.org/10.1080/00139157.2017.1325299
96. O.A. Ogunseitan, T.R. Smith, *Afr. J. Environ. Sci. Technol.* **1**(2), 27 (2007)
97. World Health Organization, *Exposure to Lead: A Major Public Health Concern: Preventing Disease Through Healthy Environments,* 3rd edn. (World Health Organization, Geneva, August 16, 2023). https://www.who.int/publications/i/item/9789240078130
98. SGS Polymer Solutions Inc., 5 Major Categories of Flame Retardants (August 23, 2016). https://www.polymersolutions.com/major-categories-flame-retardants/. Accessed 15 Feb 2025
99. A. Blum, M. Behl, L.S. Birnbaum, M.L. Diamond, A. Phillips, V. Singla, N.S. Sipes, H.M. Stapleton, M. Venier, *Environ. Sci. Technol. Lett.* **6**, 638 (2019). https://doi.org/10.1021/acs.estlett.9b00582
100. Apple, *Environmental Progress Report*. https://www.apple.com/environment/pdf/Apple_Environmental_Progress_Report_2024.pdf. Accessed 15 Feb 2025
101. Google Sustainability, A Proactive Approach to Safer Product Materials (September 2023). https://sustainability.google/operating-sustainably/stories/safer-product-materials/. Accessed 15 Feb 2025
102. Federal Register, Vol. 89, No. 223. Tuesday November 19, 2024. Rules and Regulations. Environmental Protection Agency. 40 CFR Part 751. Decabromodiphenyl Ether and Phenol, Isopropylated Phosphate (3:1). Revision to the Regulation of Persistent, Bioaccumulative and Toxic Chemicals Under the Toxic Substances Control Act (TSCA). https://www.govinfo.gov/content/pkg/FR-2024-11-19/pdf/2024-25758.pdf. Accessed 15 Feb 2025
103. European Chemicals Agency (ECHA) Brief Profile, Phenol, isopropylated phosphate (3:1), https://echa.europa.eu/brief-profile/-/briefprofile/100.066.404. Accessed 15 Feb 2025
104. X. Fu, C.A. Schuh, E.A. Olivetti, *Scr. Mater.* **138**, 145 (2017). https://doi.org/10.1016/j.scriptamat.2017.03.014
105. X. Wang, A. Kramer, C. Glaubensklee, H. He, J.M. Schoenung, "Sustainability-Based Selection of Materials for Refractory High Entropy Alloys," in *REWAS 2022: Developing Tomorrow's Technical Cycles, vol. I*, ed. by A. Lazou, K. Daehn, C. Fleuriault, M. Gökelma, E. Olivetti, C. Meskers, The Minerals, Metals & Materials Series (Springer, Cham, 2022), pp. 377–385. https://doi.org/10.1007/978-3-030-92563-5_38
106. A. Vishina, O. Eriksson, H.C. Herper, *Acta Mater.* **261**, 119348 (2023). https://doi.org/10.1016/j.actamat.2023.119348
107. C. Zeni, R. Pinsler, D. Zugner, A. Fowler, M. Horton, X. Fu, Z. Wang, A. Shysheya, J. Crabbe, S. Ueda, R. Sordillo, L. Sun, J. Smith, B. Nguyen, H. Schulz, S. Lewis, C.-W. Huang, Z. Lu, Y. Zhou, H. Yang, H. Hao, J. Li, C. Yang, W. Li, R. Tomioka, T. Xie, *Nature* **639**, 624 (2025). https://doi.org/10.1038/s41586-025-08628-5 ☐

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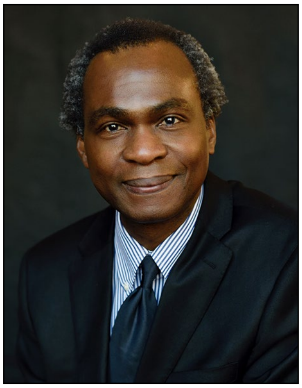

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