SUSTAINABLE CHEMISTRY REPORT

FRAMING THE FEDERAL LANDSCAPE

A Report by the
JOINT SUBCOMMITTEE ON ENVIRONMENT, INNOVATION, AND PUBLIC HEALTH
SUSTAINABLE CHEMISTRY STRATEGY TEAM
of the
NATIONAL SCIENCE AND TECHNOLOGY COUNCIL

August 2023

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About the Sustainable Chemistry Strategy Team

Congress directed an Interagency Working Group to coordinate Federal research on sustainable chemistry through the National Defense Authorization Act (NDAA) for Fiscal Year (FY) 2021.[1] In response, OSTP developed the Sustainable Chemistry Strategy Team (ST) in Fall 2021. The Sustainable Chemistry ST was configured as a NSTC ST under the Joint Subcommittee on Environment, Innovation, and Public Health (JEEP) in the Fall of 2021. The ST is co-chaired by OSTP, NIST, and NSF.

About this Document

The FY 2021 NDAA directs OSTP to establish an interagency working group; to develop a consensus definition of sustainable chemistry; to perform a landscape analysis of all current Federal sustainable chemistry activities; to develop a strategic plan to characterize and assess sustainable chemistry; to coordinate Federal efforts in the areas of regulation, R&D, and challenges; and to integrate sustainable chemistry into Federal R&D through awarded Federal grants, prizes, and loans and increase workforce training and development. OSTP and the Sustainable Chemistry ST solicited input from the public on critical research gaps and needs for sustainable chemistry. The Sustainable Chemistry ST hosted a series of webinars and also issued a Request for Information to receive public comment. This Sustainable Chemistry report establishes the Federal landscape and provides a high-level overview of

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[1] William M. (Mac) Thornberry National Defense Authorization Act for Fiscal Year 2021, (P.L. 116-283).

relevant topical areas around sustainable chemistry. **This document is a state of science report that includes gaps and opportunities for the Federal government.**

Following this report, the Sustainable Chemistry ST will develop a strategic plan for how the Federal government can leverage these opportunities in order to make significant progress in addressing the identified data gaps.

Copyright Information

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[2] See 17 U.S.C. §105

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Abbreviations and Acronyms

AI	Artificial Intelligence
AMMTO	Advanced Materials and Manufacturing Technologies Office, DOE
ARPA-E	Advanced Research Projects Agency-Energy, DOE
ASCR	Advanced Scientific Computing Research, DOE
ATSDR	Agency for Toxic Substances and Disease Registry
BAT	Best Available Techniques
BER	Biological and Environmental Research, DOE
BES	Basic Energy Sciences, DOE
BETO	Bioenergy Technologies Office, DOE
BSSD	Biological Systems Science Division, DOE
CAA	Clean Air Act
CAS	Critical Aspects of Sustainability
CCI	Centers for Chemical Innovation, NSF
CDC	Centers for Disease Control and Prevention
CO_2	Carbon dioxide
CSDM	Chemical Structure, Dynamics, and Mechanisms program, NSF
DHS	Department of Homeland Security
DOC	Department of Commerce
DoD	Department of Defense
DOE	Department of Energy
DOI	Department of the Interior
DOL	Department of Labor
DOT	Department of Transportation
DW	Drinking Water
EERE	Energy Efficiency and Renewable Energy, DOE
EFRC	Energy Frontier Research Centers, DOE
EJ	Environmental Justice
EO	Executive Order
EOP	Executive Office of the President
EPA	Environmental Protection Agency
ESOH	Environmental, Safety, and Occupational Health, DoD
ESTCP	Environmental Security Technology Certification Program, DoD
EU	European Union
FAA	Federal Aviation Administration
FAR	Federal Acquisition Regulation
FDA	Food and Drug Administration
FIFRA	Federal Insecticide, Fungicide, and Rodenticide Act
FOA	Funding Opportunity Announcement
FY	Fiscal Year
G20	Group of Twenty
G7	Group of Seven
GAO	Government Accountability Office
GDP	Gross Domestic Product
GHG	Greenhouse Gas
HAP	Hazardous Air Pollutant
HFCs	Hydrofluorocarbons
HFTO	Hydrogen and Fuel Cell Technologies Office, DOE
HHS	Department of Health & Human Services
HPC	High-performance computing

IEDO	Industrial Efficiency and Decarbonization Office, DOE
ISO	International Organization of Standards
ITA	International Trade Administration
IWG	Interagency Working Group
JSC EIPH	Joint Subcommittee on Environment, Innovation, and Public Health (also known as "the JEEP")
LCA	Life Cycle Assessments
ML	Machine Learning
MSI	Minority Serving Institution
NAICS	North American Industry Classification System
NASA	National Aeronautics and Space Administration
NASEM	National Academies of Sciences, Engineering, and Medicine
NDAA	National Defense Authorization Act
NESHAP	National Emission Standards for Hazardous Air Pollutants
NGO	Non-Governmental Organizations
NIEHS	National Institute of Environmental Health Sciences
NIFA	National Institute of Food and Agriculture
NIH	National Institutes of Health
NIST	National Institute of Standards and Technology
NSF	National Science Foundation
NSTC	National Science and Technology Council
ODS	Ozone-depleting substances
OECD	Organisation for Economic Cooperation and Development
OMB	Office of Management and Budget
OSHA	Occupational Safety and Health Administration
OSTP	Office of Science and Technology Policy
P2	Pollution Prevention
P3	People, Prosperity, Planet
PDB	Protein Data Bank
PFAS	Per- and polyfluoroalkyl substances
R&D	Research and Development
REACH	Registration, Evaluation, Authorisation, and Restriction of Chemicals
RFI	Request for Information
SBA	Small Business Administration
SciDAC	Scientific Discovery through Advanced Computing, DOE
SCIL	Safer Chemical Ingredients List
SDG	Sustainable Development Goal
SERDP	Strategic Environmental Research and Development Program, DoD
ST	Strategy Team
STEM	Science, Technology, Engineering, and Mathematics
TEA	Techno-Economic Assessment
TRI	Toxics Release Inventory
TSCA	Toxic Substances Control Act
U.S.	Unites States
UNEP	United Nations Environment Programme
USDA	United States Department of Agriculture
USGS	United States Geological Survey
WHO	World Health Organization

Executive Summary

The Biden-Harris Administration is committed to delivering clean drinking water, clean air, and safe food to all Americans, including underserved communities. To meet these goals, and in response to a directive from Congress in the William M. (Mac) Thornberry National Defense Authorization Act for Fiscal Year 2021 (NDAA for FY2021), the Office of Science and Technology Policy (OSTP) created the Sustainable Chemistry Strategy Team (ST). Sustainable chemistry can help us harness renewable energy sources, reduce demand for energy, and implement a more circular economy. This report emphasizes the importance of collaboration between government and the private sector to build a strong foundation for future research in sustainable chemistry.

Chemistry is the foundation of a competitive U.S. manufacturing sector and enables improved living standards in the United States and abroad. Chemistry supports manufacturing and high-wage jobs that drive economic growth, including in pharmaceuticals, residential buildings, and semiconductors. Chemistry is at the forefront of the transition to a low-carbon and more circular economy, providing solutions that support clean energy and renewable materials. Current approaches to chemistry to meet society's needs can have harmful impacts on human well-being and the environment. Efforts to advance sustainable chemistry are helping to secure a safe and prosperous future, while minimizing impacts on humans and the environment. More sustainable chemical products, reactions, and technologies need to be developed and applied to address emerging and growing challenges and opportunities for the economy, climate action, and environmental justice.

Definition of Sustainable Chemistry

Sustainable chemistry is the chemistry that produces compounds or materials from building blocks, reagents, and catalysts that are readily-available and renewable, operates at optimal efficiency, and employs renewable energy sources; this includes the intentional design, manufacture, use, and end-of-life management of chemicals, materials, and products across their lifecycle that do not adversely impact human health and the environment, while promoting circularity, meeting societal needs, contributing to economic resilience, and aspiring to perpetually use elements, compounds, and materials without depletion of resources or accumulation of waste.

This report outlines current Federal government sustainable chemistry activities and identifies critical data gaps and research needs, as well as other potential opportunities for strategic action, with the goal of coordinating Federal programs and activities to support sustainable chemistry. Additionally, in support of Administration priorities, this report discusses environmental justice considerations, equitable access to data and technological developments, catalyzing clean energy industries, progress towards net-zero emissions, mitigating climate change, building resilient supply chains, addressing environmental impacts, and the intersection with opportunities for biotechnology and the bioeconomy.

This report identifies key strategic areas that, when addressed, will accelerate innovation and transition to sustainable chemistry. These strategic areas include:

- Data Sharing
- Standards and Metrics Development
- Life Cycle Assessment/Modular Design
- Incentives
- Education
- Resource Access
- Alternatives
- Circularity
- Novel Methods

This report provides a roadmap for Federal agencies, collaborators, and partners. The capabilities and approaches developed in response to this report should lead to a holistic approach to sustainable chemistry. Over the next year, the ST will implement a strategic plan that coordinates activities in these strategic areas by harnessing existing research and accelerating transformative advancements. The information generated will help our nation realize its vision of clean drinking water, clean air, and safe food for all Americans.

I. Introduction

This Report outlines current Federal government sustainable chemistry activities, identification of critical data gaps and research needs, and other potential opportunities for strategic action, with the goal of coordinating Federal programs and activities in support of sustainable chemistry. This document will also serve as a frame of reference and set context for a Federal strategy to enable progress toward a more sustainable future through chemistry. This first part of the sustainable chemistry report establishes the Federal landscape and provides a high-level overview of the state of science of sustainable chemistry. Following this report, the Sustainable Chemistry Strategy Team (ST) will develop a strategic plan and implementation framework for how the Federal government can make significant progress in addressing the identified gaps and opportunities.

Chemistry is the foundation of a competitive U.S. manufacturing sector, while supporting improved living standards in the United States and abroad. From pharmaceuticals, to residential buildings, to semiconductors, chemistry supports high value-added manufacturing and high-wage jobs that drive economic growth, while supporting national well-being. Chemicals are at the forefront of the transition to a low-carbon and more circular economy, providing solutions that support clean energy and renewable materials.

The benefits which society receives from chemistry are being undermined, because chemical pollution is continuing, sometimes at catastrophic levels. We risk the loss of societal value and economic benefit when we don’t prevent pollution, or if future production is limited by insufficient supplies and recycling of resources used in chemical production, including energy (and recyclable emissions), feedstocks, water, and critical minerals. Fundamental research is needed in new chemical processes that utilize energy more efficiently and ensure feedstocks are reused.

Any gains realized in the prevention of pollution via continuous improvements in the understanding, prediction, and reduction of chemical toxicity will not be a success if the resulting innovative chemistries are not economically-viable. New innovative chemistries must meet the needs of the marketplace and meet critical performance criteria, or else they may not be successful or accepted for uses critical to public safety and national security.

Global demand for chemicals is largely cyclical, since it is linked to growth in Gross Domestic Product (GDP); the chemical industry supplies many industrial and consumer sectors, including manufacturing, infrastructure, consumer goods and food. Recent disruptions in global supply chains during the COVID-19 pandemic and the resulting impacts on critical U.S. supply chains in the medical, transportation, military and other sectors have highlighted the centrality of chemicals to our national security. As the United States seeks to secure its access to critical minerals, metals, and other materials, as well as to reestablish U.S. leadership in advanced manufacturing, chemicals will continue to play a central role in manufacturing many of these products.

Sustainable chemistry processes and products provide benefits through decarbonization, reductions in risks to human and ecological health, increased material efficiency, waste reduction, as well as through economic growth, new market opportunities, health and wellbeing, and national security. Increasing sustainable chemistry practices can reduce disruption and enhance resilience of supply chains; reduce reliance on insecure sources of raw materials; improve ability to respond to changing conditions; increase efficient use of energy and natural resources during processing and manufacturing; and increase distribution of materials recovery, reprocessing, and (re)manufacturing jobs. Furthermore, through better methods and practices, the U.S. can avoid the continuation of, and perhaps begin to remedy, the legacy of disproportionate negative impacts on overburdened and underserved communities.

Federal agencies play a key role in enabling the development and implementation of these critical technologies. The agencies represented in this report are working to advance sustainability in the practice and business of chemistry. Efforts include funding research in all areas of relevant innovation, public-private partnerships, and technology transfer; supporting best practices through standards and procurement guidelines; enforcing accountability; building incentives and enhancing profitability and competitiveness of markets; and developing responsive and timely regulatory actions based on sound scientific evidence.

Purpose

The purpose of this report is to describe the state of Federal sustainable chemistry activities and the scientific challenges, roadblocks, and hurdles to transformational progress in improving the sustainability of chemistry. In service of this goal and to reach the mandates of the NDAA for FY2021, this report:

- proposes a consensus definition of sustainable chemistry;
- proposes a working framework of attributes characterizing and considerations for evaluating sustainable chemistry;
- assesses the status of sustainable chemistry in the United States, including its applicability and utility in key sectors of the economy, key technological platforms, commercial priorities, global priorities, workforce development and education, current innovative trends, and barriers to innovation; and,
- summarizes the Federal regulations relevant to sustainable chemistry.

Additionally, in support of Administration priorities, this report addresses environmental justice (EJ) considerations, equitable access to data and technological developments,[3] catalyzing clean energy industries,[4] progress towards net-zero emissions, mitigating climate change,[5] building resilient supply chains,[6] addressing environmental impacts, and the intersection with opportunities for biotechnology and the bioeconomy[7] to provide technological solutions as critical elements of the sustainable chemistry landscape.

Upon completion of this report, the Sustainable Chemistry ST will develop a plan for Federal agencies to address the highest-priority sustainable chemistry needs. Appendix A and Appendix B provide detailed information on federally-funded sustainable chemistry activities and financial resources allocated to Federal R&D activities, respectively. This report was informed through various engagement

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[3] https://www.whitehouse.gov/wp-content/uploads/2022/04/eo13985-vision-for-equitable-data.pdf

[4] Executive Order on Catalyzing Clean Energy Industries and Jobs Through Federal Sustainability

[5] Executive Order on Tackling the Climate Crisis at Home and Abroad - The White House

[6] https://www.federalregister.gov/documents/2021/03/01/2021-04280/americas-supply-chains

[7] https://www.federalregister.gov/documents/2022/09/15/2022-20167/advancing-biotechnology-and-biomanufacturing-innovation-for-a-sustainable-safe-and-secure-american

activities with relevant stakeholders, as detailed in Appendix C. The Sustainable Chemistry ST greatly appreciates the input received from critical stakeholders throughout the development process.

Extensive research on areas involving sustainable chemistry has been published, including reports on the state of sustainable chemistry and future directions. This report builds on these previous works. Below are examples of foundational reports on sustainable chemistry and sustainability more broadly that should be consulted as background information for this report:

- White House Net-Zero Game Changers Working Group: U.S. Innovation to Meet 2050 Climate Goals (whitehouse.gov)
- White House Fast Track Action Subcommittee on Critical and Emerging Technologies: Critical and Emerging Technologies List Update (whitehouse.gov)
- GAO: Chemical Innovation: Technologies to Make Processes and Products More Sustainable | U.S. GAO
- OECD: The Role of Government Policy in Supporting the Adoption of Green/Sustainable Chemistry Innovations
- National Academies of Sciences, Engineering, and Medicine (NASEM): Enhancing the U.S. Chemical Economy through Investments in Fundamental Research in the Chemical Sciences.
- NASEM: Chemical Engineering Challenges and Opportunities in the 21st Century | National Academies
- DOE: Sustainable Chemistry in Manufacturing Processes Roundtable | Department of Energy
- US EPA: Green Chemistry | US EPA
- GAO: RECYCLING: Building on Existing Federal Efforts Could Help Address Cross-Cutting Challenges

This is not an exhaustive list, but these resources are foundational to understanding the state of sustainable chemistry in the United States and internationally.

II. Definition

Sustainable chemistry is the chemistry that produces compounds or materials from building blocks, reagents, and catalysts that are readily-available and renewable, operates at optimal efficiency, and employs renewable energy sources; this includes the intentional design, manufacture, use, and end-of-life management of chemicals, materials, and products across their lifecycle that do not adversely impact human health and the environment, while promoting circularity, meeting societal needs, contributing to economic resilience, and aspiring to perpetually use elements, compounds, and materials without depletion of resources or accumulation of waste.

Considerations for and Attributes of Sustainable Chemistry

It is the authors' intent to provide a succinct, aspirational definition for an issue that is broad and encompasses many disciplines and sectors. General scientific principles (including thermodynamics), in addition to economics, can limit whether sustainable chemistry or a specific chemical process can be realized at that moment in time. Challenges for the implementation of more sustainable chemistries than we practice today include: 1) the limits to current human knowledge and mindset, 2) the barriers to technology acceptance and adoption and expansion into commercial production, and 3) economic considerations around supply chain and trade. There are opportunities to utilize renewable energy, to extend the life of our resources, to reduce the impacts of our consumption, and to truly innovate with paradigm-shifting chemistries. As rapid progress is made in understanding the complex interplay among the United Nations Sustainable Development Goals (SDGs),[8] and the many ways in which more sustainable chemistry enables new technologies and innovation, the definition of sustainable chemistry may similarly evolve. Additionally, an understanding of sustainable chemistry needs to encompass and promote the interplay and influence of the three interrelated spheres of sustainability upon one another: environment, society, and economy. Therefore, a sustainable chemistry strategy should offer a broader multi-disciplinary approach to the practice and application of chemistry that, similar to other sustainability strategies and frameworks, strives to balance considerations of the environment, society, and the economy (Fig. 1). Sustainable chemistry encourages innovation and a trans-disciplinary approach to the environmental, societal, and economic responsibilities of all

From Green to Sustainable Chemistry

The terms sustainable chemistry and green chemistry are sometimes used interchangeably; however, they are not synonymous. Green chemistry is the design of chemical products and processes that reduce or eliminate the use or generation of hazardous substances. Green chemistry applies across the life cycle of a chemical product, including its design, manufacture, use, and ultimate disposal. Of course, the assessment of what constitutes deleterious environmental consequences of a process is complex and might include impact on air, soil, and water quality, release of greenhouse gases or ozone-depleting substances, and production of products or byproducts with incompletely-understood toxicity profiles and/or long-term fate/degradation pathways. Sustainable chemistry not only includes the concepts and principles of green chemistry, it also expands the definition to include a larger system than just the specific reaction; and "also considering the effects of processing, materials, energy, and economics." This larger context enables one to ask if a particular green process is sustainable? With the considerable amounts of research being performed in green chemistry and green engineering, sustainability considerations require assessment of whether these resulting "green technologies" improve existing chemistry and processes, across the multiple contexts including materials, energy, and economics, and are less detrimental to the environment and human health than their predecessors. Therefore, it is helpful to think of sustainable chemistry as encompassing and expanding on green chemistry to include a more holistic view of how chemistry impacts humans, the environment, and social and economic systems.

Gonzalez MA. 2017. Introduction to green and sustainable chemistry. https://doi.org/10.1016/B978-0-12-409548-9.10249-0.

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[8] https://sdgs.un.org/goals

organizations and individuals, not just chemical manufacturers and users, in order to maximize contributions to society, while avoiding harm to the planet and to current and future generations. As made clear by the definition above, sustainable chemistry spans from the research and discovery aspects to the development and adoption, requiring a holistic Federal approach (Figure 1).

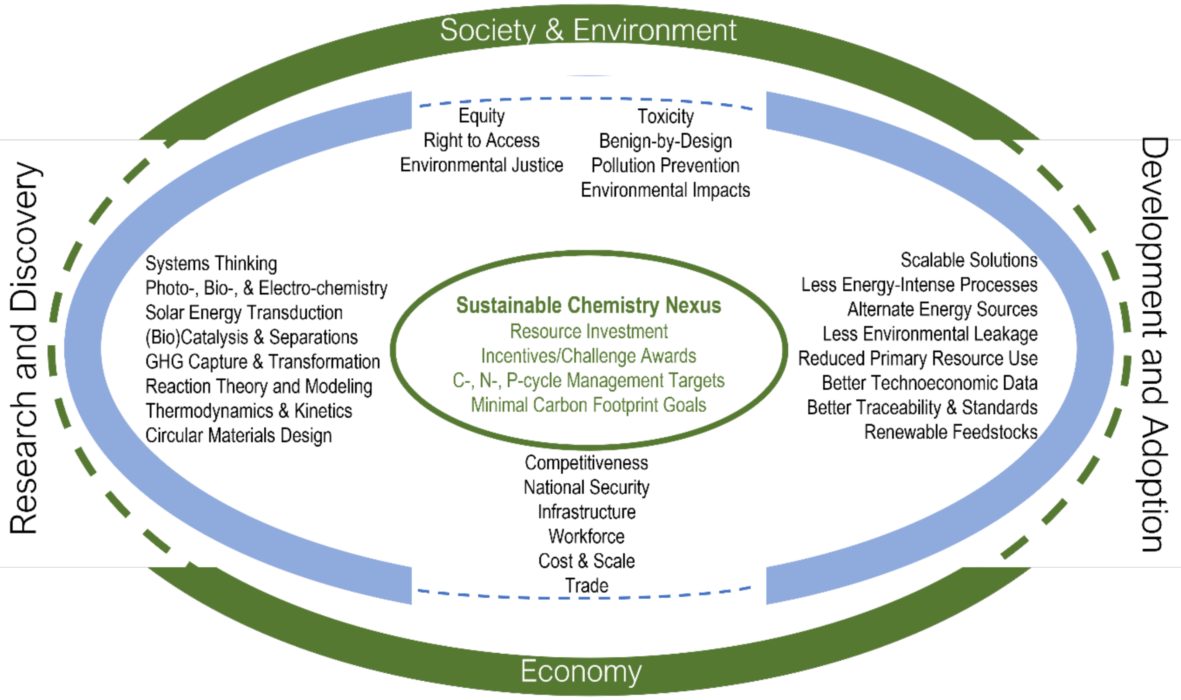

Figure 1: Visual display of the complex interplay and the spheres of relevance for sustainable chemistry.

This section presents considerations of and attributes for sustainable chemistry that help operationalize the aspirational definition. These considerations provide a broader multidisciplinary approach that considers these concepts across the full chemical enterprise, emphasizing systems thinking, which is critical to a sustainable future. The use of attributes (Table 1) to characterize sustainable chemistry allows for flexibility, progress, and operationalization of a definition; not every activity will consist of all of the attributes. Instead, these should be utilized to support continuous improvement toward sustainable chemistry. While progress will necessitate thoughtfully justified trade-offs, advancement in one of these areas should not be at the detriment of another area. This complex interplay will underlie future sustainable chemistry activities.

Table 1. Attributes and considerations to operationalize the aspirational definition of sustainable chemistry.

Attribute	Description of Attribute	Considerations
Efficiency	• Chemistry and efficiency across production and engineering, including considerations of atom economy[9] • Improve the chemistry and chemical routes, thermodynamics, kinetics and atomic mapping from educts to products, with minimal byproduct production	• Improve efficiency and performance of fundamental chemistry and process technologies • Consider elementary step and atom economy of the entire synthetic route or process; consider elements, compounds, chemicals, or materials. • Consider using alternatives (e.g., biocatalysis, other bio-based and bio-inspired processes) to traditional synthesis • Examine the overall thermodynamics of processes and of individual steps to seek and develop the most energy efficient options • Optimize the kinetics of rate-limiting steps • Support alternative needs assessment through development of platforms • Derive benchmark metrics; harness big data and facilitate data-driven research
Energy	• Drive sustainable chemical processes employing renewable energy	• Consider the source of energy input and potential alternatives (e.g., solar, electrical) and new methods to transduce alternate energy sources • Consider how to repurpose, more efficiently use or recycle critical elements • Reduce GHG footprint in process development • Diversify from over-dependence on fossil sources; expand and enhance the use of feedstock alternatives (e.g., biological renewable sources, biomass, alternative waste-streams)
Circularity	• Resource use • Continuous process thinking that leads to overall progress • Stepwise and iterative approaches	• Consider how to repurpose, more efficiently use, or recycle critical elements • Move toward true circularity with recyclable/upcyclable polymers • Strive toward a sustainable nutrient cycle; recovery and reuse of phosphates • Consider all stages of the life cycle including design, manufacture, use and end-of-life (disposal or re-use) • Develop more sustainable synthetic fuels (e.g., using hydrogen from water; reduction of CO_2 from direct air capture) • Intentionally approach each life cycle stage of design, manufacture, use and end-of-life (disposal or re-use); during these stages, chemical processes operate at maximal efficiency using building blocks, reagents, and/or catalysts that are readily available and renewable and employ renewable energy sources

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[9] Atom economy is a measure of the desired useful products formed from reactants in a chemical reaction.

Attribute	Description of Attribute	Considerations
Hazard	- Prevent release of hazardous substances to air, land, and water throughout the chemical life cycle - Toxicity reduction and hazard prevention	- Eliminate or minimize environmental and human health impacts - Prevent hazards at all stages of design, manufacture, use, and end-of-life - Develop tools to support use of less hazardous chemical substances - Consider less hazardous alternatives that are functionally comparable
Social	- Development that meets the needs of the present without compromising the ability of future generations to meet their own needs[10]	- Include equity in the prioritization, design, and access to technological advances and avoid disproportionate burden of hazards; recognize EJ considerations, as these are paramount in design, remediation, regulation, and end-of-life. - Include sustainable systems thinking in education and workforce development - Ensure equitable/enhanced access in underserved markets - Consider disproportionate burden of hazards in design, remediation, regulation, and end-of-life stages
Economic	- Viability, scalability, and distribution (including time, volume and geography) - Traceability and transparency - National security	- Consider impact of consumer wants and needs - Identify competitive technology solutions and change incentives - Use communication and traceability across the full supply chain - Consider economic viability and economic feasibility such that the cost of investing/utilizing sustainable chemistry is profitable. Competitiveness in terms of economic and other factors valued in the marketplace, including resource use - Identify policies that incentivize investments in and use of new sustainable chemistry technologies (e.g., grants) - Ensure economic resilience and national security through supply chain resilience - Contribute to U.S. National Natural Capital Accounts[11] - Enable communication and traceability across the supply chain, while protecting intellectual property, trade secrets and confidential business information - Provide equitable access to societal needs for all people without damaging the environmental resources upon which we depend.

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[10] https://www.un.org/en/academic-impact/sustainability

[11] https://www.whitehouse.gov/wp-content/uploads/2023/01/Natural-Capital-Accounting-Strategy-final.pdf

III. Federal Landscape

Below is an overview of Federal programs in sustainable chemistry. A more comprehensive overview by agency is provided in Appendix A. There are ongoing sustainable chemistry activities across the Federal agencies involved in the Sustainable Chemistry ST.

For FY 2019-2022, the estimated total expenditures on sustainable chemistry R&D and related activities across the Federal government was $1.4 billion dollars over 4 years, with DOE reporting the greatest sustainable chemistry expenditures ($730 million), followed by NSF ($364 million), DoD ($218 million), and HHS ($91 million) for 2019-2022 (for further budget information, please see Appendix B). With historic investments through the Infrastructure Investment and Jobs Act[12] and the Inflation Reduction Act of 2022,[13] the scope of Federal activities is likely to increase over the next few years. As of December 2022, in general, these research activities broadly fall into several categories, with agencies involved in each category highlighted below. For more detailed discussion of these activities, see Appendix A (Federal Research Overview) and Appendix B (BDR data).

Table 2: Federal expenditure categories and specific agency involvement within those categories.

Category	**Agency Involvement**
Funding of Grants	DoD, DOE, EPA, NSF, USDA
Research & Development	DOC/NIST, DoD, DOE, EPA, HHS/NIEHS, USDA
Demonstration Activities[a]	DoD, DOE, DOI/USGS, EPA, HHS/FDA, USDA
Data, Modeling & Simulation Resources[b]	DOC/NIST, DOE (ASCR, BES, EERE), EPA,
Procurement	DOE, EPA, USDA

[a] Activities not directly related to R&D

[b] Data, software solutions, and computational infrastructure provide enabling capabilities and tools that will be an integral part of the effective scientific strategy to address the nation's sustainable chemistry challenges. Several agencies deploy data and computational infrastructure and resources that support and accelerate research relevant to sustainable chemistry.

IV. Federal Considerations

The Federal government has a variety of roles that define its relationship with chemistry in the marketplace and the barriers and opportunities that the Federal government may present to sustainable chemistry. Most frequently considered is the Federal government's role as regulator, under statutes like the Toxic Substances Control Act (TSCA), the Federal Insecticide, Fungicide, and Rodenticide Act (FIFRA), the Clean Air Act (CAA), the Federal Food, Drug, and Cosmetic Act, and the Occupational Safety and Health Act. The Federal government writes and enforces rules that impact the development and adoption of sustainable chemistry innovations. But the Federal government is also one of the largest consumers in the world. From fighter jets and computers to cleaning supplies and

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[12] H.R. 2684. Infrastructure Investment and Jobs Act. 2021-2022. https://www.congress.gov/bill/117th-congress/house-bill/3684/text

[13] H.R. 5376. Inflation Reduction Act of 2022. https://www.congress.gov/bill/117th-congress/house-bill/5376/text

face masks, procurement statutes, policies, and preferences can make a huge difference in the incentives to invest in sustainable chemistry. The Federal government's scale and purchasing power can create market demand for sustainable products.

In addition to its role as regulator and consumer, the Federal government is an important market facilitator. Industry relies on the dissemination of information gathered and presented by the Federal government to aid investment and purchasing decisions. The Federal government also manages voluntary certification and labelling programs, such as Safer Choice, Energy Star, and USDA grades and standards, which provide consumers with reliable information to compare products and express their product preferences. These programs leverage innovation and market forces, and are positioned to accomplish such goals through sustainable chemistry. These programs can also play a significant role in the ability of domestic producers to sell in other countries, each with their own regulatory regimes.

Finally, the Federal government is the country's largest research institution, operating its own research facilities and funding third-party research. The research priorities expressed by the Federal government have a major effect on the pipeline of innovation coming to the marketplace.

Regulatory environment

The Federal government regulates the use of chemicals, emissions of chemicals, transportation, and exposure to chemicals under a variety of different statutes and under the authority of a range of Federal agencies. The scope of regulation varies across statutes. EPA has the broadest authority, with all of its authorizing statutes playing a role. First and foremost is the Toxic Substances Control Act (TSCA), which authorizes EPA to directly regulate the manufacture, use, and disposal of chemical substances. EPA can take actions to reduce the presence of hazardous chemicals in industrial, commercial, and consumer uses. The recent amendments to TSCA under the Frank R. Lautenberg Chemical Safety for the 21st Century Act[14] significantly expanded EPA's responsibility for evaluation and regulation of chemicals already on the market. Risk evaluations conducted under the amended statute have identified risks to workers, consumers, and the environment, and EPA is currently working on risk management to protections. In the long run, these evaluations and the resulting regulations will reduce the risks of older existing chemicals and will have the potential to lead to the use of alternatives, including potentially more sustainable chemicals, in the marketplace. EPA is in a position to further advance the use of more sustainable chemistry under EPA's New Chemicals program, which functions as a "gatekeeper" for chemicals new to the marketplace.

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[14] Frank R. Lautenberg Chemical Safety for the 21st Century Act. 2016. Public Law 114-182. https://www.congress.gov/114/plaws/publ182/PLAW-114publ182.pdf

Federal Regulations Related to Sustainable Chemistry

Of Federal agencies, EPA has the most direct responsibility for the regulation of the use of chemicals, emissions of chemicals, and exposure to chemicals in commerce. However, a wide range of Federal agencies also have responsibilities that are more targeted. For example:

- FDA regulates the manufacture and sale of foods, food ingredients and packaging materials, medicines, biologics, tobacco products, and medical devices.
- The Consumer Products Safety Commission can set safety standards for consumer products, including content of hazardous chemicals.
- Occupational Safety and Health Administration (OSHA) can set and enforce standards to ensure that employees work in a safe and healthy environment, including standards to protect employees from chemical hazards (e.g., individual chemical standards and permissible exposure limits, hazard communication, process safety management).
- FAA regulates the manufacture and use of aircraft and aircraft parts, which including standards of performance that, with current technology, require the use of specific chemicals.

The Federal government also regulates market activities that can have consequences for the use of chemicals. For example:

- USDA has plant protection and quarantine programs in place that rely on chemicals that are otherwise restricted.
- U.S. Customs and Border Patrol enforces prohibitions on chemical imports.

EPA also regulates the use of chemicals, emissions of chemicals, and exposure to chemicals under the Clean Air Act (CAA) in three distinct ways. First, Title II of the CAA gives EPA authority over transportation fuels, and in 2005, Congress created a Renewable Fuel Standard that requires the use of gasoline and diesel derived from renewable feedstocks. Within this framework, EPA can accelerate approval of advanced biofuel pathways that will reduce the GHG impact of transportation fuels. The substitution of fuels based on agricultural products for fuels derived from petroleum is consistent with goals of sustainable chemistry, but the use of food crops as a feedstock, such as corn and soy, or feedstocks for which the expansion of cropland may displace natural habitats, such as with palm or sugar cane, have consequences for sustainability. The hope is that advanced biofuels that use crop waste or specially grown feedstocks, such as algae, will be the basis of a more sustainable transportation fuel supply.

Second, Title VI of the CAA governs the use and release of ozone-depleting substances (ODS) and their substitutes. In recent years, EPA has used this authority to address the warming potential of Hydrofluorocarbons (HFCs), a class of chemicals that have replaced ODS in the marketplace. Congress supplemented this authority in 2020 with the American Innovation and Manufacturing Act, which requires a phase-down in the manufacture and import of HFCs. Because of the limitation of production and imports, there is a strong market incentive to recover, reclaim, and recycle HFCs currently in commerce. Better recovery programs would also have significant environmental benefits, by reducing the illegal release of these HFCs into the atmosphere.

Third, EPA regulates air emissions of chemicals under Title I, from criteria pollutants like Ozone and Lead under the National Ambient Air Quality Standards to Hazardous Air Pollutants (HAPs) like benzene and heavy metals under the National Emission Standards for HAPs. EPA's actions in these areas can promote sustainable chemistry, but it has limited discretion to change emission standards solely on that basis.

EPA also has regulatory authority over the use of chemicals, emissions of chemicals, and exposure to chemicals under many of its other statutes: CAA; Clean Water Act; the Resource Conservation and Recovery Act; FIFRA; and the Comprehensive Environmental Response, Compensation, and Liability Act. In its implementation of these acts, EPA has an impact on the adoption and promotion of sustainable chemistry.

Procurement

The Federal government is the largest purchaser of goods and services in the United States. To advance the various missions of the Federal government, acquisition and procurement programs have incorporated several sustainable chemistry-related activities that increase mission capability, reduce harm to the workforce and community, reduce life cycle costs, help ensure availability of critical products, and achieve Federal sustainability goals. Recent Federal policy directs the Federal government to use its procurement programs to advance sustainability in ways that support sustainable chemistry. Relevant executive orders (EOs) include:

- EO 13390, Protecting Public Health and the Environment and Restoring Science to Tackle the Climate Crisis[15]
- EO 14017, America's Supply Chains[16]
- EO 14030, Climate-Related Financial Risk[17]
- EO 14057, Catalyzing Clean Energy Industries and Jobs Through Federal Sustainability[18]
- EO 14081, Advancing Biotechnology and Biomanufacturing Innovation for a Sustainable, Safe, and Secure American Bioeconomy[19]

These EOs direct the Federal government to conduct several sustainable chemistry-related activities, including driving transparency across the Federal supply chains by expecting suppliers to disclose GHG emissions, prioritizing the social cost of GHGs in procurement, and prioritizing the purchase of sustainable products, such as products without added PFAS.

The Federal Acquisition Regulation (FAR) is the set of procurement rules for the Federal government. There are multiple current initiatives to update the FAR in ways that advance sustainable chemistry.

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[15] Executive Order on Protecting Public Health and the Environment and Restoring Science to Tackle the Climate Crisis - The White House. January 2021.

[16] Executive Order on America's Supply Chains - The White House. February 2021.

[17] Executive Order on Climate-Related Financial Risk - The White House. May 2021.

[18] Executive Order on Catalyzing Clean Energy Industries and Jobs Through Federal Sustainability - The White House. December 2021.

[19] Executive Order on Advancing Biotechnology and Biomanufacturing Innovation for a Sustainable, Safe, and Secure American Bioeconomy - The White House. September 2022

Federal agencies have several programs to integrate sustainable chemistry elements into their purchasing activities. For example, DoD has developed the Sustainability Analysis Guide for incorporation of life cycle environmental and human health considerations into defense acquisitions, uses the Programmatic Environmental, Safety and Occupational Health Evaluation to document environmental, safety, and occupational health (ESOH)-related considerations and eliminate ESOH risks, where possible, and has developed policy to implement sustainable procurement and supply chains that result in uninterrupted access to key supplies, materials, chemicals, and services. USDA's BioPreferred® Program requires Federal agencies and contractors to give purchasing preference to biobased products.

Market Facilitator

The Federal government gathers and disseminates information that industry and consumers use to influence their investment and purchasing decisions. This information follows broad data about the flow of goods and services into and through the economy and information about specific goods and services available in the marketplace.

Multiple agencies throughout the Federal government gather and publish data about the U.S. economy. The DOC Census Bureau is perhaps the most prominent, with the decennial Census, as required by the Constitution, and the Economic Census, the official five-year measure of American businesses providing comprehensive statistics at the national, state, and local levels. The information published by the Census Bureau and other Federal statistical agencies is key to the U.S. economy and is incorporated into business decisions at all levels, from capital investment and siting decisions to marketing and advertising.

On Earth Day 2022, the White House announced an initiative that creates a U.S. system to account for natural assets—from the minerals that power our tech economy and are driving the electric-vehicle revolution, to the ocean and rivers that support our fishing industry, to the forests that clean our air—and quantify the immense value this natural capital provides. Sustainable chemistry innovations can directly contribute to this effort by lessening impacts to these natural assets.

The Federal government also manages a series of statistical classification schemes, which help to better understand the structure of the U.S. economy and are used by the Federal government and the private sector in a variety of ways. In the context of sustainable chemistry, the Federal government could establish statistical classification to track renewable and recycled products, to demonstrate the viability and availability of these products at an industrial scale, and to encourage future investment; these considerations could be included as a classification in the North American Industry Classification System (NAICS) or in other systems in use by the Federal government.

As a market facilitator, information about specific products and services available in the marketplace is critical. Through these programs, a producer or service provider can communicate to customers some characteristic of their goods or services, backed by the Federal government. These programs are voluntary, but participants agree to abide by program regulations to ensure the targeted characteristic. The two most recognizable are DOE's Energy Star Program, which identifies the most energy efficient appliances, and USDA's Certified Organic program for farms and processors. The popularity of these programs reflects consumer preferences for these products and, in the case of Energy Star, additional incentives and subsidies from the Federal government and electric utilities to encourage energy efficiency.

There are a few examples of existing Federal certification programs that are relevant to sustainable chemistry and may have a role in promoting further innovation and investment.

The USDA BioPreferred® Program is a certification and labeling initiative for biobased products derived from plants and other agricultural, marine, and forestry materials. More than 3,000 companies participate in the program. Examples of biobased products include construction materials, custodial goods, and consumer-based personal care and packaging. Biobased products also include intermediate-use feedstocks such as biopolymers (naturally-occurring materials like wool, silk, and gelatin; and polysaccharides like cellulose and starch drawn from fungi and bacteria) and biobased chemicals used to create commercial, industrial, or consumer goods.

EPA's Safer Choice program helps consumers, businesses, and purchasers find products that perform and contain ingredients that are safer for human health and the environment. Safer Choice is an EPA Pollution Prevention program, which includes practices that reduce, eliminate, or prevent pollution at its source, such as using safer ingredients in products. About 1,900 products currently qualify to carry the Safer Choice label. Safer Choice-certified products are available for use in homes and in facilities like schools, hotels, offices, and sports venues.

Supporting the Safer Choice program is the Safer Chemical Ingredients List, which is a list of chemical ingredients, arranged by functional-use class, that the 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.

V. Key Sectors in U.S. Economy

In 2021, the chemicals and allied product industries contributed 21% of U.S. Manufacturing GDP, shipping $1.06 trillion in chemicals, plastics and other chemical-intensive products[20] and directly employing an estimated 1.41 million workers.[21] Chemical and plastics manufacturing is distributed across all 50 states, via 33,150 manufacturing facilities.[22]

The industry is typically the second or third largest national exporter, following China and the European Union (EU), sending $305.5 billion in chemicals and chemical products abroad in 2022, or $238.2 billion if pharmaceuticals are not included.[23] However, this could shift in the coming decade, due to a number of factors, including emerging chemical regulations, competitive access to feedstocks including oil and natural gas, and increases in the production of basic and specialty chemicals in Asia and the Middle East.

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[20] Department of Commerce, Bureau of the Census, Annual Survey of Manufacturers. NAICS 325 and 3261.

[21] American Chemistry Council. Guide to the Business of Chemistry: 2022. P. 7, Table 1.2.

[22] Bureau for Labor Statistics; NAICS 325; 2021 Data for Chemicals Manufacturing Facilities (includes pharma)

[23] Data from Department of Commerce, Bureau of the Census and the International Trade Administration's Trade Policy Information Systems Database. Unrevised for 2022. HS 28-40. Note this includes chemicals and some chemical intensive products such as paints, PVC pipes, and detergents.

In addition to Federal government activities, sustainable chemistry stimulates innovation across many sectors. For example, in the energy sector, no single clean energy source will likely be able to meet U.S. demand. Chemistry is supporting the development of a mix of clean energy sources and feedstocks such as nuclear and hydrogen, as well as providing coatings and other inputs that support wind and solar.[24] Nearly all goods in use every day in the United States are manufactured or otherwise produced using chemical processes and products (Figure 2). These goods are found, for example, in homes, offices, factories, pharmacies and retail grocery stores, and farms across the United States. Key sectors that rely upon chemistry include the broad manufacturing sector as well as other sectors that use chemical products, the energy sector, health, agriculture, bioeconomy-related sectors,[25] transportation, physical infrastructure, and the built environment, to name just a few.

Chemicals and materials are vital to provide the United States and our allies with the capabilities needed for defense and to maintain global security.[26] Additional relevant industries include public health and biological preparedness, defense, critical materials, information and communications technology, energy, transportation industrial base, electronics, agricultural commodities, and food products. Sustainable chemistry innovation and development needs to consider impacts among all of these key sectors, as well as balancing tradeoffs between sectors.

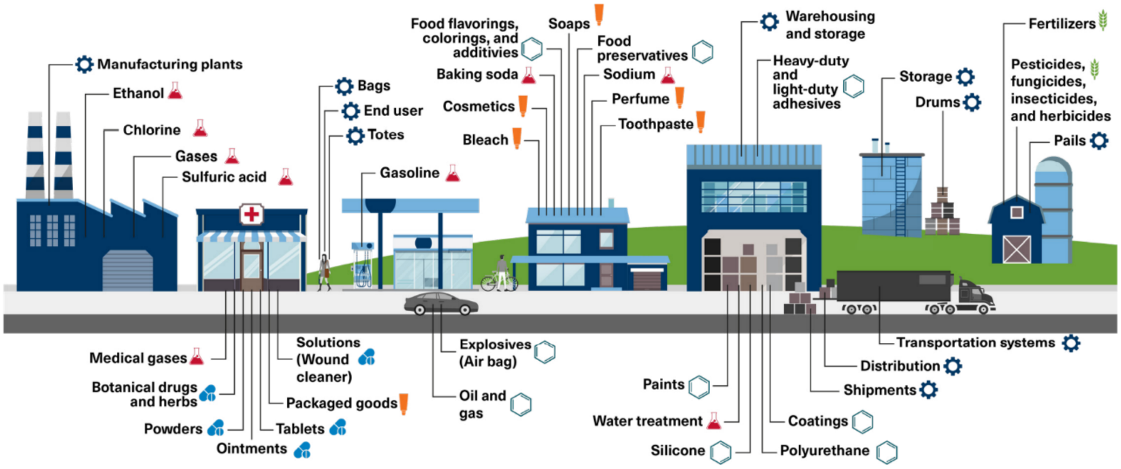

Figure 2: Examples of where chemical products are used across sectors of the economy and found in homes, offices, power plans, drug and retail grocery stores, and farms.[27] This is not a complete, comprehensive overview, but it shows the breadth of sectors that are stakeholders for sustainable chemistry.

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[24] National Academies of Sciences, Engineering, and Medicine. (2022). New Directions for Chemical Engineering. Washington, DC: The National Academies Press. https://doi.org/10.17226/26342

[25] EO 14081 directed an interagency technical working group to recommend bioeconomy-related revisions to the North American Industry Classification System (NAICS), which defines industries and sectors.

[26] Department of Defense. (2018, September). Assessing and Strengthening the Manufacturing and Defense Industrial Base and Supply Chain Resiliency of the United States.

[27] Cybersecurity and Infrastructure Security Agency. (2019, May). "Chemical Sector Profile". Fact Sheet.

Commercial Considerations

Economic factors influence the development and marketability of sustainable products. Consumers are increasingly interested in purchasing more sustainable products, which incentivizes producers, manufacturers, and retailers to consider more sustainable practices (e.g., hazard and quantity of materials in transport), as well as how consumers perceive sustainability. Progress towards sustainable chemistry relies on increased transparency, traceability, and accountability in supply chains to shed light on all of the ingredients in different products, which would help determine whether a product contains concerning substances, and whether more sustainable alternatives might be available. Transparency builds trust between various stakeholders, from industry to non-governmental organizations (NGOs) to government and consumers. However, legal barriers, such as those needed to protect intellectual property, proprietary information, and non-disclosure agreements, can present challenges when seeking greater transparency of chemical content in products. Cost is a critical consideration in advancing sustainable chemistry, and having a viable market for such products is a key precondition to commercial adoption. Ideally, more sustainable products should have improved performance, lower emissions, hazards, and costs. Increased production of products using a new, more sustainable approach will become increasingly cheaper over time due to increased economies of scale, even if it is initially more expensive. Innovative policy solutions will be needed to provide appropriate incentives for manufacturers both in the design and development stage and in the scale-up phase.

Transitions to more sustainable chemistry practices may have the potential to disrupt supply chains. This can be due to scale-up challenges, access to materials, existing capital investment in current technologies, and timing of investments in future technologies. It is important to consider the challenge of overturning well-established conventional practices when transitioning in the commercial market. However, a long-term commitment to investments that drive innovation will be necessary to promote the change needed for sustainability. As the United States transitions to more sustainable chemistry practices, the potential impact to supply chains dependent on existing chemicals must be managed to avoid economic and national security vulnerability. Sustainable chemistry increases economic benefits of products and reduces trade barriers. Increasing numbers of consumers have demonstrated their willingness to pay for products that demonstrate sustainable chemistry, increasing demand and incentivizing firms to produce more to preserve their market share, maintain their reputation, or increase profits.[28] Consumers are changing their behavior, with searches for sustainable goods increasing globally by 71% since 2016,[29] and their increased willingness to pay more for sustainable products.[30] Corporations are responding, particularly in the cosmetics, pharmaceutical, fashion, and food sectors. For example, 65% of the businesses surveyed in the fashion and textile industry have committed to sourcing sustainably produced raw materials, and 60% of businesses now collect data on supply chain sustainability.[31] A 2021 survey by Statista of U.S. consumers identified a number of factors

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[28] United States Government Accountability Office (GAO). (2018, February). Chemical Innovation Technologies to Make Processes and Products More Sustainable. Technology Assessment.

[29] The Economist Intelligence Unit. (2021). An Eco-Wakening: Measuring Global Awareness, Engagement and Action for Nature.

[30] The Nielsen Company. (2015, October). The Sustainability Imperative. New Insights on Consumer Expectations. Global Sustainability Report, 2.

[31] The Economist Intelligence Unit. (2020). Is Sustainability in Fashion? Industry Leaders Share their Views.

they identified as characterizing sustainable consumption, including 27% that prioritized "no use of environmentally harmful raw materials," 23% that prioritized "resource saving production," and 40% that emphasized environmentally friendly packaging.[32] Additionally, a McKinsey study found that between 2018 to 2022, sales of products with environmental, social, and governance claims grew by roughly 28% compared to 20% for products that made no social or sustainability claims.[33] Standardized sustainable chemistry metrics can also facilitate international trade. Along the trade and climate nexus as an example, common life cycle assessment standards formally adopted by governments could reduce trade frictions for carbon-related border adjustments and provide a more comparable picture of carbon intensity of products traded.[34]

In the United States, innovation and new products are an important driver of industry revenue. A market survey conducted by the American Chemistry Council indicates that in the past decade, new products contribute between 14% to 17.8% of U.S. chemical companies revenues and averaged 14.7% in 2021.[35] Data from the National Science Board indicate that U.S. companies' R&D investments as a percentage of revenue may lag at 2.2% when compared to top chemicals manufacturers in other countries, including Germany 5.8%, Japan 5.9%, and China 6.6%. In absolute terms, China invested $24 billion, followed by the United States ($9.5 billion), Japan ($8.07 billion), and Germany ($5.09 billion).[36] In 2019, the Organisation for Economic Cooperation and Development (OECD) in its research on R&D intensity by industry, ranked the U.S. chemicals industry as average among OECD member countries.[37] These lower levels of R&D investment in the United States are likely due in part to the significant production of building block/commodity chemistries in the United States, in which levels of R&D investment are lower than in specialty chemistries. In non-market economies, it should be noted that private sector investments in R&D are not easily distinguished from public sources, including government.

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[32] Statista. Global Consumer Survey: Consumer Insights Sustainable Consumption. February 2021. Available online at www.statista.com

[33] McKinsey and Nielsen IQ. "Do Consumers Care About Sustainability and ESG Claims." February 2023. https://gcc02.safelinks.protection.outlook.com/?url=https%3A%2F%2Fwww.mckinsey.com%2Findustries%2Fconsumer-packaged-goods%2Four-insights%2Fconsumers-care-about-sustainability-and-back-it-up-with-their-wallets&data=05%7C01%7Cholmes.brooke%40epa.gov%7C9ce6f3a785114f4a4e4408db6b792385%7C88b378b367484867acf976aacbeca6a7%7C0%7C0%7C638221940313710291%7CUnknown%7CTWFpbGZsb3d8eyJWIjoiMC4wLjAwMDAiLCJQIjoiV2luMzIiLCJBTiI6Ik1haWwiLCJXVCI6Mn0%3D%7C3000%7C%7C%7C&sdata=k1Us2uy9ZbEP0jf4NX%2Fm0UKvtp4g04hmlgEPT2Cx5bU%3D&reserved=0

[34] Benson, E. (2021, October). The OECD and Carbon Life-Cycle Assessments. Center for Strategic and International Studies.

[35] American Chemistry Council. Guide to the Business of Chemistry: 2022. Table 7.1, p. 50.

[36] Boroush M and Guci L. National Science Board. *Science & Engineering Indicators. Research and Development. U.S. Trends and International Comparisons. Table RD-14.* Business expenditures for R&D, by selected countries and top R&D performing industries: 2018 or most recent year. Published April 22, 2022. Available: https://ncses.nsf.gov/pubs/nsb20225/table/RD-14.

[37] Organization for Economic Cooperation and Development. ANBERD (Analytical Business Enterprise Research and Development Database. R&D Intensity by Industry, 2019. https://www.oecd.org/innovation/inno/anberdanalyticalbusinessenterpriseresearchanddevelopmentdatabase.htm.

Another aspect of competitiveness in the business of chemistry is linked to the cost of operations in promoting more sustainable management of chemicals. For example, in the United States, increasingly, companies are providing sustainability services to downstream users of chemistry, to promote safe and efficient use, while promoting circularity by capturing and reusing waste. Notably, in the electronics industry, chemical companies may "lease" chemicals to semiconductor companies to process chips, managing the used chemicals and waste. In the automobile sector, coatings companies run the entire coatings operation.

Sustainable chemistry principles potentially address important industry environmental abatement costs which translate to increased profitability. In 2011, a report on the economic benefits of green chemistry published by the University of Massachusetts found that negative environmental outcomes, measured in terms of environmental lawsuits and toxic releases, reduce the market value of an average firm in the U.S. chemical industry by an estimated 31.2% of the replacement value of assets and that appropriately designed regulations support innovation, productivity, and employment in the chemicals sector.[38] Sustainable chemistry initiatives may boost U.S. economic competitiveness by reducing abatement costs associated with producing and using chemical products.

Addressing the Challenges

U.S. leadership in sustainable chemistry will support enhanced environmental sustainability, means to address climate change, national security and economic competitiveness, and improve supply chain resilience.

VI. Global Perspectives

To be a scientific and technological leader in sustainable chemistry, the United States must acknowledge the global nature of the chemical industry. Global coordination and harmonization strengthen supply chain resilience and security, which is crucial to national and economic security. However, a long-term commitment to investments that drive innovation will be necessary to promote the change needed for sustainability. As the United States transitions to more sustainable chemistry practices, the potential impact on supply chains dependent on existing chemicals must be managed to avoid economic and national security vulnerability. Consistency in metrics and data quality, interoperability, and alignment with international regulations and standards promotes competitiveness and stability in U.S.-based supply chains. The ability to lead on a global scale depends on understanding the global perspectives of our allies and partners; additionally, these interactions provide opportunities to share best practices, innovations, and lessons learned across nations. Below are examples of sustainable chemistry activities across the globe, including how the United States is currently engaging and opportunities for further engagement. This is not meant to be comprehensive, but instead provide evidence of the complexity of sustainable chemistry as an international issue.

The impact of regulation on the sustainable chemistry field, both within the United States and internationally, must be considered. Greater consistency in chemical and chemical product regulations and standards has the potential to increase commercial manufacture of more sustainable products.

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[38] Heintz J and Pollin R. 2011. Political Economy Research Institute, University of Massachusetts, Amherst. Blue Green Alliance, The Economic Benefits of a Green Chemical Industry in the United States, 6-7.

This includes regulation of the products themselves and regulation of the packaging that those products are transported in. However, regulations by other countries that may place a greater emphasis on taxing pollution or incentivizing more sustainable chemistry may push the development of more sustainable products by product manufacturers. Because of the international nature of our supply chain, these companies must consider non-U.S. regulations when developing new products and processes to avoid trade barriers. U.S. leadership is needed to drive harmonization of regulations that support sustainable chemistry initiatives. Different rules related to sustainability could lead to trade barriers where products designed to meet a certain market could inhibit their sale in a different market.

Development of International Sustainability Standards and Metrics

According to the Department of Commerce,[39] approximately 93% of global trade is affected by standards or technical regulations. To promote the use of standards as an enabler of trade and innovation, the United States advocates that countries, in line with their obligations via the World Trade Organization Technical Barriers to Trade Agreement, participate in the development of technical regulations and utilize international standards. The application of this approach in the United States is supported via U.S. trade statues and trade agreements, as well as the Office of Management and Budget (OMB) Circular A-119: Federal Participation in the Development and Use of Voluntary Consensus Standards and in Conformity Assessment Activities,[40] which directs U.S. Federal agencies to use international standards developed or adopted by voluntary consensus standards bodies rather than government-unique standards, except where inconsistent with applicable law or otherwise impractical.

There are several international standards and certification systems related to sustainable chemistry. These standards and certification systems vary widely, but tend to focus on the use of chemicals in specific processes for subsectors of chemicals products. Some stakeholders in the sustainable chemistry community report that there may be a need for more standards across sectors to define and to assess the sustainability of chemical processes and products. They believe that the lack of these standards inhibits the advancement of the goals of sustainable chemistry.[41,42]

In the United States, our voluntary consensus standards system is bottom-up, industry-driven, and sector-focused.[43] Federal agencies could expand interagency coordination and information exchange activities to support Federal and private sector engagement and ensure effective engagement of the United States in the development and use of international standards and related tools. Furthermore, Federal agencies such as NIST could fulfill an enhanced role in maintaining measurement methods, data, and models that underpin standards for sustainable chemistry and its attributes. This should be supported by enabling transferable, transparent information to flow along the value chain and across stakeholders.

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[39] Okun-Kozlowicki J. 2016. Standards and Regulations: Measuring the Link to Goods Trade. United States Department of Commerce Office of Standards and Investment Policy.

[40] https://www.whitehouse.gov/wp-content/uploads/2020/07/revised_circular_a-119_as_of_1_22.pdf

[41] United States Government Accountability Office (GAO). (2018, February). Chemical Innovation Technologies to Make Processes and Products More Sustainable. Technology Assessment.

[42] Tickner JA and Becker M. 2016. Mainstreaming Green Chemistry: The Need for Metrics. *Current Opinion in Green and Sustainable Chemistry*, vol. 1.

[43] Oltholff, J. (2022). Setting the Standards: Strengthening U.S. Leadership in Technical Standards.

Economic Security

When considering participation in international investments or programs, Federal agencies should evaluate how participation might enhance U.S. competitiveness or create vulnerabilities in our absence, especially if competitors fill the void in U.S. presence in a manner that is detrimental to U.S. national or economic security interests.[44] Trade and other agreements should also consider sustainability with respect to availability of raw materials, technology practices used by partner countries, and EJ and equity factors when compared against domestic sources and practices, as well as UN Sustainable Development Goals.

National Security

Sustainable chemistry-related technologies are critical to national security,[45] as they support our industrial base and economic resilience. Access to chemicals and materials is required for our nation's warfighters to sustain and strengthen deterrence with our most consequential strategic competitors.[46] Although there is no commercial market for certain national security capabilities, commodity items, such as chemicals, are integral components and enable the defense industrial base, and at times create unique strategic advantage.[47] As such, as commercial markets adopt sustainable chemistry principles and accelerate change away from existing chemicals, it is important to consider the impact to dependent national security capabilities. For example, the pace of change from existing chemicals may outpace the chemical and defense sector's ability to develop and adopt new chemical technologies, which could increase reliance on foreign suppliers or result in the loss of capability. Likewise, as regulations drive adoption of sustainable chemistry principles, it is important that the U.S. interagency assess impacts to key capabilities and engage with allies and industry partners to develop strategies to maintain industrial base resilience.

As supply chains have become more global in scale, there has been decreased visibility into sub-tiers of supply chains—which exacerbates the issues with defense supply chains. As sustainable chemistry initiatives increase transparency, traceability, and accountability in supply chains, this will enable strategies to address vulnerabilities and identify if more sustainable alternatives might be available.

The innovation created by sustainable chemistry initiatives is a national security opportunity. Innovations are essential to military preparedness—like highly specialized lithium-ion batteries—and require an ecosystem of innovation, skills, and production facilities that the United States currently

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[44] https://www.whitehouse.gov/wp-content/uploads/2022/01/010422-NSPM-33-Implementation-Guidance.pdf

[45] CISA. There are 16 critical infrastructure sectors whose assets, systems, and networks, whether physical or virtual, are considered so vital to the United States that their incapacitation or destruction would have a debilitating effect on security, national economic security, national public health or safety, or any combination thereof. Presidential Policy Directive 21 (PPD-21): Critical Infrastructure Security and Resilience advances a national policy to strengthen and maintain secure, functioning, and resilient critical infrastructure. (https://www.cisa.gov/topics/critical-infrastructure-security-and-resilience/critical-infrastructure-sectors).

[46] United States Department of Defense. (2022). Fact Sheet: 2022 National Defense Strategy. https://www.defense.gov/Spotlights/National-Defense-Strategy/

[47] United States Department of Defense. (2022). Securing Defense-Critical Supply Chains. An action plan developed in response to President Biden's Executive Order 14017.

lacks.[48] It is important to build domestic production capacity for those supply chains that are critical for national defense. The U.S. government can leverage its investment authorities for domestic production in certain sectors, and sustainable chemistry principles can shape development of new technologies that reduce pollution and waste generation and advance national security capabilities.

International cooperation and collective action are needed to promote resilience, competitiveness, and innovation.[49] As supply chains incorporate sustainable chemistry principles, there can be decreased interoperability with our partners without engagement and collaboration between partners and allies. Through cooperation with partners and allies, supply chains can increase resilience and improve our ability to recover quickly from disruption.

Related United States Policy

EO 14017, America's Supply Chains, declares the need for the United States to achieve resilient, diverse, and secure supply chains to ensure our economic prosperity and national security.[1] This includes investments in high road labor and environmental standards and developing domestic supplies, cooperating with allies and partners to diversify supply chains, developing workforce capabilities, enhancing access to financing, expanding research and development to broaden supply chains, and addressing risks posed by climate change. The U.S. government identified critical sectors and drivers of supply chain vulnerability, including limited international coordination and misaligned incentives and short-termism in private markets. Additionally, the *National Strategy for Advanced Manufacturing* identifies the importance of environmental sustainability, climate change, national security, as key factors in advancing national manufacturing capabilities.[2] **This report complements U.S. government initiatives to advance resilient supply chains by leveraging a life cycle perspective to achieve sustainable chemistry**.

[1] https://www.whitehouse.gov/wp-content/uploads/2021/06/100-day-supply-chain-review-report.pdf

[2] https://www.whitehouse.gov/wp-content/uploads/2022/10/National-Strategy-for-Advanced-Manufacturing-10072022.pdf

Relevant International Organizations' Initiatives

United Nations Environment Programme (UNEP). UNEP developed the *Green and Sustainable Chemistry: Framework Manual,*[50] which includes scientific, technical, and policy aspects of sustainable chemistry. The framework presented aligns with the UN SDGs. Additionally, UNEP's *10 Objectives and Guiding Considerations for Green and Sustainable Chemistry* provide additional detail, including green molecular

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[48] White House. (2021). Building Resilient Supply Chains, Revitalizing American Manufacturing, and Fostering Broad-Based Growth. 100-Day Reviews under Executive Order 14017.

[49] White House. (2021). Interim National Security Strategic Guidance.

[50] United Nations Environment Programme. (2021). Green and Sustainable Chemistry: Framework Manual. https://wedocs.unep.org/20.500.11822/34338.

design, a life cycle perspective, and ensuring chemistry works to address societal needs. In 2022, the United Nations Environmental Assembly, UNEP's governing body, launched negotiations on the establishment of a science policy panel on chemicals and waste management and on an international legally binding instrument on plastic pollution, both of which could have implications for U.S. policies in sustainable chemistry and potential opportunities for increased harmonization of regulatory practices. Interagency working groups led by the State Department have been established to prepare the U.S. delegations for both negotiations.

World Health Organization (WHO). WHO's Chemicals Road Map[51] details sound management of chemicals throughout their life cycle, with SC being a critical strategy. This road map links to the UN SDGs.

There is potential for more U.S. engagement with international bodies on research coordination and promoting cohesion in regulations and private sector, voluntary standards. For example, on the specific topic of plastic pollution, separate dialogues, studies, and statements have been pursued in recent years by the OECD, G7, G20, and the Asia-Pacific Economic Cooperation, in addition to the UN. This is complemented by concurrent work in both the International Organization of Standards and ASTM International, and in the relevant international research communities.

International Landscape

European Union Initiatives

There are several initiatives in the EU that will impact the local and global chemical industry, as well as users of chemical products. The *Chemicals Strategy for Sustainability Towards a Toxic-Free Environment*[52] is part of the *European Green Deal*[53] and establishes a vision and contains sustainable chemistry principles that are being used to guide policy development across sectors. The chemicals strategy strives for a toxic-free environment, where chemicals are produced and used in a way that maximizes their contribution to society, while avoiding harm to the planet and to current and future generations. The implementation of the chemicals strategy contains over 50 measures that will have far-reaching consequences for the chemical industry and the users of chemical products.

In December 2022, the EU elaborated on its Chemicals Strategy by publishing a framework for how it will assess safe and sustainable by design chemicals and materials Commission Recommendation: EU 2022/2510. The stated aim of the framework is to place the EU "at the forefront of research and innovation, and to promote use of the latest scientific knowledge to meet the highest levels of ambition for safety and sustainability in innovation." It included several areas of focus including:

> *"substituting as much as possible the production and use of substances of concern; for promoting the use of sustainable resources and feedstock for the production of chemicals and materials; for minimizing the impact of the production and use of chemicals and materials, throughout their life*

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[51] World Health Organization. (2017, July). Chemicals Road Map. https://www.who.int/publications/i/item/WHO-FWC-PHE-EPE-17.03

[52] EU. Chemicals Strategy. https://environment.ec.europa.eu/strategy/chemicals-strategy_en

[53] https://commission.europa.eu/strategy-and-policy/priorities-2019-2024/european-green-deal_en.

> *cycle, on the climate, on the environment, and on human health; and for driving industries and public authorities' R&D investments in the right direction."*

The Commission seeks to refine the framework, via a testing period, in which EU member states and stakeholders will be encouraged to report on its applicability and the development of case studies. The Commission will then consider if the framework should be used with additional aspects in terms of safety, sustainability, and social impact. The framework seeks to establish ambitious principles to support investments in research and innovation, while relying upon EU regulatory frameworks when assessing safety and sustainability performance.

Australian Initiatives

Australia's Commonwealth Scientific and Industrial Research Organisation is the leading scientific agency in Australia. Aligning with the SDGs, this organization has wide-ranging research around sustainability.[54] Recent reports include proposals for bio-based plastics, strategies around sustainable weed and pest control, and opportunities for circular economy and waste management.

Chinese Initiatives

Since at least 2016, China has included priorities around the greening of its industries, including chemistry. These priorities included modernizing chemical production technologies to reduce air and water emissions, as well as moving to less-toxic formulations in agriculture and other chemical sectors. The 14th five-year national plan, published in March 2021, covers the years 2021 through 2025. This plan emphasizes the push to a low-carbon transition, with China's aiming for its economy to peak in energy use by 2030 and to reach net zero by 2060. Notably the plan includes binding targets for capping energy and carbon intensity per unit of GDP, rather than the total tonnage of CO_2 equivalent emissions.

Since the plan's issuance, China has issued several subplans, focused on traditional industries, such as petrochemicals and the automotive industry, that similarly will seek to set peak GHG emissions targets, as well as plans linked to specific commitments, including support to the expansion of the circular economy, advanced manufacturing, and greening industry. China also published plans on clean production and the Industrial Green Development Plan. Chemicals and green targets are referenced across several of these plans. The plans suggest that China will promote a holistic approach to reduce the GHG emissions across heavy industries—including chemicals—focused on enhancing the efficiency of production and access to renewable energy and materials as well as carbon capture technologies and bio-based feedstocks. Coal is anticipated to stay in China's energy mix in the near term.

In terms of other sustainability criteria for chemicals, China's ambition is in line with its chemicals regulations to move towards the use of less toxic substances, with a prioritization to develop alternatives for priority chemicals. China's Clean Production Plan also references a plan to reduce reliance on persistent organic pollutants and volatile organic compounds, including referencing China's commitments via the Kigali Agreement to the Montreal Protocol to move away from the use of HFCs. In addition to industrial plans and policies in support of these objectives, China notes in the 14th Plan its intent to establish unified green product standards, certifications, and labeling systems,

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[54] https://www.csiro.au/en/research/environmental-impacts/sustainability

particularly for energy and water efficiency. It does not specifically reference plans to develop standards for green or low- carbon chemicals, but there are references across the document to develop standards for circularity and recyclability of chemical intensive products, such as batteries.

In 2018, the State Council[55] developed a three-year action plan to reduce emissions, including GHG emissions, and achieve cleaner air. This plan updated the legal framework and increased financing to adjust industrial production, increasing pollution control, and transition towards a cleaner, more efficient energy system, including efficiency improvements across all end-use sectors.

VII. Environmental Justice Considerations

Executive Order 14096[56] defines environmental justice as the just treatment and meaningful involvement of all people, regardless of income, race, color, national origin, Tribal affiliation, or disability, in agency decision-making and other Federal activities that affect human health and the environment so that people: (i) are fully protected from disproportionate and adverse human health and environmental effects (including risks) and hazards, including those related to climate change, the cumulative impacts of environmental and other burdens, and the legacy of racism or other structural or systemic barriers; and (ii) have equitable access to a healthy, sustainable, and resilient environment in which to live, play, work, learn, grow, worship, and engage in cultural and subsistence practices.

This EO aims to advance equity for all, including people of color and others who have been historically underserved, marginalized, and adversely affected by persistent poverty and inequality. The disproportionate historical impacts of chemicals on the health, well-being, and quality of life of these communities is an issue that can be improved by employing sustainable chemistry activities.

Environmental Justice Considerations

Negative impacts of chemicals on human health and quality of life are frequently concentrated near locations where those chemicals are manufactured and along routes where they are transported or disposed. These manufacturing and disposal facilities are often located in communities that have been historically underserved and marginalized and the presence of manufacturing or disposal facilities serves to increase inequality for those who live nearby.

Widespread use of sustainable chemistry principles by facilities located in or near marginalized communities will result in processes that release fewer, less-harmful chemicals into the environment throughout the manufacturing, use, and disposal phases of the chemical lifecycle. These resultant reductions in exposure to potentially harmful chemicals will serve to increase equity by lessening the disproportionate burden currently borne by people of color and others who have been historically underserved or marginalized.

EJ principles and stakeholder engagement will be important considerations when developing sustainable chemistry. Creating an inclusive and participatory decision framework for sustainable chemistry necessitates understanding the breadth and diversity of all communities that could be

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[55] http://english.www.gov.cn/premier/news/2018/06/13/content_281476183699292.htm

[56] EO 14096. “Revitalizing Our Nation's Commitment to Environmental Justice for All.” https://www.whitehouse.gov/briefing-room/presidential-actions/2023/04/21/executive-order-on-revitalizing-our-nations-commitment-to-environmental-justice-for-all/

affected by changes in chemical processes. Engaging communities from the initiation of a decision-making process through completion and evaluation of results is a mechanism to build public trust. This could also increase equity in decision making and mitigation outcomes by ensuring engagement with underrepresented and disproportionately impacted groups. Therefore, any plan for sustainable chemistry activities should start with engagement of stakeholders, collaborators, and partners that ranges from researchers and community scientists to public health experts, industries, governments (Federal, state, local, Tribal, and territorial), non-governmental organizations, and civil society. Building these relationships will provide the opportunity to understand the concerns, values, and perspectives of collaborators and partners, as well as allow for transparency, openness, and clear communication.

While a transition to use of sustainable chemistry will have many benefits for EJ communities, there are challenges that must be addressed during this transition. In order to effectively increase equity, the transition should be prioritized at manufacturing facilities in historically marginalized or disadvantaged areas. If the transition to sustainable chemistry does not follow this model, and is instead first initiated at manufacturing sites in wealthy communities, it may have the opposite effect and could further burden historically marginalized communities relative to other areas.

Economic considerations for a transition to the use of sustainable chemistry must also be examined. If transition to use of sustainable chemistry practices results in increased costs for goods and services, people with limited financial resources will be least likely to benefit from sustainable chemistry, as they may not be able to afford sustainably produced products or services. It will be important to minimize any cost increases in manufacturing and disposal of chemicals to ensure that all people benefit from a transition to sustainable chemistry.

VIII. Education and Workforce

The Federal government currently makes significant investments in science, technology, engineering, and mathematics (STEM) education. The NSTC Committee on STEM Education's (CoSTEM) strategic planning process identified 129 Federal programs with a total FY 2020 investment of $2.25 billion directly or indirectly supporting partnerships among Federal agencies, educational institutions, employers, museums, and other community organizations to leverage resources and expertise across STEM education ecosystems to maximize the impact of educational efforts. It also identified 165 programs with a total FY 2020 investment of $3.3 billion directly or indirectly supporting diversity, equity, and inclusion in STEM.[57]

These foundational investments, which in part support chemistry education at all levels, present an opportunity for specifically advancing sustainable chemistry education. A February 2018 GAO[58] technology assessment found that "integrating sustainable chemistry principles into educational programs could bolster a new generation of chemists and advance student achievement in the field."

Some Federal government funding is already spurring enhanced collaborations to integrate research and education, drive innovation, and broaden participation in chemistry and allied disciplines. For

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[57] OSTP. "Progress Report on the Implementation of the Federal Stem Education Strategic Plan" - https://www.whitehouse.gov/wp-content/uploads/2022/01/2021-CoSTEM-Progress-Report-OSTP.pdf

[58] https://www.gao.gov/assets/gao-18-307.pdf

example, the NSF Centers for Chemical Innovation (CCI), research centers that include scientists from across academic institutions, tackle major chemical research challenges to produce transformative research, while also organizing educational outreach programs for elementary, middle, and high schools, colleges and universities, and the community to increase understanding about sustainable chemistry. Educating students early is critical to building a workforce knowledgeable in sustainable chemistry. Additionally, innovative ways to work with non-traditional students, including those who may transfer into four-year colleges and universities from community colleges, is an important consideration. Finally, investment in Historically Black Colleges and Universities (HBCUs) and other minority serving institutions (MSIs)' chemistry programs represents an important path to equitably increasing sustainable chemistry education. One successful model is the long-standing NSF Partnership for Research and Education in Materials program, which supports MSIs to partner with larger centers and facilities, such as the Materials Innovation Platforms conducting research in sustainable polymer chemistry. A recently launched sister program, the NSF Partnerships for Research and Education in Chemistry, is funding MSIs to partner with CCIs, including those focused on sustainable chemistry topics to build a more diverse pipeline into sustainable chemistry science.

Federal government investments in workforce development are another set of existing opportunities into which sustainable chemistry education and training could be integrated. As GAO noted, "new training to upgrade the chemistry and manufacturing workforces could encourage innovation." Some of these workforce development efforts include those administered by DOL's Employment and Training Administration—programs established through the Workforce Innovation and Opportunity Act,[59] which help job seekers access employment, education, training, and support services to succeed in the labor market and to match employers with the skilled workers they need. Existing worker safety and health training efforts, such as NIEHS's Worker Training Program and OSHA's Training Institute Education Centers,[60,61] could train the workforce on safer chemistry, driving demand for sustainable chemistry innovation and supporting implementation of these technologies throughout all sectors of the economy.

Federal government engagement with other key stakeholders, including academic institutions, industry associations, and non-governmental organizations, is also critical for sustainable chemistry education and workforce development efforts. To date, many of these stakeholders have significantly advanced sustainable chemistry education efforts.

Advancing diversity is also a critical goal of current chemistry education efforts and should be a fundamental consideration for future sustainable chemistry education efforts. The National Academies of Science, Engineering, and Medicine has noted that diversifying the chemical workforce and the chemical engineering profession is essential to the field.[62, 63] Several existing Federal efforts, such as the U.S. Federal TRIO program, NIH Build Initiative, NSF Planning Grants, and DOE Reaching a New Energy Sciences Workforce awards support DEI and Diverse Individuals in the Chemical Sciences.

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[59] https://www.dol.gov/agencies/eta/wioa/programs

[60] https://www.niehs.nih.gov/careers/hazmat/about_wetp/index.cfm

[61] https://www.osha.gov/otiec/

[62] https://nap.nationalacademies.org/download/26342#

[63] https://nap.nationalacademies.org/download/26568# (p. 124).

IX. Key Technological Considerations

Technological support is crucial to implementing a robust sustainable chemistry strategic plan. Technology will be foundational to advancing sustainable chemistry, as it can support dramatic improvements in fidelity, scalability, and throughput. Specific technologies relevant to innovations in sustainable chemistry warrant attention. In 2018, GAO published a Technology Assessment on Chemical Innovation[64] that identified three primary technologies that would advance sustainable chemistry: (1) technologies to make catalysts more sustainable; (2) technologies to make solvent use more sustainable; and, (3) technologies as more sustainable alternatives to batch processing. This analysis was based on extensive input from experts across the government, industry, and academia. In addition to these specific chemical innovation needs, there are additional areas where technological development will advance sustainable chemistry.

Data sharing platforms are critical for comprehensively addressing sustainable chemistry across the life cycle of materials. These platforms should house information that aligns with the considerations of sustainable chemistry presented above, including benchmarks or evaluation metrics. Development of these platforms should prioritize harmonization with existing platforms and transparency to allow for this information to be more widely available to all stakeholders, including the Federal government, academics, state and local governments, private companies, and the public.

Artificial intelligence and machine learning (AI/ML) have the potential to accelerate materials discovery and process design, as well as provide information on hazard potential and environmental sustainability. High-throughput screening and computational toxicology could provide relevant expertise and analytical techniques that are crucial for screening to help indicate where more in-depth toxicological studies are needed to complete hazard characterization. In order to seize the benefits of AI/ML, we must manage any risks involved with its design, deployment, and usage.

Circular technologies and infrastructure are key to sustainable chemistry. These technologies rely on used materials and chemicals continually reentering the supply chain, including technologies related to developing chemicals from recycled and recovered materials.

Synthetic biology represents another technological opportunity to advance innovation in sustainable chemistry. This field focuses on reengineering organisms (e.g., to gain a new ability, produce a new substance, etc.). This allows researchers to harness the power of nature for innovative solutions.

Efforts to transition basic research findings to application and commercialization will also be central to advancing sustainable chemistry. Transitioning fundamental scientific discoveries into new technologies has been and continues to be a significant challenge. However, the successful integration of basic and applied sustainable chemistry research could provide notable societal benefits, for instance, through the development of more sustainable commercial products and of more efficient technologies.

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[64] GAO-18-307. *Chemical Innovation: Technologies to Make Processes and Products More Sustainable.* https://www.gao.gov/products/gao-18-307.

X. Current Innovation Trends and Opportunities in Sustainable Chemistry

Sustainability concepts must be at the forefront of chemical research. While recent innovations provide continued strides toward an idealized circular economy, opportunities exist from the basic science level to the technology transition space to continue to accelerate this process. Computational and data-intensive sciences coupled with AI/ML can also play an important role in advancing sustainable chemistry.

Highlighted below are example approaches to sustainable chemistry innovation, specifically: 1) energy inputs and energy balancing in chemical reactions and processes, 2) circularity, including safe and sustainable by design, chemical fate, and waste resource management, 3) foundational feedstocks for sustainability, and 4) catalysis and separations. Crosscutting challenges and opportunities for innovation present themselves across these areas, providing a roadmap for future investment.

Energy Inputs and Energy Balancing in Chemical Processes

For many decades, the chemical industry has been structured primarily around thermal conversions and separations, with highly engineered balance of plant considerations maximizing efficiency. However, in moving toward a sustainable industrial complex, considerations regarding both the energy source for chemical reactivity and separation, as well as holistic accounting of the energetic and environmental impacts of processes are needed.

Many opportunities exist to leverage energy inputs that do not use energy-intensive thermal processes in chemical conversions, particularly given the enormous potential of solar energy and the possibility of transducing solar, wind, and geothermal energy into stored electrical energy with improved renewable energy generation and storage technologies. These have been explored in many contexts (e.g., electrification of chemical processes, photochemical methods, coupling of photo(electro) conversions, and mechanochemistry), but much research remains to overcome both fundamental (increasing efficiency) and practical (improving durability and utilizing system components with robust and sustainable supply chains) challenges in these areas. Moving beyond redox-driven transformations in such processes presents another opportunity, which could expand the scope and accessibility of reactions and reaction systems and impact the fine chemical space (e.g., pharma). For example, biological systems demonstrate the ability to utilize solar power to drive complex molecule biosynthesis and incorporate nitrogen and oxygen, and exquisitely build molecular complexity with control of stereochemistry. And while ‘artificial leaf’ approaches have begun to provide prototypes for such bioinspired approaches, the swath of chemical space yet to be explored with such systems is immense.

Beyond the energy source-mediating processes, expanding the types of methods utilized and the scale of their deployment remain active areas of exploration. The challenges of scaling photo- and electro-mediated reactions can be unique in an industry heavily entrenched in thermal processes. However, recent examples in the pharmaceutical industry demonstrate potential for scaling photoredox and electromediated reactions.[65,66] While a recognized challenge, a continued push towards methods that prioritize flow over batch processes is another goal aligned with more efficient and sustainable methods.[67]

Beyond the energy inputs, methods, and scale of chemical processes, accounting for energy and emissions management considerations through a life cycle of resources, production, use, and end of life is critical to achieve truly sustainable systems. This requires an awareness of process scales and a recognition that reactions may also require coupling to off-cycle processes (e.g., CO_2 capture and storage, see below) to be viable. Moreover, opportunities continue to exist to develop a range of both transient and long-term energy storage vehicles, either chemical or electrical in nature. Versatility in this space is key, given the requirements of one sector vary widely with respect to another, such as comparing energy needs for a continuous, unmanned facility to those of a heavy-duty transport vehicle.

Circular Processes/Circularity

Generally, chemical/material performance and cost during production and use have been primary drivers within chemical manufacturing. Considerations of impact post-use have played secondary roles or were non-factors, with those costs frequently borne by local governments and taxpayers. As such, great opportunity exists to consider full life cycle ramifications and design of more sustainable chemicals and materials while concurrently examining waste sources as potential feedstocks.

New design concepts for circular chemical and materials synthesis remain an active area of research. Topics of current study include introduction of “Trojan horse” elements within the chemical/material to permit for on-demand breakdown and materials responsive to stimuli (light, heat, etc.).[68] Moreover, circular design methods can move beyond just generation and regeneration of feedstock/product to connect to deconstruction to intermediates of value that might integrate into other sustainable life cycles. Such cascade value chains are an alternative to the feedstock/product cycle that may prove more advantageous in certain situations. Much work remains in integrating circular design concepts into areas, including concrete production and metallurgy, which inherently can involve challenges associated with environmental considerations, emissions, significant energy demands, and scarce or geopolitically-fraught supplies.

Resource recovery and management is the second key consideration to transition to a circular economy. Many opportunities exist in this waste-to-resource space, including: 1) ability to selectively deconstruct materials on demand and often in mixed feeds containing additives/impurities, 2) harnessing/retaining the inherent chemical complexity of the feedstock to provide value-added products, 3) design for recycling, 4) moving beyond carbon management to consider cycling of other critical elements (hydrogen, nitrogen, and phosphorous, specifically), 5) considering resources that indirectly enter into product life cycle (e.g., water, solvents, etc.), 6) targeting key sectors or product

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[65] *The importance of synthetic chemistry in the pharmaceutical industry*, *Science*, **2019**, DOI: 10.1126/science.aat080.

[66] Decarboxylative Cross-Coupling: A Radical Tool in Medicinal Chemistry *ACS Medicinal Chemistry Letters* **2022** *13*(9), 1413-1420, DOI: 10.1021/acsmedchemlett.2c00286.

[67] Asymmetric Organocatalysis in Continuous Flow: Opportunities for Impacting Industrial Catalysis, ACS Catal. 2015, 1972–1985, DOI: 10.1021/acscatal.5b00002.

[68] Near-complete depolymerization of polyesters with nano-dispersed enzymes, Nature, 2021, 592, 558-563, DOI:10.1038/s41586-021-03408-3.

formats with little chance of recycling being economically viable (e.g., personal care, multi-layer packaging), and 7) substantively decreasing the energetic costs of circular processes.

Foundational Feedstocks for Sustainability

Although the chemicals, plastics, and other materials used today primarily originate from hydrocarbon sources, the feedstocks of a circular economy will derive from more readily available molecules, including water, carbon dioxide, and nitrogen. Complex but renewable feedstocks (e.g., biomass) will also play an important role. The current landscape for each feedstock class and opportunities to advance impact on chemical sustainability are highlighted below.

While hydrogen remains a key component underpinning the chemical industry, the source of the molecule is critical to a sustainable future. Though the majority of hydrogen generated today is produced through natural gas stream methane reforming with substantial CO_2 emissions, scalable clean hydrogen production through approaches such as water electrolysis is ramping up. This area is of clear national interest, given the DOE Energy Earthshot – Hydrogen Shot™, with a goal to reduce the cost of clean hydrogen by 80% to achieve $1 per kg of hydrogen in one decade.[69] Much opportunity remains in the space to enable clean hydrogen production, delivery, storage, and end use, which covers multiple technologies. This challenge spans both chemistry and materials science, across hydrogen and fuel cell technologies, with a need, for example, to discover and develop more efficient, earth-abundant catalysts to achieve high activity, while also meeting cost, efficiency, and durability requirements.

Bio-based material success stories

Recent success stories in this area include development of bio-based chemicals and materials like polylactic acid and polyhydroxyalkanoate, which are now being commercialized. Another example, polybutylene adipate terephthalate, now on the market, combines attributes of both petroleum-derived and bio-based polymers. Much opportunity exists to improve property performance of these materials; it remains an area where strides in data/science MC methods and automation, discussed in detail in other sections of this report, can accelerate discovery.

Roadmap to biodegradable plastics-current state and research needs, *ACS Sustainable Chemistry & Engineering,* **2021**,*9*, 6170-6187, DOI:10.1021/acssuschemeng.1c00801

The impact of CO_2 as a greenhouse gas is well known, and efforts are underway to capture and store CO_2 reservoirs and in value-added products. Relevant to sustainable chemistry, CO_2 can play a unique role in a circular economy, given its potential to act both as a feedstock and a product of combustion and various industrial reactions. As a reactant in chemical processes, much effort is being pursued in the electrocatalytic reduction of CO_2. Given the disparity of scales between fine chemicals and fuels, means of capturing and storing CO_2 must also be pursued in tandem with chemical conversion. Key to many of the potential systems is reactive capture and storage of CO_2 as small-molecule organics or inorganic minerals (e.g., carbonates). Understanding the geochemical formation and persistence of these salts in the subsurface is key to environmental decarbonization of manufacturing and the chemical industry.

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[69] https://www.energy.gov/eere/fuelcells/hydrogen-shot.

While biomass is a more complex feedstock, it can function as both a renewable carbon pool and one that serves as an alternative oxidized carbon source to CO_2 for hybrid biocatalytic/synthetic processes. Many advances have been made in this area in the past few decades, with a variety of routes from the main components of biomass (cellulose and lignin) to value-added chemicals and fuels being developed. Although conversion of biomass to co-products and fuels can be demonstrated at or near economically viable levels, much work remains to target commodity chemicals at appropriate scales.

Catalysis and Separations

Catalysis is a central component to most industrial reactions, given its ability to accelerate reactions and direct reaction selectivity towards desired products. From an industrial perspective, this enables both lower capital and operating expenses, as well as decreased energy demands and emissions burdens per unit of product. These advantages translate directly from traditional fossil fuel-based feedstocks to sustainable feedstocks—the primary difference reflecting a corresponding switch from fossil energy-mediated thermal processes to sustainable energy, direct or indirect electrical processes. Thus, the future of catalysis for sustainable chemistry will come in the form of greater reliance on electrocatalysis, mechanocatalysis, photocatalysis, and renewable energy-based thermal catalysis. The search for efficient technologies for converting sustainable electricity to thermal energy has prompted research around alternative energy sources such as microwave or radio-frequency catalyst heating, cold plasma-assisted catalysis, novel reactor designs for efficient electrical resistance heaters, and even small fission nuclear reactors for electricity generation. Beyond the alternative energy sources required for sustainable industrial chemistry, many research opportunities exist for tailoring catalysts to the new energy sources. Catalyst design and discovery can impact many aspects of sustainable processes, including: (1) improving the robustness of catalysts and ability to tolerate a wide variance of environmental conditions; such advances could provide self-healing or switchable catalysts that have the durability necessary for the range of catalysis required for both distributed and modular manufacturing discussed above; (2) enzyme engineering can also be used to specifically tailor catalyst reactivity/selectivity; exploiting the specificity of natural active sites with the combinatorial techniques of artificial enzyme development provide a unique way to explore a given chemical reaction; and, (3) biochemical and chemical catalysts may also be integrated, as hybrids or used in sequenced cascades. These systems could blur the boundaries of traditional catalytic fields and permit transformations inaccessible to any current catalyst class. While such advances offer exciting research opportunities for coupling sustainable energy sources—through advanced catalyst designs—to sustainable chemical manufacturing, significant challenges remain, especially in chemical process scalability. Traditional fossil feedstock hydrocarbon reactions are characterized by high rates and throughput but suffer from poor product selectivity and the need for energy-intensive downstream processes (e.g., separations, recycling, treatment of waste products, etc.). In contrast, enzyme catalysis offers exquisite selectivity for specific target molecules, but at rates and throughput generally incompatible with demand for commodity chemicals. There are clearly opportunities to increase process efficiencies here by addressing such challenges to improve titers, material throughput while reducing volumes and aqueous effluents.

Separations are another key process that underpin modern chemical conversions and sustainable chemistry. Sustainable production of fuels and chemicals and a large number of pollution prevention and environmental clean-up processes rely on chemical separations. In addition, a notable amount of in-plant industrial energy use in the United States can be attributed to chemical separations. Innovations in this space that can contribute to sustainability include: 1) coupling conversion and separation to drive desired reactivity,[70] 2) moving beyond distillation, through study of melt/bulk phase reactivity (e.g., solvent-free reactions) or using alternative separation media and energy sources (membranes, organometallic complexes, mechanochemistry, electro-, magneto- and photo-excitation, etc.), and 3) extended investigation of solid-liquid interfaces and how solvents impact fluid transport in confined environments within porous materials.

Finally, the ability to model, simulate, and create digital twins of complex chemical systems with improved fidelity, scalability, and throughput will be foundational to advancing sustainable chemistry.

XI. Barriers to Innovation

There are various kinds of barriers to innovation for sustainable chemistry. These include technological barriers, business-related concerns, industry-wide concerns, and sector-specific challenges, among other issues.

Technological Barriers

The technological barriers identified include issues throughout the life cycle of a chemical product, including the need to consider alternatives. Among the technological barriers, there are specific fundamental and applied science challenges, which are related to the need for additional national dialogue, research, and investment support from the Federal government. The Federal government should consider leading in piloting or de-risking technological efforts, and coordinating cross-field/sector efforts.

There is a lack of research support for modular or mono-material processing and design, which can extend the lifetime of a chemical or product (including its ability to repair, refurbish, or recycle) or reduce the time required for decomposition, while simultaneously making it safer and cheaper (see section XIII below for additional details).

Alternatives

There are many unaddressed needs related to improving the discovery, development, and implementation pipelines of alternative chemicals and alternative chemistry processes, which constitute major barriers.

Consideration of renewable alternatives to existing chemicals has unique barriers, which include variability of feedstocks that could present issues due to regional or seasonal availability affecting supply and disrupting production. There is an additional barrier, however, to adapting new alternatives when they do not readily plug into the existing industrial infrastructure. Similarly, the challenge that safer/more sustainable alternatives will often not be drop-in ready replacements presents a barrier in being able to use existing end-of-use infrastructure to recover materials safely and effectively, such as sorting technology at materials recycling facilities.

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[70] https://www.nationalacademies.org/our-work/a-research-agenda-for-a-new-era-in-separations-science

Supporting Business Models that Enable a Circular Economy

Support or incentives are needed to promote business models that enable circular economy through recycling, refurbishment and product sharing. For example, with regard to the end life of existing chemicals that may be considered hazardous, such as pesticides, pharmaceuticals, and flame retardants, there is a need to develop new approaches for their elimination, replacement and/or destruction. Similarly, clear technical definitions, measurements, methods and prioritized goals are critical to establishing a credible marketplace for circular chemicals and materials.

Standardization and Scale-Up

There is a need for coordinated action on issues like advanced plastic recycling technologies that include improved mechanical methods and increased efficiency of chemical processes, which can produce high-purity chemical and material feedstocks from plastic waste.

Inability to measure or assess sustainability disincentivizes businesses or consumers in considering sustainability broadly. It presents a barrier to all stakeholders along the value chain from having confidence in their choices. Without agreement on how to measure the sustainability of chemical processes and products, companies may be hesitant to invest in innovation they cannot effectively quantify, and end users are unable to make meaningful comparisons that allow them to select appropriate chemical products and processes. Without a standard set of attributes to compare and make decisions about sustainability, it is very difficult for customers, decision makers, and others to compare the sustainability of various products to make informed decisions. There is a need to provide better information on product content throughout the supply chain, and more sufficient data on the health and environmental impacts of chemicals throughout their life cycle to compare sustainability of products. Using a variety of metrics and including variation in the underlying factors included in their calculation hinders the ability of companies and others to compare the sustainability of chemical processes or products.

There is a risk of supply chain disruption when switching to alternative chemistry that may be considered more sustainable. These issues include scaling up and addressing the problems that arise in supply chains and raw material availability if relevant. Additionally, existing capital investments in current technologies may serve as a disincentive to newer companies that might want to enter a field full of well-established businesses.

XII. Strategic Areas of Opportunity

Overarching opportunities for transformational progress in improving the sustainability of the chemical sciences are presented below.

Standards and Metrics Development

Metrics Needs

Process metrics such as E-factor, carbon factor, atom, or mass efficiency and yield must be balanced against performance metrics such as durability, cost, end of use recovery pathways, and societal metrics, such as environmental leakage, health risks, and mitigation strategies. That will require models and data frameworks that challenge the status quo, and the use of Findability, Accessibility, Interoperability, and Reuse (FAIR) data principles that ensure equitable access and quantitative, reproducible outcomes.

Measurement methods for reliable and transparent data and metrics are not widely available to quantitatively inform decision making when complex systems-level determinations are needed from all stakeholder perspectives. Metrics should align with the definition and attributes of sustainable chemistry. Therefore, metrics need to be flexible in both definition and in weighting. Resulting information must move consistently and uniformly along the full value chain, with fixed meaning. It is likely that metrics or indicators will be needed for each attribute identified above. Additionally, an important component of metrics is understanding the baseline to measure progress. When evaluating metrics, it is important to remember that a goal for sustainable chemistry progress is that improvements in one aspect of sustainability should not lead to reductions in another equally important metric.

There is a lack of standardized tools and information regarding chemical or product sustainability. The lack of standardized tools increases the uncertainty in decision making and may slow down improvements, as companies would not want to incur costs from making changes that are ultimately not more sustainable, or which may make them vulnerable to accusations of "greenwashing."[71] Reducing this uncertainty through standardized tools is an approach to support broader commercial adoption of more sustainable approaches. For example, environmental product declarations have emerged as a standardized life cycle assessments (LCA) approach to communicate the environmental performance of a product.[72,73]

This report demonstrates the need for transparent, consistent, standardized, and harmonized metrics across sustainable chemistry activities. The development of consensus metrics necessarily depends on the definition and attributes of sustainable chemistry. Metrics should align with and evaluate attributes. Getting broad buy-in on these attributes across stakeholders will allow for a more robust conversation

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[71] "Greenwashing" is a form of misinformation often used to entice an aspiring green consumer. Companies promising to be sustainable, biodegradable, or environmentally conscious sometimes fail to meet the promises they make to consumers.

[72] Borghi, A. (2013). LCA and communication: Environmental Product Declaration. Int J Life Cycle Assess https://link.springer.com/article/10.1007/s11367-012-0513-9.

[73] Passer, A., et al. (2015). Environmental product declarations entering the building sector: critical reflections based on 5 to 10 years experience in different European countries. Int J Life Cycle Assess https://link.springer.com/article/10.1007/s11367-015-0926-3.

of how to evaluate those attributes. The need for these methods and metrics is critical to developing policy actions and implementing sustainable chemistry activities. Therefore, the development and identification of metrics (including when and where to use metrics and how to balance trade-offs) will be a critical immediate activity in the forthcoming strategic plan.

Data Sharing

Access to trusted data sources that allow comparison of information that is easily translated to meaningful outcomes is necessary to support movement toward sustainable chemistry. The leading issues for advancing access to trusted data sources include standardizing metrics and measurement methods, including how to harmonize different reporting mechanisms, interoperability, and computational advancement. Standardizing and harmonizing data is essential for moving forward and normalizing or prioritizing sustainable chemistry decisions. These decisions, which lead to claims and declarations, must be based on consistent and comparable information. Moreover, these decisions should follow and adhere to FAIR data principles to ensure equitable access, and quantitative, reproducible outcomes.

Continuous improvement to more sustainable practices can only occur if claims such as biodegradability, recycling, toxicity, and greenhouse gas emissions are expressed using consistent terms and measures based in quality data collection. Harmonization refers to the reconciliation of various data types, sources of data, and formats for compatibility and comparison across various platforms and communities. For example, measurements can only be compared if made on the same material types in the same measurement units; otherwise, the usefulness of those data may be severely limited. Having a comparable view of data from various sources is critical to understanding the full landscapes of sustainable management of materials. Lack of harmonization prevents effective communication. Given the many sources in which data can be collected, standardization in methodology or protocols for the collection, analysis, and preparation of data can serve as an opportunity to promote greater collaboration among stakeholders and interested parties to support quality assurance. This builds trust within the scientific community and with stakeholders and the public. The use of accrediting bodies, to ensure standardized processes are employed, also helps in the quality of the information and data that is being used. Development of trustworthy and privacy-preserving AI methods, and techniques for processing, reduction, curation, intelligent analysis, and integration of massive and heterogeneous data, as well as for extracting structured information from publications and legacy data, is critical to address these challenges. Generation of this data ecosystem can also accelerate and broaden workforce development and education opportunities.

Intellectual Property Sharing

Further important challenges in data science include access to data and enabling intellectual property sharing. How do we spread technologies that are game changing, while providing frameworks that enable companies to share comparable information? This relates to interoperability: sharing and accessibility to data for the greater good. The Protein Data Bank (PDB) is a good example of a data-sharing mechanism that has proven to be sustainable and effective, successful in garnering international participation by the protein structure community worldwide. This mechanism has allowed protein crystallographers to share the three-dimensional coordinates of protein structures in a format compatible with a large array of software/computational tools that can import and manipulate these data. The PDB contents have, in turn, served as a data set for the development of ML approaches that now have fundamentally transformed how we can predict protein structure, including AlphaFold and RoseTTAFold. The knowledge gained from this use of data sharing, ML, and chemistry informs biomedical breakthroughs for prevention and treatment of disease. This example also emphasizes the role for computational advancement and AI in maximizing data access and the potential for life cycle data and accessibility/application/translation to transform material choices, supply chains, and ultimately sustainable chemical and material supply systems for a circular economy.

The Federal government houses and manages huge amounts of data and can provide infrastructure for trusted sources of data, aggregating data, curating data, and translating data. Chemical, process, and product life cycle analysis is a key approach to understanding environmental impact; publicly accessible data that can be applied to products and can be translated for public understanding are required for educating industry and the public in chemical choices for reduced environmental impact and for advancing a circular economy. Interoperable and harmonized data platforms across all stakeholders—including international partners—is critical to advancing innovation in sustainable chemistry without duplicating efforts.

Life Cycle Assessment/Modular Design

Beyond these specific fields intimately tied to chemical conversion, for design of energy-efficient, decarbonized, circular processes to be successful, systems-level approaches that integrate and leverage computational methods must be considered from the outset. Holistic analyses which begin with molecular-level insights into atom and energy economy and end with process engineering considerations on the macroscale must be conducted. This integrated way of thinking ensures an accurate and complete picture of a process is developed. Intimately coupled with systems thinking is integrated cradle to grave assessments, such as LCA, techno-economic assessment (TEA), and sustainability assessments (SA), incorporating the entirety of the process (acquisition, manufacturing, separation, material use, end-of-life, and product disposal/recovery). LCAs, TEAs, and SAs should consider important factors other than GHG footprint, such as elemental footprint, ecosystem quality, and EJ impact. For example, DoD's Sustainability Analysis Guide[74] suggests consideration of life cycle

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[74] https://denix.osd.mil/esohacq/

cost and impacts such as GHG footprint, resource availability, human health, and ecosystem quality during defense acquisitions.[75]

Modular or mono-material design that can extend the lifetime of a chemical or product (including the ability to repair, refurbish, or recycle a product) or reduces the time required for decomposition should be explored. For example, reducing material complexity can help reduce plastic burden by simplifying recycling of the material, and as a result, decrease landfill build-up of the material in question.

Incentives

Economic motivation can provide a strong market demand for sustainable chemistry. Environmentally preferable purchasing can continue to harness the power of demand from the Federal government and provide standards for defining not just environmentally preferable purchasing but also sustainable chemical purchasing. Programs that currently exist to support green, safer, and sustainable chemistry can expand to inform choices that are lower impact and enable circularity (Safer Choice, BioPreferred, Energy Star, Water Sense). Additionally, fiscal policies and tax incentives that help companies manage the transition to and scale-up of sustainable chemistry activities could accelerate innovation and progress.

The U.S. government and its partners can leverage existing private sector and public interest (e.g., NGO, philanthropic, etc.) to better support sustainable chemistries. This could include academic, public interest, and private sector sustainability standards boards, as well as programming and resources to bring more specific definitions and focus areas to environmental, social, and governance investment. The recent appropriation for EPA to support 'Green Banks' to support shifts to lower-carbon emissions is a concept that could be expanded to include investments in sustainable chemistry, not just carbon emissions reduction.

Education

Educating students early is critical to building a workforce that is knowledgeable in sustainable chemistry. Additionally, innovative ways to work with students, including those who may transfer into four-year colleges and universities from community colleges, is an important consideration. Finally, investment in MSI chemistry programs represents an important path to equitably increasing sustainable chemistry education.

Another aspect of education related to sustainable chemistry is around educating consumers. Public behavior related to choosing more sustainable products is a result of consumer choices and socioeconomic status, and it is commonly raised as a major barrier to adoption of more sustainable products and technologies. Educating the public about the impacts of their consumption will not enable the level of change needed for a safe, sustainable and circular society without leadership action by industry and government.

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[75] In DoD, the term acquisition encompasses the design, engineering, testing, deployment, sustainment, and disposal of defense systems.

There is significant opportunity to better understand consumer and community behavior, and support change and adaptation to new technologies and norms by investing in robust interdisciplinary partnerships that include the social sciences. Development of decision science tools that support different approaches for planning and risk mitigation, including digital twins for the many choices made at the individual and local level, can help improve outcomes along the full value chain. If the benefits of taking a more sustainable approach are valued and can be afforded by consumers, companies may be able to recoup the higher costs by charging higher prices because of higher-quality, longer-lasting products. However, if the benefits are not easily understood and measurable (e.g., long-term health benefits), or are external to consumers (e.g., broader environmental impacts), then consumers may not be willing to pay higher prices for more sustainable products.

Resource Access

Resource access and stability of supply chains is a practical and important component to advancing sustainable chemistry. On the one hand, reducing reliance on critical minerals in catalytic processes and advancing the chemistry of earth abundant metals is a desired step toward creating a sustainable chemical enterprise within the United States. On the other hand, continued focus on optimizing catalytic turnover, increasing access to and usage of critical elements, and improving methods for their recycling is equally important, as are efforts to recycle rare earth elements, as critical components in the electronics, battery, and magnet industries. Moreover, leveraging the unique reactivity of base metals may provide unexpected opportunities that exceed performance of existing systems.[76]

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[76] Using nature's blueprint to expand catalysis with Earth-abundant metals, SCIENCE, 2020, 369, DOI: 10.1126/science.abc3183

Biocatalysis-based process chemistry success stories

With the advent of directed enzyme evolution methods[1] and biological pathway engineering, the past two decades have seen a notable transformation among some in academia and industry on the realm of the possible for bio-based routes into value-added products. Processes of note include the engineering of biological pathways from glucose to catechol[2] or to cap off the synthesis of anti-malarial artemisinin.[3] The development of an artificial transaminase evolved nearly from scratch to near perfection, which enzymatically set the stereochemistry of the anti-diabetes agent, sitagliptin,[4] was recognized with the Presidential Green Chemistry Award. More recently, the development of a nine-enzyme, largely biocatalytic route into the anti-HIV drug, ilsatravir, in which five of these enzymes were re-engineered by directed evolution[5] stands out as a beacon for the future when "biocatalytic retrosynthesis"[6] is paired with traditional retrosynthesis in designing new processes for value-added products.

[1] Arnold, FH. "Directed Evolution: Bringing New Chemistry to Life" Angew. Chem. Int. Ed. 2018, 57, 4143 – 4148; DOI: 10.1002/anie.201708408

[2] Li, Wensheng; Xie, Dongming; Frost, John W. "Benzene-Free Synthesis of Catechol: Interfacing Microbial and Chemical Catalysis" J. Am. Chem. Soc. 2005, 127, 2874-2882; DOI: 10.1021/ja045148n

[3] Dietrich, J, Yoshikuni, Yasuo; Fisher, Karl J.; Woolard, Frank X.; Ockey, Denise; McPhee, Derek J.; Renninger, Neil S.; Chang, Michelle C. Y.; Baker, David; Keasling, Jay S. "A Novel Semi-biosynthetic Route for Artemisinin Production Using Engineered Substrate-Promiscuous P450BM3" ACS Chem. Biol. 2009, 4, 261–267; DOI: 10.1021/cb900006h

[4] Savile, Christopher K.; Janey, Jacob M.; Mundorff, Emily C.; Moore, Jeffrey C.; Tam, Sarena; Jarvis, William R.; Colbeck, Jeffrey C.; Krebber, Anke; Fleitz, Fred J.; Brands, Jos; Devine, Paul N.; Huisman, Gjalt W.; Hughes, Gregory J. "Biocatalytic Asymmetric Synthesis of Chiral Amines from Ketones Applied to Sitagliptin Manufacture" Science 2010, 329, 305-309; DOI: 10.1126/science.1188934

[5] Huffman, Mark A.; Fryszkowska, Anna; Alvizo, Oscar; Borra-Garske, Margie; Campos, Kevin R.; Canada, Keith A.; Devine, Paul N.; Duan, Da; Forstater, Jacob H.; Grosser, Shane T.; Halsey, Holst M.; Hughes, Gregory J.; Jo, Junyong; Joyce, Leo A.; Kolev; Joshua N.; Liang, Jack; Maloney, Kevin, M.; Mann, Benjamin F.; Marshall, Nicholas M.; McLaughlin, Mark; Moore, Jeffrey C.; Murphy, Grant S.; Nawrat, Christopher C.; Nazor; Jovana; Novick, Scott; Patel, Niki R.; Rodriguez-Granillo, Agustina; Robaire, Sandra A.; Sherer, Edward C.; Truppo, Matthew D.; Whittaker, Aaron M.; Verma, D.; Xiao, L.; Xu, Yingju; Yang, Hao "Design of an in Vitro Biocatalytic Cascade for the Manufacture of Islatravir" Science 2019, 368, 1255-1259; DOI: 10.1126/science.abs1954

[6] Turner, Nicholas, O'Reilly, Elaine "Biocatalytic retrosynthesis." Nat. Chem. Biol. 2013, 9, 285–288; DOI: doi.org/10.1038/nchembio.1235

Small- and medium-sized enterprises play a pivotal role in the chemistry supply chain and experience unique challenges in adapting to change. Efforts to facilitate their participation via ability to comply with new certifications and adopt new technologies will be a rapid facilitator of the transition and expanded demand for a distributed, trained workforce. This is complemented by enabling innovative solutions from subject matter experts to take hold in the marketplace with support for the necessary R&D.

Alternatives

There is a critical opportunity to leverage sustainable chemistry solutions for the continued use of hazardous substances that impact human health and the environment. National priorities for sustainable chemistry solutions—PFAS, surfactants, solvents, preservatives, other chemicals on state, federal, and global agendas for elimination—address issues faced by industry when faced with phase-outs.

Development of alternative elements (e.g., non-critical and non-rare elements), alternative chemicals (e.g., new platform molecules), and alternative chemistry processes (e.g., bio-based or natural chemicals and chemical inputs, biomass processing methods, carbon capture and renewable energy for chemical production) are key to fundamentally shift from toxic to sustainable chemistry. For alternative chemicals, ideally net-zero alternatives that minimize natural resource demand, and environmental and health threats in manufacture and use need to be developed. For alternative processes, manufacturing that is distributable, flexible in scale, uses lower pressure and heat or alternative energy sources, and generates less waste and emissions should be supported. Another alternative that requires research support is identifying natural chemicals produced by terrestrial and marine microbes that may substitute for petrochemical-derived raw materials and ingredients. This includes needing an understanding of platform bio-based chemicals or processes with the ability to go from plant waste to a series of useful chemicals, ranging from bulk/commodity chemicals to specialty chemicals.

Circularity

Research to support circularity, including a focus on chemical disposal, recyclability, reusability, degradability and biodegradability, recapture, remanufacture, and recovery, as well as fundamental design for facilitated entry into all of those pathways after use. Ensuring a firm understanding of environmental impacts and human health effects of chemicals and materials remains essential to more circular economic advances that are consistent with the broader goals of sustainable chemistry.

Novel Methods

An important consideration in advancing the field of sustainable chemistry are new hazard assessment methods under development for regulatory use. New hazard assessment methods can include new approach methodologies such as *in chemico*, *in vitro*, and *in silico* methods that can supplement or potentially replace existing *in vivo* mammalian tests. Computational chemistry, including the use of AI/ML, high-throughput screening, and computational or predictive toxicology are additional areas of opportunity. In addition to the benefits these methods offer in reducing the time and costs associated with *in vivo* testing, many of the new hazard assessment methods allow for rapid hazard screening of theoretical or planned chemical substances. These methods can be an invaluable aid in the design of safer alternative chemicals, while accelerating R&D to market timelines. Another advantage of these methods is the potential to assess biological variability: variability in the toxicological response to a chemical among the human population and within susceptible subpopulations.

XIII. Summary and Next Steps

This report summarizes the current sustainable chemistry landscape and identifies data gaps and research needs critical to progressing sustainable chemistry R&D. It provides information for the development of a Federal strategic plan, in which coordination and collaboration across agencies will greatly expedite progress. Additionally, there is a need for coordination between the Federal government and state, local, Tribal, and territorial entities, as well as outreach activities that engage or inform the public. Coordination with international partners is also critical for economic and national security. The strategic areas identified above provide a roadmap for sustainable chemistry activities that, when addressed, will generate actionable information to guide Federal agencies and sustainable chemistry collaborators and partners.

The Administration has accelerated efforts to advance sustainable chemistry practices. The capabilities and approaches developed in response to this report should lead to a holistic treatment of sustainable chemistry. Over the next year, the Sustainable Chemistry ST will operationalize a strategic plan and implementation framework that organizes and coordinates activities in these strategic areas by harnessing existing research and accelerating transformative advancements. The Sustainable Chemistry ST will be developed through and informed by engagement of stakeholders, collaborators, and partners that ranges from researchers and citizen scientists to public health experts, industries, governments (Federal, state, local, Tribal, and territorial), non-governmental organizations, and civil society. The information generated will inform sustainable chemistry standards and metrics, decarbonization, circularity, the use of novel methods for assessing sustainable chemistry, and fuel other innovative public health actions and help our nation realize its vision of clean drinking water, clean air, and safe food for all.

Appendix A – Federal Sustainable Chemistry Activities

This is a snapshot of the activities ongoing in the Federal agencies as of October 2022. We note that activities in agencies are evolving rapidly in response to the call for more sustainable activities; therefore, this should be treated as a living inventory of activities. The ST will continue to gather this information in order to best leverage agency expertise to address the strategic areas identified in the report. The forthcoming strategic plan will align these existing activities with areas of focus to prioritize areas needed to supplement ongoing activities as well as synergize collaborations across agencies with complementary activities. The activities presented below provide a holistic overview of sustainable chemistry activities more broadly. Appendix B provides financial resources allocated to Federal R&D activities, which supplements the information provided here.

Department of Commerce

National Institute of Standards and Technology

Manufacturing Processes and Alternate Technologies

- Managing the Manufacturing USA Program to streamline the deployment of new innovation into the commercial sector.
- Property models and data for commercial chemical process modeling software
    - Data and modeling from 647 are used extensively in commercial chemical process design software (such as AspenTech)
- Fundamental polymer design and processing strategies for end-of-life solutions (experimental and computational)
- Engineering Biology Program—focuses on biometrology, technologies, and standards to promote engineering biology and related innovations and translation
    - Efforts in microbial systems aim to deliver measurements and workflows for prediction, control, and design
    - Efforts in mammalian systems focus on the development of robust engineering tools, cell lines, and measurements
- Methods to measure carbon uptake in cements and concrete
- Material marketplaces for industrial scrap
- Advancement of manufacturing science that will enable more agile manufacturing facilities that are able to pivot to new products more ably as more sustainable chemistry solutions are available

Thermodynamics and Kinetics

- Simulation Methods for determining the thermodynamics and phase behavior of bulk fluids and mixtures
- (Thermo)dynamics and Virial Coefficients of Confined Fluids
- Experimental measurement of thermodynamic and transport properties (density, vapor pressure, heat capacity, viscosity, thermal conductivity, etc.) of fluids and mixtures

Adsorption and Separations

- FACT Lab

  - Facility for Adsorbent Characterization and Testing (FACT): providing impartial testing and characterization of material sorption properties, establishing testing procedures, and disseminating reliable sorbent material property data and measurement best practices
- Alternative Separations (ALTSEP) Advisory Committee: “Sustainable Separation Processes- A Roadmap to Accelerate Industrial Application of Less Energy-Intensive Alternative Separations” (Report available).
- Co-Sponsor of National Academy of Science and Engineering and Medicine Report “A Research Agenda for Transforming Separation Science” (Report available).
- Polymer Membranes and Transport Media (for water purification and separations)
- Adsorption metrology for the direct capture of CO_2 from air.

Sustainable Manufacturing/Decision Tools

- Documentary standards engagement (ASTM International, ISO, etc.) to define metrics and methods for sustainable manufacturing and circular economy.
- Decision tool development:
  - BIRDS: Building Industry Reporting and Design for Sustainability
  - BEES: Building for Environmental and Economic Sustainability
- Gap analysis and intercomparison studies of decision tools (current focus on polymers)
- Membership in Federal LCA Commons

Assessments and Benchmarking (includes measurement support for environmental impact assessment)

- Assessments and Benchmarking, which includes measurement support for environmental impact assessment, reference material development, and measurements and metrology for plastics pollution; development, implementation, and validation of reliable data analysis tools, including AI and machine learning (ML) NIST also hosts several data resources that provide data relevant to various aspects of sustainable chemistry:
  - Development of robust cell-based toxicity methods
  - Reference material development and method development strategy for the determination of chemical residues in foods (currently pesticides)
  - Food Safety and Nutrition Quality Assurance Program regularly tackles environmental and packaging contamination of foods
  - Measurements and metrology for plastic pollution (bulk and particulate)

Data Resources

- NIST Chemistry Webbook**
  - Provides access to data compiled and distributed by NIST under the Reference Data Program
- NIST Mass Spectral Library
  - Develops evaluated mass spectral libraries and provides related software tools
  - Intended to assist compound identification by providing reference mass spectra for Gas Chromatography/Mass Spectrometry (by electron ionization) and Liquid Chromatography-Mass Spectrometry/Mass Spectrometry (by tandem mass spectrometry) as well as gas phase retention indices for Gas Chromatography

- Thermodynamics Research Center
    - Develops tools and standards for archival and dissemination of experimental thermodynamic data, especially critically evaluated data
    - Develops electronic database products
- NIST REFPROP
    - Provides high-accuracy data on selected industrial fluids and their mixture
- adsorbents.nist.gov: database of adsorption data collected from literature
- JARVIS
    - Tools/data repositories to automate materials discovery and optimization using classical force-field, density functional theory, machine learning calculations and experiments.
    - Includes data for a variety of materials (solar cells, infrared, piezoelectric, topological, thermoelectric, etc.)
    - JARVIS-ML includes a wide range of tools for searching databases and making predictions
- Interatomic Potentials Repository
    - Source for force fields, related files, and evaluation tools to help researchers obtain interatomic models and judge their quality and applicability
    - Materials: metals, semiconductors, oxides, and carbon-containing systems
    - Related variety of scripting tools for creating, representing, manipulating, and analyzing large-scale atomic systems of atoms

Department of Defense

- DoD funds research to develop products using more sustainable chemistry that also meet performance needs. DoD's SERDP funds basic and applied research and advanced technology development on contaminants of concern to DoD, and DoD's ESTCP funds validation and demonstrations of new, more sustainable chemistry technologies and products, among other activities.
- SERDP is jointly managed by DoD, EPA, and DOE and research funding priorities for both programs are identified by these agencies, experts, and by DoD's Emerging Contaminants program. SERDP and ESTCP fund federal organization and award contracts to universities and private industry.
- Special Targeted Initiatives/high-level core activities
    - After Camp Edwards was shut down in part because hazardous chemicals from flares were leaching into the community water supply, SERDP funded research to develop new flares without the chemicals of concern.
    - DoD has invested in research on new paint technologies that eliminate carcinogenic hexavalent chromium in paint primers and in research into methods for reducing or eliminating solvents.
    - ESTCP funded research at the Army Armament Research, Development and Engineering Center to validate the performance of nontoxic, biodegradable bio-based cleaner, lubricant, and preservative products as potential alternatives to petroleum-

  based products or other products containing chemicals that may cause eye, skin, and respiratory irritation.
  - SERDP and ESTCP have demonstrated and validated fluorine-free foams for suppression of liquid pool fires and developed a new military specification, MIL-PRF-32725, to enable acquisition of these products and allow the DoD to meet the 2020 NDAA requirement that prohibits use of aqueous film forming foams (AFFF) that contain perfluoro alkyl substances (PFAS) for shore-based fires as of 1 OCT 2024.
  - SERDP and ESTCP have developed methodologies to detect PFAS at the 1 ppb level and have developed a series of technologies, including filtration and incineration, to fully degrade PFAS from contaminated sites into components that do not pose significant environmental risk.
  - The Army's Safe Alternative For Readiness (SAFR) program funds research within the Army on development of low global warming potential refrigerants, sustainable coatings, toxic metal reduction for sustainable metal finishing, airborne lead reduction and other ordinance environmental efforts for sustainable munitions, and sustainable fluids and lubricants.
- The Sustainable Technology Evaluation and Demonstration Program evaluates, demonstrates, and transitions sustainable technologies and products at DoD and other Federal agency facilities.
- The Army's Safe Alternative For Readiness (SAFR) program funds demonstration and validation efforts on sustainable coatings, toxic metal reduction for sustainable metal finishing, and airborne lead reduction and other ordnance environmental efforts for sustainable munitions.
- The National Defense Center for Energy & Environment (NDCEE) funds demonstration, validation, and other RDT&E to transition sustainable chemistry to use in the DoD. The mission of the Navy's Environmental Sustainability Development to Integration (NESDI) program is to provide solutions by demonstrating, validating, and integrating innovative technologies, processes, materials, and by filling knowledge gaps to minimize operational environmental risks, constraints, and costs while ensuring Fleet readiness.
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Department of Energy

- The **Office of Advanced Scientific and Computing Research (ASCR)** in DOE's Office of Science supports research and capabilities to advance applied mathematics and computer science; deliver the most sophisticated computational scientific applications in partnership with disciplinary science; and to develop future generations of computing and networking hardware and software tools for science and engineering in partnership with the research community, including U.S. industry. ASCR supports state-of-the-art capabilities that enable scientific discovery through computation in strategic areas such as sustainable chemistry.
- The IIJA (aka BIL) included multiple provisions across technologies related to sustainability in manufacturing and recycling. For example (from HFTO) Provisions 815 and 816 address clean hydrogen manufacturing and recycling as well as clean hydrogen electrolysis with an open FOA covering materials, component, and system level R&D relevant to sustainable chemistry

(including non-PFAS polymers, low PGM and PGM-free catalysts, etc.). On the deployment side, Provision 813 will provide substantial funding for the clean H2 hubs- expected to include sustainable chemical end-uses.

- The **Mathematical, Computational, and Computer Sciences Research** program in ASCR supports research activities for both data intensive and computationally intensive science. Computational and data intensive sciences coupled with Artificial Intelligence and Machine Learning (AI/ML) are central to progress at the frontiers of science and to our most challenging engineering problems, including in sustainable chemistry. The ASCR Computer Science and Applied Mathematics activities provide the foundation for increasing the capability of the national high-performance computing (HPC) ecosystem and scientific data infrastructure by focusing on long-term research to develop intelligent software, algorithms, and methods that anticipate future hardware challenges and opportunities as well as domain needs. This program also supports the Computational Partnerships activity which includes the Scientific Discovery through Advanced Computing (SciDAC) program. SciDAC partnerships portfolio includes interdisciplinary teams of chemists, materials scientists, applied mathematicians and computer scientists that focus on the effective use of HPC resources and expertise to tackle critical challenges in chemistry and materials. The Computational Partnerships activity includes collaborations in the areas of data analysis that enable large, distributed research teams to share data and develop tools incorporating AI/ML for real-time analysis of the massive data flows from the scientific user facilities, as well as R&D of software to support a distributed advanced computing data infrastructure and computing environment.
- The **High-Performance Computing (HPC) and Network Facilities** subprogram supports the operations of forefront computational and networking user facilities. ASCR operates three HPC user facilities: the National Energy Research Scientific Computing Center at Lawrence Berkeley National Laboratory (LBNL), which provides HPC resources and large-scale storage to a broad range of researchers; and the two Leadership Computing Facilities at Oak Ridge National Laboratory and Argonne National Laboratory, which provide leading edge HPC capability to the U.S. research and industrial communities. ASCR’s high performance network user facility, ESnet, delivers highly reliable data transport capabilities optimized for the requirements of large-scale science. ASCR HPC facilities participated in COVID-19 HPC Consortium, a partnership between industry, national and international federal agencies, national laboratories, and academia and deployed customized computing hardware to better address COVID-19 research needs such as high throughput drug candidate screening and advanced data analytics. These additional HPC resources are available for peer-reviewed, competitive research with emphasis on biological, chemical and medical research including research in sustainable chemistry.
- The **Exascale Computing Initiative** develops and deploys an exascale-capable computing system with an emphasis on sustained performance for a wide-range of applications including those for sustainable chemistry. The Exascale Computing Project develops a suite of applications and software technologies that might be leveraged by efforts making use of computing at all scales.

The following DOE ASCR/BES solicitation has recently supported sustainable chemistry research:

SciDAC Partnerships in Basic Energy Sciences Funding Opportunity Announcement (FOA), an FY 2021 solicitation focused on interdisciplinary teams to establish partnerships between domain scientists – in the fields of materials science, condensed matter physics, chemical sciences, geosciences, and energy-related biosciences – and applied mathematicians and/or computer scientists to overcome barriers between these disciplines. Specifically two topical areas of interest were targeted: Quantum phenomena of many-particle systems driven far from equilibrium such as coherence, entanglement, and novel states of matter by going beyond the use of existing quantum based methods in their traditional regimes and predictive control of reaction pathways for chemical mechanisms in complex nonequilibrium and field-driven environments important in synthesis of materials and chemicals, and deconstruction of macromolecular structures such as plastics for polymer upcycling. Several awards focused on sustainable chemistry related topics, including data-driven design and control of chemical and material systems, modeling chemical reactivity in complex systems such as catalysts for chemical up-cycling of polymers.

- The **Office of Basic Energy Sciences (BES),** in DOE's Office of Science, supports fundamental research to understand, predict, and ultimately control matter and energy at the electronic, atomic, and molecular levels. BES research provides the foundations to develop new energy technologies, to mitigate climate and environmental impacts of energy generation/use, and to support DOE missions in energy, environment, and national security. BES accomplishes its mission through scientific discovery in the energy sciences and through stewardship of world-class scientific user facilities that enable cutting-edge R&D. Several core programs in the BES portfolio in **Materials Sciences and Engineering** and **Chemical Sciences, Geosciences, and Biosciences** support sustainable chemistry -related research. These programs span chemical transformations, fundamental interactions, photochemistry, biochemistry, geochemistry, and materials discovery, design, and synthesis. Research at BES-supported user facilities, such as the Nanoscale Science Research Centers, addresses large scale, complex R&D challenges relevant to sustainable chemistry.

DOE BES center efforts associated with the sustainable chemistry space include the **Energy Frontier Research Centers (EFRCs)** and the **Energy Innovation Hubs.** The EFRCs support multi-disciplinary scientific teams to tackle scientific challenges preventing advances in energy technologies. These centers take advantage of powerful new tools for characterizing, understanding, modeling, and manipulating matter from atomic to macroscopic length scales. They also train the next-generation scientific workforce by attracting talented students and postdoctoral researchers interested in energy science. EFRCs specifically related to sustainable chemistry address challenges in the upcycling and redesign of polymers, battery design, light driven catalysis, new catalyst design strategies, carbon-neutral hydrogen production and utilization, and the energy-water nexus. The Energy Innovation Hubs focus on collaborative fundamental research to overcome key scientific barriers for major energy challenges. The Hubs funded and managed by BES bring together teams of experts from multiple disciplines to address two grand challenges in energy: (1) Fuels from Sunlight and (2) Batteries and Energy Storage. The Fuels from Sunlight Hub awards aim to understand, design, and develop chemical processes and new materials for directly converting sunlight into storable fuels using only water and carbon dioxide.

The following cross-divisional DOE BES solicitations have recently supported sustainable chemistry research:

Chemical and Materials Sciences to Advance Clean Energy Technologies and Low-Carbon Manufacturing Funding Opportunity Announcement (FOA), an FY 2022 solicitation focused on single PI to small team efforts to advance basic and fundamental chemical and materials sciences that underpin clean energy technologies and low-carbon manufacturing and create foundational knowledge to support the development of approaches that will minimize climate impacts of energy technologies and manufacturing. Multiple awards involve the sustainable chemistry space, including strategies to selectively oxidize polymers in mixed feeds, study of catalytic clean hydrogen generation and storage in thermal and electrocatalytic systems, and development of earth abundant catalysts for water electrolysis.

Chemical Upcycling of Polymers FOA, an FY 2021 solicitation focused on single investigators and teams to support fundamental experimental and theoretical efforts that advance chemical upcycling of polymers and circular design of next-generation plastics. Several awards focused on sustainable chemistry related topics, including design of next generation plastics, base metal mediated deconstruction and up conversion of polymers to value added molecules and materials, and the selective deconstruction of specific plastic classes in mixed feedstock streams.

Critical Mineral & Materials: Chemical and Materials Sciences Research on Rare Earth and Platinum Group Elements FOA, an FY 2021 solicitation focused on single investigator and multi-disciplinary teams to support experimental and theoretical research to advance chemical and materials sciences relevant to critical elements and critical materials that provide essential functionality in key technologies and have no easy substitutes. This FOA sought an understanding of the fundamental properties and mechanisms of critical minerals, elements, and materials to improve separation and extraction processes and to enable discovery and design of alternates that reduce or eliminate the need for critical elements, thus diversifying the supply, development of substitutes, and improving reuse and recycling of critical minerals and materials. One sustainable chemistry-relevant project focuses on new synthetic strategies to confine nanoparticle catalysts to improve durability and decrease reliance on high platinum group loadings.

Data Science to Advance Chemical and Materials Sciences FOA, an FY 2021 solicitation focused on expanding the integration of data science/AI/ML methods with BES research disciplines, to accelerate scientific discovery and overcome difficult challenges in these fields. The FOA supported teams of investigators for synergistic computational, experimental, and theoretical research emphasizing science-based, data-driven approaches for fundamental basic energy sciences challenges and integrating novel data science, uncertainty quantification, and other AI and ML approaches with domain sciences to uniquely advance the understanding of fundamental properties and processes relevant to chemical and materials systems, and achieve predictability of functions and behavior under dynamic conditions. An award related to sustainable chemistry involved acceleration of enzyme engineering for base metal catalysis development.

- The **Office of Biological and Environmental Research (BER)** in DOE's Office of Science supports fundamental research to integrate observations, experimental capabilities, and computational resources to advance predictive systems-level understanding from microbes and plants to ecosystems and the earth system for energy and infrastructure security. The BER **Biological Systems Science Division (BSSD)** integrates across disciplines for discovery- and hypothesis-driven genome-enabled science to understand, predict, manipulate, and design plants and microbial systems that can contribute to sustainable chemistry efforts. BER-supported researchers in the **Genomic Sciences Program** are using experimental and computational tools with plant and microbial systems to pursue innovative early-stage research that could lead to development of future transformative bio-based products, clean energy opportunities, and next-generation technologies for the burgeoning bioeconomy. BSSD's diverse portfolio is helping to illuminate the functional principles that drive living systems at different scales, enabling rapid advances in biotechnology and bioengineering. Biological processes within the BSSD portfolio hold the potential to underpin opportunities in sustainable chemistry. BSSD specific research on sustainable chemistry pertains to the upcycling of polymers and plastics.
- The DOE **Advanced Materials and Manufacturing Technologies Office (AMMTO)** within DOE EERE researches, develops, and demonstrates next-generation materials and manufacturing technologies needed to increase U.S. industrial competitiveness and to drive economy-wide decarbonization. AMMTO also sponsors a series of RD&D consortia. These consortia help coordinate applied RD&D across the public and private sector around high-priority technology areas that support AMMTO's vision & mission. Specific efforts in the sustainable chemistry space include the REMADE Institute, which seeks to bring together innovators across academics, industry, and the national lab complex to enhance the nation's industrial competitiveness and champion the transition to a circular economy within the United States.
- The DOE **Industrial Efficiency and Decarbonization Office (IEDO)** within DOE EERE supports innovation in technologies and the adoption of practices to enable the industrial sector to cost-effectively reduce greenhouse gas emissions. IEDO funds cooperative RD&D and technical assistance across several research areas to drive economy-wide decarbonization. Decarbonization of chemicals production is a high priority for IEDO since the chemicals sector is the highest CO_2-emitting industrial subsector. Recent investments have included a FOA topic on Sustainable Chemistry Practices—which focused on advancing platform molecules, materials and processes that can contribute to the principles of sustainable chemistry and foster decarbonization of the chemicals industry—and a topic on decarbonizing high volume energy intensive chemicals through next generation unit operations like advanced separations and advanced reactors, and process heating technologies.
- IEDO also supports the Rapid Advancement in Process Intensification Deployment Manufacturing USA Institute, established in 2017 to support development for modular manufacturing using process intensification principles. The institute convenes companies, universities, industrial research organizations, and National Laboratories to focus on new technologies that maximize processes at the molecular level to save energy with every chemical reaction.

- In November 2020, the Advanced Manufacturing Office, the precursor office to IEDO, co-hosted a virtual roundtable on Sustainable Chemistry in Manufacturing Processes with the Green Chemistry & Commerce Council, to collect industry stakeholders' perspectives on incorporating sustainable chemistry practices into the manufacturing of consumer and commercial products. In March 2023, IEDO held a second roundtable titled Sustainable Chemistry in RD&D to Transform the Chemicals Industry with the Green Chemistry & Commerce Council. The roundtable focused identifying impactful sustainable chemistry RD&D to achieve chemical sector decarbonization and environmental justice.
- Within DOE EERE, the **Bioenergy Technologies Office (BETO)** supports research, development, and demonstration to enable the sustainable use of domestic biomass and waste resources for the production of biofuels and bioproducts. BETO funds work in collaboration with industry, academia, and DOE national laboratories to develop advanced technologies and innovative solutions to reduce the costs of biofuels, from harvesting and preprocessing to conversion of biomass and waste. Projects aims to efficiently convert organic materials and biomass into affordable biofuels and bioproducts which will help decarbonize the transportation sector while mitigating greenhouse gas emissions. Specific efforts in the sustainable chemistry space include the Bio-Optimized Technologies to keep Thermoplastics out of Landfills and the Environment (BOTTLE™) consortium. This activity conducts high-impact R & D to re-imagine recycling, which includes improving catalytic and biocatalytic recycling strategies to break down today's plastics into chemical building blocks for manufacturing higher-value products (upcycling) while also focusing on the design of tomorrow's plastics to be recyclable-by-design (circular). The BETO 'ChemCatBio' Consortium for advanced catalytic conversion of biomass feedstocks into sustainable fuels and products.
- The DOE **Hydrogen and Fuel Cell Technologies Office (HFTO)** focuses on research, development, and demonstration of hydrogen and fuel cell technologies across multiple sectors enabling innovation, a strong domestic economy, and a clean, equitable energy future. Efforts supported by HFTO include fuel cell RD&D, hydrogen production RD&D, hydrogen storage and delivery infrastructure RD&D, systems development and integration RD&D, and associated analysis. It also funds lab-led consortia to coordinate national laboratory RD&D activities and serve as a resource for universities and industry. HFTO also conducts outreach activities to increase awareness and understanding of the technologies, technology acceleration activities to provide financial and technical assistance for use of hydrogen and fuel cell systems in early market applications, and safety, codes, and standards efforts to develop information resources and best practices.
- The **Advanced Research Projects Agency-Energy (ARPA-E)** advances high-potential, high-impact energy technologies that are too early for private-sector investment. ARPA-E awards target development of entirely new ways to generate, store, and use energy. Research funded by ARPA-E supports advances relevant to sustainable chemistry.
- **Cross-agency Activities:** The **Energy Earthshots Initiative**, coordinated through the Office of Science and Innovation, targets the complete spectrum of RD&D, with specific targets to slash GHG emissions and provide the pathway for national decarbonization by 2050. The current

portfolio consists of six individual Energy Earthshots™, with broad focus areas including hydrogen, long duration energy storage, and carbon negative technologies. These and the other Shots provide a metric driven roadmap to integrate sustainable chemistry and circular process design concepts across basic science, applied, and deployment programs within DOE.

- GreenBuy Award program recognizes DOE sites for excellence in "green purchasing" that extend beyond minimum compliance requirements. Sites receive recognition for purchasing programs that obtain sustainable products and services, save energy, conserve water, and reduce negative health and environmental impact.

Department of the Interior

- The U.S. Department of the Interior (DOI) is committed to enhancing sustainable uses of chemicals in its daily operations across its bureaus and offices, and to foster innovative practices that promote sustainability. For example, DOI is committed whenever feasible to replacing toxic chemicals used in its operations with less toxic chemicals. Sustainable practices are similarly of high priority in the DOI bureaus and offices with laboratory facilities that make use of chemicals and/or that provide chemical analyses.

United States Geological Survey

- The U.S. Geological Survey (USGS) has the majority of laboratory facilities within DOI that make use of chemical reagents and generate chemical wastes. USGS is committed to reducing its contaminant footprint on the hazardous waste side by replacing toxic reagents with less-toxic alternatives. For example, the USGS National Water Quality Laboratory (NWQL) is the primary USGS fee-for-service lab that analyzes tens of thousands of environmental samples annually for a wide range of chemicals. NWQL has adapted methods to incorporate less-toxic reagents in its analyses, such as replacing cadmium with nitrate reductase in the high-use nitrate + nitrite nutrient analytical method. NWQL and other USGS labs are also leaders in the development of analytical chemistry methods for environmental samples that miniaturize the volumes of sample required for analysis and that thereby greatly reduce the volumes of reagents needed for the analyses.
- The USGS conducts research on the potential for contaminant exposures in the environment that might originate throughout the life cycle of energy and mineral resource extraction, use, recycling/reuse, and disposal. This life cycle approach includes research focusing on the transportation, storage, extraction, waste management, releases, and restoration of chemicals and materials used in energy and mineral extraction and use. For example, laboratory and field studies work to understand the benefits and potential risks associated with beneficial reuse of unconventional oil and gas-associated materials such as produced waters. Research on the extraction of critical minerals and other mineral commodities is exploring the use of engineered materials to sorb metal contaminants at point of release. The USGS is also doing research to inform restoration plans prior to resource extraction activities.
- USGS plays a leadership role in the assessment of the global geologic occurrences of, supplies of, supply chains for, and demands for the critical minerals and other mineral commodities that are essential for the nation's sustainable energy production and used in sustainable chemical manufacturing.

Environmental Protection Agency

- Toxics Release Inventory (TRI): A resource for learning about toxic chemical releases and pollution prevention activities reported by industrial and federal facilities. U.S. industry facilities must report annually how much of each chemical is released to the environment and/or managed through recycling, energy recovery and treatment. TRI data support informed decision-making by communities, government agencies, companies, and others. Section 313 of the Emergency Planning and Community Right-to-Know Act created the TRIChemical Safety for Sustainability (CSS) research program: The Chemical Safety for Sustainability research program provides the decision-support tools needed safely produce, use, and dispose of chemicals, while advancing ways to evaluate chemicals, conduct risk management, and prioritize time-critical research.
- The Chemical Safety for Sustainability national research program in EPA's Office of R&D is focused on addressing the pressing environmental and health challenge of a lack of sufficient information on chemicals needed to make informed risk-based decisions. Included in the program is research focused on informing life cycle risk assessments for new and existing chemicals, and providing support for alternatives assessments, through the development of tools and models, and through the generation of data.
- **Chemical Property Information, Estimation, and Prediction Tools:** Assessment methods, databases, and predictive tools to help evaluate what happens to chemicals when they are used and released to the environment and how workers, citizens, and the environment might be exposed to and affected by them. (https://www.epa.gov/tsca-screening-tools)
  - https://comptox.epa.gov/dashboard/
    - The CompTox Chemicals Dashboard provides chemistry, toxicity and exposure information for over 900,000 chemicals, with over 300 individual chemical lists. The available data includes bioactivity data from the ToxCast and Tox21 projects, exposure data associated with the ExpoCast program and toxicity data.
  - https://www.epa.gov/chemical-research/toxicity-estimation-software-tool-test
    - The Toxicity Estimation Software Tool (TEST) allows users to estimate the toxicity of chemicals using Quantitative Structure Activity Relationships (QSARs) methodologies.
- **Safer Choice:** Safer Choice helps consumers, businesses, and purchasers find products that perform and contain ingredients that are safer for human health and the environment. Safer Choice is an EPA Pollution Prevention (P2) program, which includes practices that reduce, eliminate, or prevent pollution at its source, such as using safer ingredients in products.
- **Environmentally Preferable Purchasing Program:** The Environmentally Preferable Purchasing Program has developed Recommendations of Specifications, Standards, and Ecolabels for Federal Purchasing, including chemical purchasing categories such as custodial cleaners, hand soaps, commercial dishwasher detergents, and deicers.
- P3 – People Prosperity Planet: The P3 is a competition that is open to teams of college/university students working to design solutions for a sustainable future. This annual, two-phased research grants program challenges students to research, develop, and design

innovative projects that address real world challenges involving all areas of environmental protection and public health.

- **EPA Regional Engagements and Pollution Prevention P2 grants**
- The Pollution Prevention grant program currently makes grant awards for projects that align with the five P2 National Emphasis Areas. Specifically, the Chemical Manufacturing, Processing, and Formulation National Emphasis Area can support – among other things – projects that promote research, development, and marketing of green chemistry products and processes that reduce or eliminate the generation of hazardous substances. P2 grants include:
    - EPA Region 1 supports the Vermont Department of Environmental Conservation PFAS Pollution Prevention Project to reduce PFAS use and identify safer alternatives in the metal finishing and aerospace industries.
    - EPA Region 2 supports Rowan University, who is partnering with ExxonMobil Corporation to investigate lubricant formulation blending operations at the ExxonMobil facility in Paulsboro, New Jersey to reduce the amount of downgraded oil produced from cleaning and blending operations.
    - EPA Region 9 supports the University of California, Berkeley as they research safer chemical alternatives to (PFAS) in the carpet and food packaging industry sectors.
    - EPA Region 10 supports the Washington State Department of Ecology Green Chemistry program.
    - EPA Region 10 supports the Oregon Department of Environmental Quality as they offer the Pacific Northwest OSHA Education Center's Transitioning to Safer Chemicals Course, alternatives assessment training to support implementation of the Toxics Free Kids Act, and training for government purchasing officials and commercial product vendors on the use of EPA Safer Choice.
- Through their Healthy, Resilient, and Sustainable Communities grant program, EPA Region 10 is supporting the Pollution Prevention Resource Center as they build a technical assistance program to guide chemical manufacturers through the Safer Choice certification process.
- **Green Chemistry Challenge Awards.** The Green Chemistry Challenge Awards promote the environmental and economic benefits of developing and using novel green chemistry. These prestigious annual awards recognize chemical technologies that incorporate the principles of green chemistry into chemical design, manufacture, and use. The 2022 Green Chemistry Challenge Awards categories are:
    - Focus Area 1: Greener Synthetic Pathways
    - Focus Area 2: Greener Reaction Conditions
    - Focus Area 3: The Design of Greener Chemicals
    - Small Business (for a technology in any of the three focus areas developed by a small business)
    - Academic (for a technology in any of the three focus areas developed by an academic researcher)
    - Specific Environmental Benefit: Climate Change (for a technology in any of the three focus areas that reduces greenhouse gas emissions)

- The California Environmental Protection Agency, the Oregon Department of Environmental Quality, and the Washington State Department of Ecology have entered into an MOU called the West Coast Green Chemistry and Safer Products Memorandum of Understanding.

Health and Human Services

Food and Drug Administration

- The FDA does not have specific authorities related to sustainable chemistry. However, the agency is engaged in activities that are framed in the broad concept of sustainable chemistry. Examples of these activities include:
    - Implementation of laboratory procedures that enable the reduction of the use of chemicals
    - Fostering the use of laboratory procedures that are less reliant on toxic chemicals
    - Implementation of recycling programs for specific laboratory chemical waste streams
    - Fostering the development and approval of veterinary drugs, especially for food-producing animals, that are expected to reduce impact in the environment
    - Supports the use of recycled plastics for food contact articles through safety review of recycling processes
    - Fostering the development and approval of drugs manufactured with innovative technologies, such as continuous manufacturing, distributed manufacturing and point-of-care manufacturing, that are expected to reduce the use and/or generation of hazard chemicals, reduce energy needed for manufacturing, storage and distribution and ensure agile and robust supply chains.
    - Continued rigorous assessments for the appropriate dosing of drugs including antibiotics to treat and prevent disease can lead to the use of lower drug doses or shorter drug regimens, reducing their environmental burden.

National Institute of Environmental Health Sciences

- NIEHS undertakes and funds basic and applied research to understand the links between chemical exposures and disease.
- NIEHS has been involved in a number of efforts to translate the knowledge derived from toxicological studies to design for safer chemistries.
- The National Toxicology Program includes a specific focus on Safe & Sustainable Alternatives, a program focused on the human health side of the R&D activities aimed at identifying potential alternatives to chemicals listed as carcinogenic or toxic to reproduction.

National Science Foundation

Foundation-wide the most influential cross-divisional support for sustainable chemistry research is housed under a metaprogram:

- The Foundation-wide **Critical Aspects of Sustainability (CAS**) metaprogram supports basic research through core disciplinary programs aimed at improving the sustainability of resources for future generations while maintaining or improving current products in order to offer technologically-advanced, economically competitive, environmentally-benign and useful materials to a global society.

- More specifically, the CAS Dear Colleague Letters encourage the science and engineering communities to develop forward-thinking research in this topic area.
- **CAS: Innovative Solutions to Climate Change** is a call to action that encourages the submission of certain types of proposals to appropriate existing NSF core programs to lay the foundation for disciplinary and interdisciplinary research and to answer fundamental questions related to novel approaches and solutions to climate change. Project descriptions should clearly articulate climate relevance and contribute to new approaches regarding innovative solutions that address climate change mitigation and adaptation.
- **CAS: Innovative Solutions to Sustainable Chemistry** is a call to seek research ideas to improve the efficiency with which resources are used to meet human needs for chemical products and materials while reducing use of hazardous substances and the generation of waste. This effort to minimize, reduce, and recycle includes the design of sustainable chemicals as well as sustainable materials, engineering process optimization, resource management (e.g., elimination or reduction of scarce and depletable resources such as rare earth elements, developing responsible, bio-based alternatives), and environmental remediation.

Mathematical and Physical Sciences Directorate

- In the **Division of Chemistry** most core programs support sustainable chemistry -related research, particularly:
    - The Environmental Chemical Sciences program supports experimental and computational research on the fundamental chemistry of processes in the environment including approaches to discover, explain, and predict environmental phenomena at the molecular scale.
    - The Chemical Catalysis program supports experimental and computational research directed towards the fundamental understanding of the chemistry of catalytic processes, including polymerization catalysis, single site catalysis, organocatalysis, inorganic, organometallic, and photoredox catalysis, electrocatalysis, and biologically-inspired catalysis. Fundamental studies of energy-related catalytic processes (such as in water splitting and fuel cells) and photocatalysis (such as in solar energy conversion) are also included.
    - The Chemical Structure, Dynamics, and Mechanisms (CSDM) program supports research projects that have strong implications for advancing the foundational knowledge of chemical systems. The Program supports research on the nature of chemical structure, chemical structure property studies, chemical dynamics, and chemical mechanisms. The CSDM Program is divided into two sub-programs, CSDM-A, focusing on frontline problems in experimental physical chemistry and applied computational physical chemistry, and CSDM-B, the venue for physical organic and physical inorganic chemistry.
    - The Macromolecular, Supramolecular, and Nanochemistry Program focuses on basic research that addresses fundamental questions and advances knowledge regarding the chemistry of macromolecular, supramolecular, and nanoscopic structures. Topics

  of interest include transformative approaches to efficient and inexpensive synthesis of polymers or nanostructures using renewable feedstocks or earth abundant elements; and innovative research that enhances the understanding of efficient use and recycling of polymers and critical elements or the conversion of energy from renewable sources, and more.

- The **Centers for Chemical Innovation** (**CCI**) program supports research centers focused on major, long-term fundamental chemical research that collaboratively address grand challenges in the field. Among the larger Phase II CCIs, the Center for Aerosol Impacts on Chemistry of the Environment, Center for Sustainable Polymers, Center for Sustainable Nanotechnology, Center for Synthetic Organic Electrochemistry, Center for Genetically Encoded Materials, Center for the Chemistry of Molecularly Optimized Networks and Center for Selective C–H Functionalization, in particular, have themes related to sustainable chemistry.
- The **Division of Materials Research** similarly supports sustainable chemistry-related research through all its core programs as well as the programs supporting research teams and center-scale research. All core programs are part of the CAS metaprogram. For example:
  - The Polymer program supports research on biosourced and environmentally benign polymeric materials and on preventing plastics waste, including from micro-and nanoplastics.
  - The Solid State and Materials Chemistry and the Ceramics programs support research developing materials containing earth-abundant elements, for example for next generation batteries and solid-state lighting. Another focus of these programs is on preparing materials in a more sustainable fashion, for example at lower temperatures than what traditional syntheses and processes use.
  - The Metals and Metallic Nanostructures program supports projects that impact or take into consideration sourcing, cost and availability of metals and plays a role when it comes to lightweighting and recycling.
  - Other solicitations that call out sustainable materials and green sustainable energy include:
    - Designing Materials to Revolutionize and Engineer our Future, which is an inter-directorate program in which the Mathematical and Physical Sciences Directorate, the Directorate for Engineering, and the Computer and Information Science and Engineering Directorate, https://www.nsf.gov/pubs/2021/nsf21522/nsf21522.htm
    - Materials Research Science and Engineering Centers, https://www.nsf.gov/publications/pub_summ.jsp?WT.z_pims_id=5295&ods_key=nsf21625
    - And the Materials Innovation Platforms competition 2020, https://www.nsf.gov/pubs/2019/nsf19526/nsf19526.pdf
- **National High Magnetic Field Laboratory:** The National High Magnetic Field Laboratory uses high magnetic fields to better understand existing energy sources and to explore new ones, and support environmental studies, especially in petroliomics.

Directorate for Engineering

- **Chemical, Bioengineering, Environmental, and Transport Systems** Programs that support sustainable chemistry-related research include:
    - The Catalysis program supports research on catalytic materials and reactions that use synthetic, theoretical and experimental approaches. The program goal is to increase fundamental understanding in catalytic engineering science and to advance the development of catalytic materials and reactions that are beneficial to society.
    - The Electrochemical Systems program supports electrochemical or photochemical engineering research for the sustainable production of electricity, fuels, chemical and other specialty and commodity products.
    - The Interfacial Engineering program supports fundamental research with the potential to advance industrial chemical or biochemical processes, focusing on atomic- and molecular- scale interfacial phenomena or on engineering interfacial properties, processes and materials. Fundamental understanding of the thermodynamic, kinetic, and transport properties of interfacial systems underpins improvements in chemical process efficiency and resource utilization.
    - The Process Systems, Reaction Engineering, and Molecular Thermodynamics program supports fundamental engineering research on the rates and mechanisms of chemical reactions, systems engineering, and molecular thermodynamics as they relate to the design and optimization of chemical reactors and the production of specialized materials that have important impacts on society.
    - The Nanoscale Interactions program supports fundamental research on the interactions of nanomaterials and nanosystems with biological and environmental components in various media.
    - The Environmental Sustainability program supports engineering research that balances ecological protection and stable economic conditions through five general research areas: industrial ecology, green engineering, ecological engineering, Earth systems engineering, and circular bioeconomy engineering.
    - The Environmental Engineering program supports fundamental research focused on reducing pollution and its environmental impacts through closing resource loops; smart amendments; environmental manipulation; or remediation with engineered processes.
- **Directorate for Biological Sciences** the **Division of Molecular and Cellular Biosciences** includes the **Systems and Synthetic Biology** and **Molecular Biophysics** programs that support biological routes to understand and design enzymes, organisms and communities of organisms that can contribute to biological/biochemical routes to a circular/sustainable bioeconomy.

The **Directorate of Geosciences** has core programs across their four Divisions/Offices that support sustainable chemistry -related research.

- Division of Earth Sciences core program of **Geobiology and Low-Temperature Geochemistry** supports the intersection of earth materials and human health with a focus on geochemistry and supports fundamental research on the interactions between the chemistry of earth's materials and their interactions with solutions, gases, and biota. The **Hydrologic Sciences Program** supports fundamental research about water on and beneath the Earth's surface, as well as relationships of water with material and living components of the environment. Many projects involve the study of hydrologic transport (e.g., of dissolved solutes) and coupling of hydrological processes with other systems (e.g., geochemical cycles). These programs co-funds awards on projects focused on fate and transport of chemicals introduced into the natural environment, including environmental remediation strategies. The **Sedimentary Geology and Paleobiology Program** funds research that includes deciphering the production, transport, and deposition of chemicals in the geologic record to investigate means for a sustainable future from a paleo-perspective. The **Critical Zone Collaborative Network** supports Thematic Clusters or Coordinating Hubs whose observational network includes data to understand chemical processes within carbon, nutrient, and hydrological cycles.

United States Department of Agriculture

- Within USDA, a range of supportive programs exist in the Rural Development Agency on biobased feedstocks, ranging from grants to loan to technical advice and support.
- The Biorefinery, Renewable Chemical, and Biobased Product Manufacturing Assistance Program provides loan guarantees up to $250 million to assist in the development, construction and retrofitting of new and emerging technologies including renewable chemicals and biobased products. USDA National Institute for Food and Agriculture (NIFA) has grant programs that include topics like fertilizer production and use, pesticide production and use, biomass feedstock production (corn grain, oilseeds, lignocellulosic feedstocks), circularity and waste resource management, and antimicrobial resistance and alternatives to antibiotics, fate in the environment.
- USDA's BioPreferred program is designed to increase the purchase and use of biobased products.
- USDA Agricultural Research Service has sustainable chemistry research in the following national programs: Food Safety (National Program 108), Product Quality and New Uses (NP 306), Animal Health (NP 103), Veterinary, Medical, and Urban Entomology (NP 104), Aquaculture (NP 106), Crop Protection and Quarantine (NP 304), Water Availability and Watershed Management (NP 211), Soil and Air (NP 212), Sustainable Agricultural Systems (NP 216); AgSTAR is a collaborative program with EPA that promotes the use of biogas recovery systems to reduce methane emissions from livestock waste.[77]
- USDA National Institute for Food and Agriculture (NIFA)
- Other USDA agencies to ask for information about relevant programs include: Farm Service Agency, Natural Resources Conservation Service, National Agricultural Statistical Service, Economic Research Service
- Several USDA agencies (Agricultural Research Service, National Institute for Food and Agriculture, Economic Research Service, and National Agricultural Statistical Service) have ongoing research on fertilizer production/use/environmental fate, circularity and waste resource management, pesticide production/use/environmental fate, biomass feedstock production (corn grain, oilseeds, sugar crops, switchgrass and other lignocellulosic feedstocks), biomass conversion, biochar, anaerobic digestion, per- and polyfluoroalkyl

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[77] https://www.epa.gov/agstar

substances (PFAS) in food systems, food safety related to chemical contamination, antimicrobial resistance/alternatives to antibiotics/antimicrobial fate in the environment, life cycle analysis of bioenergy systems and nitrogen and phosphorus use.

Appendix B – Budget Data Request

OMB issued a Budget Data Request to collect information about sustainable chemistry R&D and related activities expenditures from 2019-2021, as well as estimated expenditures for 2022. It is the first snapshot of sustainable chemistry R&D spending for fiscal years 2019-2022. Responding departments included DOC, DoD, EPA, HHS, and USDA; responding independent agencies included NSF. The total estimated sustainable chemistry expenditures were $1.4 billion dollars over 4 years, with DOE reporting the greatest R&D expenditures ($730 million), followed by NSF ($364 million), DoD ($218million), and HHS ($91 million) over the four fiscal years.

Summary information for each responding department and agency are provided below. These data are the first such data collected by OMB. There may be some aspects that impact the accuracy of the results. Some agencies reported difficulty in parsing which of their R&D money was specifically spent on sustainable chemistry. In many cases, agencies estimated their reported expenditures in part because many budget data systems do not track R&D funding down to specific projects. A specific difficulty with estimating expenditures for sustainable chemistry includes the lack of consensus definition for sustainable chemistry.

Overall, the summary information should be treated as a general indication of spending and distribution of funding within departments and agencies for sustainable chemistry R&D; however, it may not represent spending with full accuracy. The information provided here should be viewed in concert with the information in Appendix A, which provides a more holistic view of sustainable chemistry activities ongoing in agencies. The spending data presented below are solely focused on sustainable chemistry R&D activities. The development of a consensus definition in this report can help with tracking and reporting in the future.

Agency	Bureau	Category	Initiative Title	FY 2019 Actual ($M)	FY 2020 Actual ($M)	FY 2021 Actual ($M)	FY 2022 Estimated ($M)
Department of Commerce	National Institute of Standards and Technology	R&D	Sustainable Chemistry	1.00	1.00	2.00	2.00
Subtotal				1.00	1.00	2.00	2.00
Department of Defense	Department of Defense	R&D	SERDP	16.5	17.0	19.32	18.3
	Department of Defense	Demonstration	ESTCP	8.5	9.0	9.58	10.8
	Department of Defense	Technology Transfer	O&M Chemical Risk Management	0.80	0.80	0.30	0.90
	Department of Defense	R&D	Army CCDC SAFR	10.6	21.3	11.9	20.8
	Department of Defense	R&D	NDCEE	4.9	5.0	5.2	5.3
	Department of Defense	R&D	NESDI	4.3	4.4	6.1	6.2
Subtotal				45.5	57.6	52.52	62.3
Department of Energy	Department of Energy	R&D	Sustainable Chemistry	164.20	171.03	175.66	218.59
Subtotal				164.20	171.03	175.66	218.59
Environmental Protection Agency	Environmental Protection Agency	Commercialization	Environmentally Preferable Purchasing	0.00	0.00	0.00	0.00
Subtotal				0.00	0.00	0.00	0.00
Department of Health and Human Services	National Institutes of Health	R&D	A Specialized Platform for Innovative Research Exploration (ASPIRE)	10.00	8.24	6.94	8.10

	National Institutes of Health	R&D	ASPIRE	0.05	3.89	4.30	3.20
	National Institutes of Health	Demonstration	2022 Chemistry & Biology of Peptides Gordon Research Conference & Gordon Research Seminar	0.00	0.00	0.03	0.00
	National Institutes of Health	Commercialization	Novel Genomic Technology Development	0.07	0.64	0.48	0.00
	National Institutes of Health	Commercialization	Novel Nucleic Acid Sequencing Technology Development	2.23	3.45	1.41	0.43
	National Institutes of Health	R&D	Novel Genomic Technology Development	2.90	3.95	5.09	5.41
	National Institutes of Health	R&D	Novel Nucleic Acid Sequencing Technology Development	1.59	2.01	2.73	2.81
	National Institutes of Health	R&D	Novel Synthetic Nucleic Acid Technology Development	0.00	0.00	1.77	3.54
	National Institutes of Health	R&D	Data-driven, evolution-based design of proteins	0.00	0.00	0.32	0.32

	National Institutes of Health	R&D	Ultrahigh Throughput Microscale Mass Spectrometry for Pharmaceutical Prenylation Enzyme Engineering	0.00	0.00	0.25	0.00
	National Institutes of Health	Education	Grants—Education	0.30	0.32	0.41	0.21
	National Institutes of Health	R&D	Grants—Research & Development	0.14	0.00	0.00	0.00
	National Institutes of Health	Training	Grants—Training	3.64	0.25	0.00	0.00
Subtotal				20.91	22.75	23.71	24.02
National Science Foundation	National Science Foundation	R&D	NSF-funded Basic Research	71.45	87.00	74.94	82.00
	National Science Foundation	Demonstration	NSF-funded Basic Research	0.73	1.42	0.89	1.00
	National Science Foundation	Technology Transfer	NSF-funded Basic Research	0.73	1.42	0.89	1.00
	National Science Foundation	Commercialization	NSF-funded Basic Research	13.49	11.72	5.01	6.50
	National Science Foundation	Training	NSF-funded Basic Research	1.07	0.63	1.19	0.72
Subtotal				87.47	102.19	82.92	91.22
	US Department of Agriculture	R&D	NIFA—Hatch	0.19	0.27	0.40	0.40

U.S. Department of Agriculture	US Department of Agriculture	R&D	NIFA—Hatch (Multi-Sate)	0.22	0.22	0.38	0.38
	US Department of Agriculture	R&D	NIFA—McIntire-Stennis	0.00	0.00	0.01	0.01
	US Department of Agriculture	R&D	NIFA—AFRI	0.00	1.53	0.92	0.92
	US Department of Agriculture	R&D	NIFA—1890 CBG Program	0.50	0.00	0.00	0.00
	US Department of Agriculture	R&D	NIFA—Other Programs	0.00	0.00	0.42	0.42
	US Department of Agriculture	R&D	NIFA—SBIR	0.20	0.00	0.11	0.11
Subtotal				1.11	2.03	2.25	2.25
Total				**320.2**	**356.6**	**338.86**	**400.38**

Appendix C – Summary of Stakeholder Outreach Activities

On April 4, 2022, OSTP posted a Request for Information (RFI) on sustainable chemistry.[78] This RFI requested input from interested parties on sustainable chemistry. OSTP requested comments on preferred definition for sustainable chemistry, as well as how sustainable chemistry could impact the following: the role of technology, Federal policies that may aid or hinder sustainable chemistry initiatives, future research to advance sustainable chemistry, financial and economic considerations, and Federal agency efforts. Comments provided in response to this RFI were used in development of this report. Additionally, the input received will be used in the development of the follow-up strategic plan for Federal R&D sustainable chemistry activities.

OSTP received 47 total responses to the RFI. These came from a range of organizations, including industry, academia, international entities, NGOs, and state governments. A high-level summary of the responses to each question are provided below:

- For the first question, on the definition of sustainable chemistry, we received responses from nearly all respondents. The main themes that came out across all submissions is that a sustainable chemistry definition should consider resource use, hazard and risk reduction, and environmental, social, and economic factors. There was a mix in preference for a broad versus narrow definition. However, there was more consensus around the overlap with green chemistry—most respondents felt that sustainable chemistry is more holistic and should encompass and build on green chemistry.
- The second question focused on technological needs to support sustainable chemistry. There were several specific technologies suggested, including advanced recycling technologies, bio-based and petrochemical-alternative technologies, biotechnologies, and technologies for reducing chemical risks. Additional suggestions included fossil fuel-based technologies and biofuels, but these seemed to be a lower priority across the responses.
- There were several fundamental research areas identified. These included methods for conducting and implementing life cycle assessments (LCAs), methods for conducting and implementing chemical hazard and risk assessments, computational chemical research (including AI and MC, high-throughput screening, and computational or predictive toxicology), research to support chemical circularity, research to support the transition to sustainable chemistry (barriers, opportunities, supply-chain issues) and enabling policies, tools, and instruments, and development of chemical alternatives and alternative chemistry processes.
- On metrics, there was general consensus that metrics need to be flexible in definition and weighting. Many respondents suggested the Strategy Team look at and align with existing metrics, including international metrics.
- Respondents emphasized that financial and economic considerations are key components of sustainable chemistry. There was an emphasis on market forces being a driver of development and adoption. Market viability and widespread adoption is needed to make industrial chemistry more sustainable, and we need sustainable chemical products to be economically accessible to all.

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[78] https://www.federalregister.gov/documents/2022/04/04/2022-07043/request-for-information-sustainable-chemistry

- There was substantial input on policy considerations. There were overarching suggestions for the Strategy Team to participate in and leverage international community; consider ethical, social, and EJ factors and needs; use a cross-government, coordinated, or universal approach; use market forces; and integrate life cycle assessments and analyses. There were also suggestions for specific policies focused on: increasing government and chemical transparency; grant funding; education and training; encouraging the use of sustainable chemistry practices and products; phasing out hazardous substances and unsustainable chemicals and chemistry processes, and raising awareness of sustainable chemistry.
- The final question received a range of responses. However, there were a few themes that popped up: consider social factors, ethics, justice, national security needs, and potential economic impacts and viability when investing in sustainable chemistry; have broad stakeholder engagement (public, private, non-profit, policymakers, regulators) to build awareness and make progress; align sustainable chemistry with broader goals of sustainability; and use sustainable chemistry to advance the bioeconomy and create jobs.

OSTP hosted a series of three webinars to further gather input on various topics. The Strategy Team held a webinar with professional societies in March 2022 and a webinar around science, technology, and innovation needs in the chemical enterprise in May 2022. This webinar included discussion around the needs of the chemical industries, including carbon capture, sustainable process design, and chemical separation technologies. And the third webinar in June 2022 was on data and tools to inform sustainable chemistry decisions. The webinars are all available online: https://www.nist.gov/mml/nstc-webinar-series-sustainable-chemistry.