IDENTIFYING OPPORTUNITIES FOR **GREEN CHEMISTRY RESEARCH**

TO ADVANCE SUSTAINABLE DEVELOPMENT



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EXECUTIVE SUMMARY

Green and sustainable chemistry aims to minimize the potential negative impact of chemicals and their production on human health, ecosystems, biodiversity, and the environment. Accelerating adoption of green and sustainable chemistry is critical to meeting United Nations <u>sustainable development goals</u> (UN SDGs) and addressing climate change, pollution, and biodiversity loss in the coming decades.

Funders and researchers alike could benefit from a common method of connecting research to these societal goals. The method could be used to evaluate the impact of funding portfolios and better align research initiatives with impact on sustainable development. Such alignment will be critical to reaching UN SDGs by 2030.

To establish an overview of the current funding landscape for green and sustainable chemistry, the ACS Green Chemistry Institute (ACS GCI), with funding from the Gordon and Betty Moore Foundation, undertook a year-long project to elucidate opportunities for public and private funders to contribute to achieving the UN SDGs and climate-mitigation goals.

The Moore Foundation is a charitable foundation that invests in areas such as science and environmental conservation, with an eye toward achieving large-scale, enduring impacts. The foundation is exploring the potential of funding high-risk challenges in green chemistry that are not adequately addressed by existing funding streams and that bring about a quantifiable impact on sustainable development.

ACS GCI's mission is to catalyze implementation of green chemistry and engineering throughout the chemical enterprise by facilitating innovation and communicating core values and benefits of green and sustainable chemistry and engineering. The ACS Campaign for a Sustainable Future is a strategic initiative aimed at positioning ACS as a leader in advancing chemistry innovations that address challenges articulated in the UN SDGs.

THE PROJECT CONSISTED OF THREE OBJECTIVES:

- Convene funding organizations to share information about current and near-future funding interests.
- Analyze emerging areas of research anticipated to have a catalytic impact on green chemistry and UN SDGs by developing a hierarchical neural network approach.

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• Prioritize and analyze emerging areas of research.

The team used the scientific research database Dimensions to collect data on grants focused on basic research in green and sustainable chemistry that were awarded globally by all funding institutions between 2013 and 2022.

Of the nine fields the study examined, analytical chemistry and theoretical and computational chemistry were found to have the lowest funding levels. While funding for theoretical and computational chemistry increased during the study period, it remains the lowest-funded field. Because of their relevance to the fundamental chemical and process design, increased funding for analytical chemistry and theoretical and computational chemistry could have a catalytic impact toward meeting the UN SDGs.

Additionally, of the grants and funding awarded globally between 2013 and 2022 for basic research in the chemical sciences, industrial biotechnology, and chemical engineering, 64% of the total funding and 81% of individual grants awarded had no connection to UN SDGs. Funding for green and sustainable chemistry applications must increase if we are to reach societal goals such as UN SDGs.

Funding agencies can collaborate and amplify the impact of investment by facilitating sharing of experimental data, fostering interdisciplinary and cross-sector collaborations with industry, and funding high-risk projects. Furthermore, researchers and funders must mutually connect their basic research or research portfolios to UN SDGs to evaluate impact on sustainable development. Striving for the 2030 sustainable development goals will indeed necessitate that research in the chemical sciences be considered through the lens of green and sustainable chemistry.

BACKGROUND

Green and sustainable chemistry aims to minimize the potential negative impact of chemicals and their production on human health, ecosystems, biodiversity, and the environment. Accelerating adoption of green and sustainable chemistry is critical to meeting United Nations <u>sustainable development goals</u> (UN SDGs) and addressing climate change, pollution, and biodiversity loss in the coming decades.¹ The UN Environment Programme's 2021 <u>Green</u> <u>and Sustainable Chemistry: Framework Manual</u> references the potential of green and sustainable chemistry to help achieve UN SDGs.²

Green and sustainable chemistry is integral to climate priorities in the US. The National Science and Technology Council's 2023 Sustainable *Chemistry Report* resulted from an endeavor to coordinate efforts and analyze and promote federal funding related to green and sustainable chemistry.³ This report builds on work such as the Net-Zero Game Changers Initiative, which the White House announced in its 2022 report U.S. Innovation to Meet 2050 Climate Goals.⁴ The 2022 report prioritized five areas—efficient building heating and cooling, net-zero aviation, net-zero power grid and electrification, fusion energy at scale, and industrial products and fuels for a netzero, circular economy—for critical progress if the US is to meet its 2050 climate goals.

Investment that advances green and sustainable chemistry will be critical for reaching the goals in both the UN SDGs and the Net-Zero Game Changers. Federal funding of earlystage research is critical for maintaining a sustainable innovation pipeline. The US federal government awards grants related to green and sustainable chemistry through the Department of Defense, the Department of Energy, the Environmental Protection Agency, the National Science Foundation, and the US Department of Agriculture. It funds its own research and development; demonstration activities; data, modeling, and simulation resources; and procurement related to green and sustainable chemistry.³ It also supports small science and technology businesses through its Small Business Innovation Research and Small Business Technology Transfer programs.⁵

But funders beyond the federal government will need to support the advancement of green and sustainable to make meaningful progress on UN SDGs. David Berkowitz, director of the National Science Foundation's Division of Chemistry, says that challenges such as moving away from fossil carbon sources, developing truly recyclable polymers and plastics, and achieving material circularity "would benefit greatly from engagement by community organizations and not-for-profits and foundations." In realms such



as powering ground and air transportation that are inherently global and industrial, Berkowitz says, "Foundations, such as those dedicated to facilitating public-private partnerships and those committed to building bridges to international relationships in this space, will likely play a very important role." Since the budgets of most foundations are limited in comparison with those of federal governments, foundations may seek out areas that are not adequately supported by federal funds and that contribute tangibly to societal goals, such as UN SDGs.

Funding must touch the entire value chain, from bench to market and beyond, to achieve a truly significant shift. In addition to federal agencies and private foundations funding basic and applied research, venture capital must be available for start-ups to bring new technologies to market.

"There's a greater demand from the market for safer and sustainable chemistry than there is capital to fund it," says Marty Mulvihill, a general partner with Safer Made, a venture capital firm focused on green and sustainable chemistry investment.

"Chemistry and materials are central to safety and sustainability," Mulvihill says. He cites carbon emissions from chemical and materials companies and water pollution from manufacturing processes, as well as the need to produce food more efficiently and with fewer pesticides, as areas where green and sustainable chemistry can make progress toward UN SDGs. "Throughout many of the UN Sustainable Development Goals and energy transition goals, it comes back to the development and deployment of new materials. And that's where chemistry has a role to play," Mulvihill adds.

Mulvihill says foundations can help bridge the gap between early-phase research, where the goal is to publish an academic paper, and the point at which a young company can produce and sell product, which is typically when venture funding comes in.

It is difficult for funders to get involved without a sufficient understanding of the mechanisms through which investment in fundamental research impacts UN SDGs. Funders presently do not require researchers to identify the potential connections of their proposed work to specific UN SDGs, and there is no existing framework by which researchers can evaluate the impact of their work through this lens. To that end, funders and researchers alike could benefit from a common method of connecting research to societal goals. Such a method would allow the impact of funding portfolios to be evaluated, which in turn would help the chemistry community better align its research initiatives with impact on sustainable development. Such alignment will be critical to reaching the UN SDGs by 2030.

Aligning fundamental research with impact on sustainable development also requires application of a comprehensive, systems-based approach to research—one that considers the impact of the chemical process; the fate, transport and hazard profile of the chemicals

or materials produced; and the lifecycle impact, including chemical or material use and circularity. Green and sustainable chemistry should not be funded to the exclusion of fundamental research; rather, because of the time pressure involved in meeting the UN SDGs, funders should prioritize research that can be connected to these goals.

GREEN AND SUSTAINABLE CHEMISTRY DEFINITIONS

The US Environmental Protection Agency <u>defines green chemistry</u> as "the design of chemical products and processes that reduce or eliminate the use or generation of hazardous substances."⁶

The White House's August 2023 report <u>Sustainable Chemistry Report: Framing the Federal</u> <u>Landscape</u> defines sustainable chemistry as "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."³ In a more simplified definition, the <u>UMass Lowell Sustainable Chemistry Catalyst and partners</u> defines sustainable chemistry as "the development and application of chemicals, chemical processes, and products that benefit current and future generations without harmful impacts to humans or ecosystems."⁷

PROJECT SUMMARY

Understanding where green and sustainable chemistry investment have contributed to the advancement of global sustainability goals—and where the current gaps in investment lie—is critical for meeting societal goals such as UN SDGs.

To establish an overview of the current funding landscape for green and sustainable chemistry, the ACS Green Chemistry Institute (ACS GCI), with funding from the Gordon and Betty Moore Foundation (Moore Foundation), undertook a year-long project to elucidate opportunities for public/private funders to contribute to achieving the UN SDGs and climate-mitigation goals.

The Moore Foundation is a charitable foundation that invests in areas such as science and environmental conservation with an eye toward achieving large-scale, enduring impacts. The foundation is exploring the potential of funding high-risk challenges in green chemistry that are not adequately addressed by existing funding streams and that bring about a quantifiable impact on sustainable development.

ACS GCI's mission is to catalyze implementation of green chemistry and engineering throughout the chemical enterprise by facilitating innovation and communicating core values and benefits of green and sustainable chemistry and engineering. The ACS Campaign for a Sustainable Future is a strategic initiative aimed at positioning ACS as a leader in advancing chemistry innovations that address challenges articulated in the UN SDGs.

The project consisted of three objectives:

- Convene organizations to share information about current and near-future funding interests.
- Analyze emerging areas of research anticipated to have a catalytic impact on green chemistry and UN SDGs by developing a hierarchical neural network approach.
- Prioritize and analyze emerging areas of research.

The team used the scientific research database Dimensions to look at grants awarded globally by all funding institutions between 2013 and 2022. To focus on basic research in green and sustainable chemistry, the team narrowed the scope to all grants that met the targeted fields of research, were consistent with fundamental as opposed to applied research, and met at least one of the UN SDGs. (See appendix on page 22 for a full explanation of the methods.)

Some of the project's key findings are as follows:

 Analytical chemistry and theoretical and computational chemistry are the least-funded of the nine fields of study examined. Funding for theoretical and computational chemistry increased during the study period, but it remains the lowest-funded field. Because of

their relevance to the fundamental design of molecules, increased funding for analytical chemistry and theoretical and computational chemistry could have a catalytic impact toward meeting UN SDGs.

- Of the individual grants and total amounts of funding awarded globally between 2013 and 2022 for basic research in the chemical sciences, industrial biotechnology, and chemical engineering, 81% of grants and 64% of funding had no connection to UN SDGs. (The amount of funding associated with each grant varies.) Funding for green and sustainable chemistry applications must increase if we are to reach societal goals such as UN SDGs. Researchers and funders must adopt a method for connecting their fundamental research or research portfolios to UN SDGs.
- US-based institutions received the most funding for basic research in the chemical sciences, industrial biotechnology, and chemical engineering that met at least one

UN SDG—about one-third of the funding awarded worldwide. For work related to UN SDGs in the chemical sciences, industrial biotechnology, and chemical engineering, seven of the nine fields of study examined chemical engineering, industrial biotechnology, inorganic chemistry, macromolecular and materials chemistry, organic chemistry, physical chemistry, and theoretical and computational chemistry—are funded primarily by government agencies. Medicinal and biomolecular chemistry and analytical chemistry are funded primarily by private foundations.

 Funding agencies can collaborate and amplify the impact of investment by developing a common repository of experimental data, fostering interdisciplinary and academiaindustry collaborations, and funding high-risk projects.

PROJECT NARRATIVE

1. CONVENE ORGANIZATIONS TO DISCUSS FUNDING LANDSCAPE

The project's first objective was to convene representatives from federal funding agencies, private foundations, and organizations with interests in green and sustainable chemistry to survey current and near-future requests for proposals in the field, including magnitude of funding, time scale, and type of research team being funded.

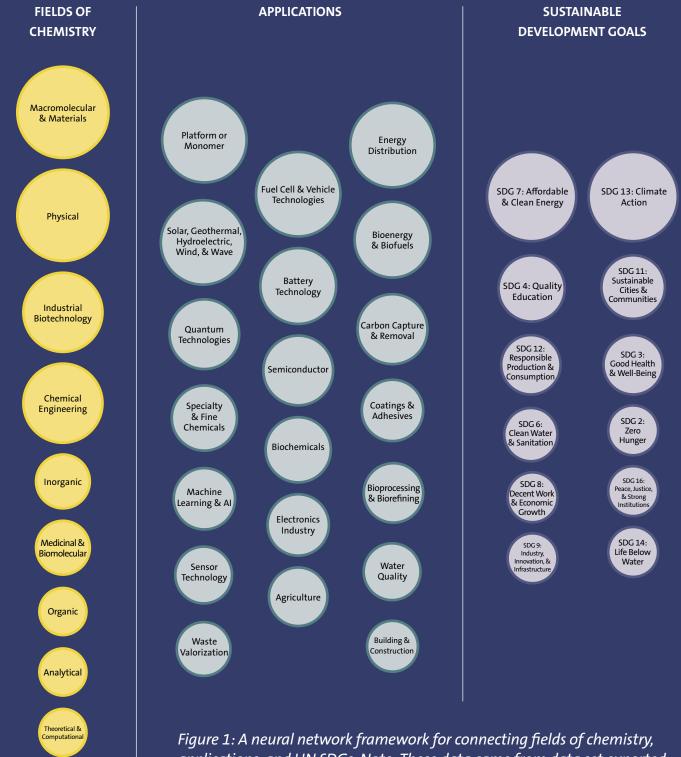
To this end, in February 2023, the ACS GCI hosted the "Future of Green and Sustainable Chemistry Funding Workshop." Representatives attended from the National Institute of Standards and Technology, the National Science Foundation, the US Department of Energy, the US Environmental Protection Agency, and the White House Office of Science and Technology Policy, as well as from the Alfred P. Sloan Foundation; the American Chemical Society; the Arnold and Mabel Beckman Foundation; the Camille and Henry Dreyfus Foundation; the Moore Foundation; the National Academies of Science, Engineering and Medicine; Schmidt Futures; and the Research Corporation for Science Advancement.

In the workshop, ACS GCI representatives introduced the landscape of green and sustainable chemistry funding and how it connects to UN SDGs. They highlighted preliminary findings regarding funding and knowledge gaps that could better position the scientific community to address the UN SDGs. The preliminary findings informed a facilitated discussion among attendees. The group explored topics and collaborations to accelerate or amplify impact on the UN SDGs.

Attendees of the workshop identified several opportunities for funders to collaborate and amplify the impact of investment in green and sustainable chemistry:

- Amplify funding impact by integrating fundamental science with supply chains and environmental justice partners in both education and research.
- Accelerate research by developing a common repository of experimental data. The repository must include validation for data quality, possibly leveraging existing AI tools to do so.
- Nucleate partnerships by fostering interdisciplinary collaborations, especially with community leaders and social scientists. Greater transparency around existing collaborative funding opportunities can better position funders to offer such opportunities.
- Accelerate innovation by promoting academiaindustry collaboration on basic research. IP issues continue to be a difficult challenge in this area.
- Spur transformative innovation by funding highrisk projects.

A NEURAL NETWORK FRAMEWORK FOR CONNECTING FIELDS OF CHEMISTRY, APPLICATIONS, AND UN SDGS.



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Angure 1: A neural network framework for connecting fields of chemistry, applications, and UN SDGs. Note: These data came from data set exported in June 2023.

2. ANALYZE EMERGING AREAS OF RESEARCH

The project's second objective was to develop a hierarchical neural network approach for identifying high-impact research areas. Figure 1 shows a network map of grants from 2013 to 2022 for basic research in the chemical sciences, industrial biotechnology, and chemical engineering that meet at least one UN SDG from global funders to US recipients. The size of each bubble corresponds to the research funding for each field, application, and UN SDG. Using such a framework, one can draw connections between fields of chemistry and applications and connect those applications with UN SDGs. As a proof of concept, the project team manually mapped fields of chemistry to applications and UN SDGs using information available in Dimensions. Such a framework provides a starting point for looking at research through the lens of UN SDGs.

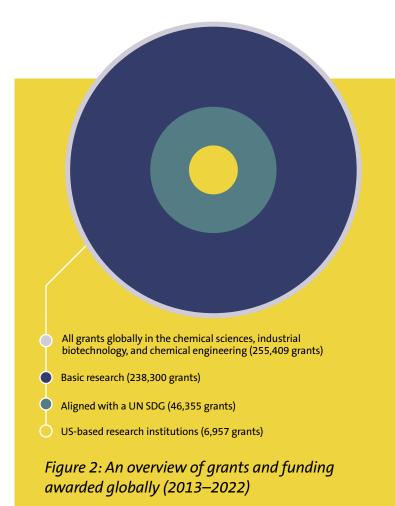
3. PRIORITIZE AND ANALYZE KEY AREAS

The project's final objective was to prioritize and analyze emerging areas of research for which a deeper understanding of the funding and research landscape is needed, plus to analyze various types of funding mechanisms.

The study looked at starting grants from 2013 to 2022 for basic research in the chemical sciences, industrial biotechnology, and chemical engineering that meet at least one UN SDG from all funders to global recipients. The results were analyzed at the global and agency levels, as well as by field of research and application.

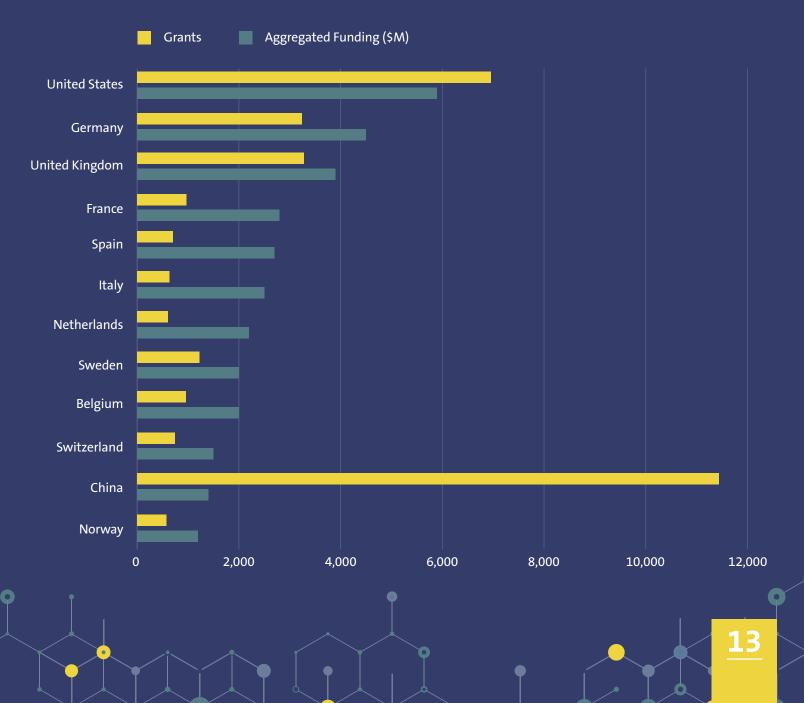
GLOBAL FUNDING LANDSCAPE OF BASIC CHEMISTRY RESEARCH

The data set consisted of 255,409 grants in chemical sciences, industrial biotechnology, and chemical engineering. Of these, 46,355 grants were aligned with a UN SDG, amounting to \$18.4 billion of funding awarded between 2013 and 2022. Of the grants and funding awarded globally for basic research in the chemical sciences, industrial biotechnology, and chemical engineering, the majority (81% of grants and 64% of funding) were found to have no direct



connection to the UN SDGs, as shown in Figure 2. However, the dollars per grant for the UN SDGrelated research in this category (\$399,094) was more than twice the dollars per grant for non-UN SDG-related research (\$173,487). US-based research institutions received close to one-third of worldwide basic science funding in the chemical sciences, industrial biotechnology, and chemical engineering that aligns with at least one UN SDG. Among countries receiving more than \$1 billion in aggregated funding, US-based institutions received the most funding for basic research in the chemical sciences, industrial biotechnology, and chemical engineering that meets at least one UN SDG. The US is followed by several countries in the EU and the UK.

Figure 3: Funding received by institutions in each country receiving more than \$1 billion in aggregated funding (2013–2022)

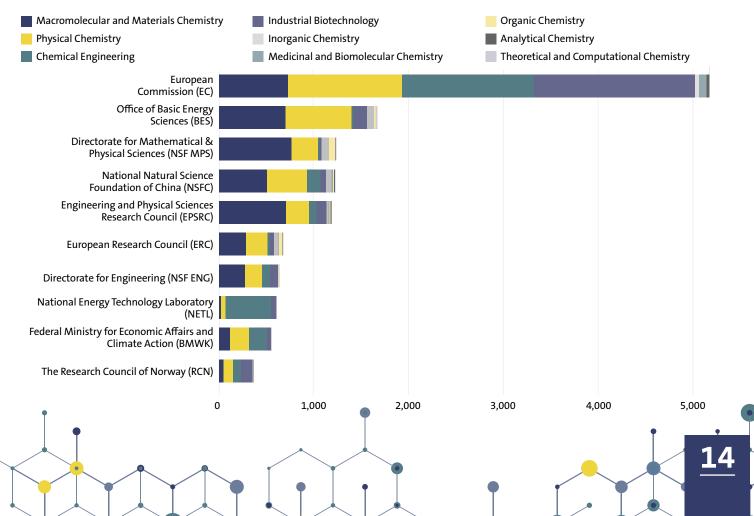


FUNDING BY AGENCY AND FIELD

The analysis also examined funding agencies that have substantial chemistry portfolios. Figure 4 shows the investment of the top 10 funders invested in UN SDG-related basic research in the chemical sciences, industrial biotechnology, and chemical engineering from 2013 to 2022.

Half of the agencies shown here fund all nine fields of study. US-based agencies account for four of the top 10 funders. Some agencies are very discipline-specific: for example, the US National Energy Technology Laboratory funds only five areas, with about 80% of the funds being distributed to chemical engineering research. Additionally, the project team looked at the top funders for each field of research. Only two fields - medicinal and biomolecular chemistry and analytical chemistry-have private institutions as their top funders; these foundations do not figure among the top funders of UN SDG-related basic research in the chemical sciences, industrial biotechnology, and chemical engineering globally. The Wellcome Trust contributes the most funding toward medicinal and biomolecular basic research grants related to UN SDGs (\$46 million), while the Canada Foundation for Innovation funds the most UN SDG-related basic research grants in analytical chemistry (\$19 million). Medicinal and biomolecular chemistry also receives UN SDGrelated funding from the fewest number of top grant funders.

Figure 4: Chemistry portfolio investment in \$ millions by field of research for top 10 worldwide funders of UN SDG-related basic research in the chemical sciences, industrial biotechnology, and chemical engineering globally (2013–2022)



The analysis also explored investment, both in terms of aggregated funding and number of grants, by field of research for UN SDG-related basic research in the chemical sciences, industrial biotechnology, and chemical engineering from 2013 to 2022.

Figure 5 shows a clear breaking-off point between the most-funded fields in terms of financing and grants (macromolecular and materials chemistry, physical chemistry, chemical engineering, and industrial biotechnology) and the leastfunded. Analytical chemistry and theoretical and computational chemistry are the two leastfunded fields, with 83 grants totaling \$70 million for analytical chemistry and 52 grants totaling \$42 million for theoretical and computational chemistry. Together, they account for only 1.6% of grants and 4.4% of funding worldwide.

Taken together, investment in UN SDG—related research in the four most-financed fields increased 750% from 2013 to 2022—twice the increase of the five least-financed fields, as shown in Figure 6. Funding for physical chemistry and theoretical and computational chemistry saw the largest increase, although even in 2022, basic research in theoretical and computational chemistry received the least funding of any of the nine fields. Inorganic chemistry and medicinal and biomolecular chemistry saw the lowest increase in funding.

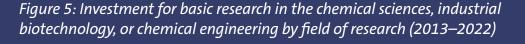
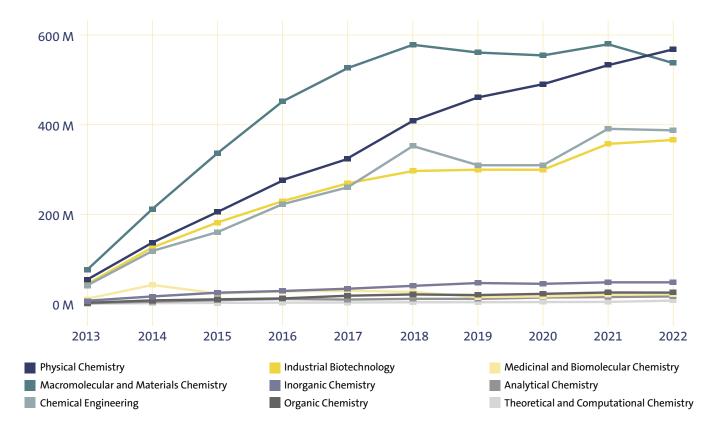




Figure 6: Investment for basic research in the chemical sciences, industrial biotechnology, or chemical engineering by field of study over time



FUNDING BY SUSTAINABILITY-RELATED APPLICATIONS

Finally, the analysis examined the connections between fields of research and 20 applications related to sustainability. The team created filters to better understand the potential future applicability of this research and its alignment with UN SDGs.

All four of the top-funded fields — macromolecular and materials chemistry, physical chemistry, chemical engineering, and industrial biotechnology—have research related to all 20 applications. In contrast, the least-funded fields—analytical chemistry and theoretical and computational chemistry—connect to very few applications related to sustainability: quantum technologies, machine learning and AI, and electronics for theoretical and computational chemistry, and agriculture and specialty chemicals for analytical chemistry.

It is worth noting that, while investments in machine learning and AI are generally on the rise, the chemical sciences, industrial biotechnology, and chemical engineering have contributed comparatively little to date. The number of starting grants in these areas that relate to machine learning and AI increased but remained low during the study period (2013–2022).

AREAS FOR INVESTMENT: ANALYTICAL CHEMISTRY AND THEORETICAL AND COMPUTATIONAL CHEMISTRY

The works shows that funding for analytical chemistry and theoretical and computational chemistry have remained low over the past decade. Analytical chemistry is the science of obtaining, processing, and communicating information about the composition and structure of matter.⁸ According to *Nature*, theoretical chemistry "seeks to provide theories and explanations for chemical observations whilst also posing questions to be answered by future experiments," while computational chemistry "describes the use of computer modelling and simulation . . . to study the structures and properties of molecules and materials."^{9,10}

Green and sustainable chemistry requires chemists to return to the fundamental design of molecules of chemicals to develop safer chemistries. Both analytical chemistry and theoretical and computational chemistry will be critical areas in which to fund research.

Mulvihill says that new analytical techniques and innovations are critical for characterizing the fate and transport of chemicals of concern and for lowering the cost and developing new types of remediation. "Innovations in analytical chemistry can have an outsized impact on the perception of the need for safer chemistry throughout society," he says. "There's a catalytic role that better analytical chemistry techniques focused on these areas could play."

Most of analytical chemistry's environmental impact comes from high-throughput industrial facilities running quality assurance or quality control analyses, says Kevin Thurbide, a professor of analytical chemistry at the University of Calgary. Reducing instrument size and thus the energy, space, and waste required to operate them and exploring novel, green solvent media to reduce the emission of harmful organic vapors are two areas where Thurbide says advances in analytical chemistry could drive progress toward UN SDGs.

According to Anastassia Alexandrova, a theoretical and computational chemist at the University of California, Los Angeles, the field contributes to green and sustainable chemistry by resolving mechanisms in green synthesis, predicting better catalysts and capture agents for CO₂ capture and conversion, and guiding the development of better fuel cells. Theoretical chemistry is also integral to catalysis for renewable energy. And according to Jakub Kostal, a professor of computational chemistry and director of the Environmental and Green Chemistry Program at the George Washington University, computational chemists can identify new chemical solutions using artificial intelligence and characterize their performance, hazards, and persistence using quantum mechanics and molecular simulations. Theoretical and computational chemistry can also be used to design new polymers and materials for circularity.

To take a closer look at funding in action, we aggregated grant data from six prominent chemists working in analytical chemistry and theoretical and computational chemistry. Of the 59 grants these researchers won during the study period, only 5 (8%) are in the chemical sciences and align with analytical chemistry or theoretical and computational chemistry, and none of those grants align with UN SDGs. However, of the 736 papers these researchers published during the study period, 139 (19%) are in the chemical sciences and align with analytical chemistry or theoretical and computational chemistry, and 4 of those (0.5%) align with at least one UN SDG.

That analytical chemistry and theoretical and computational chemistry show up more frequently in publications than in grant abstracts may indicate that researchers in these littlefunded fields are being resourceful in obtaining funding, either by collaborating, soliciting internal funds, or strategically targeting better-funded fields in their grant-writing. It may also represent a limitation of this study, as some grants could incorporate work in analytical chemistry or theoretical and computational chemistry without being categorized as such in Dimensions.

Thurbide says that funding for analytical chemistry can vary a lot by country but that it tends to be heavily supported by industry. "Efforts that encourage strategic partnerships with industrially supported analytical research will greatly help analytical chemistry to assist industry in achieving their [sustainability] goals," he says.

On funding for theoretical and computational chemistry, Alexandrova says, "There are certainly ways to fund theoretical research on problems of sustainability through many different routes in NSF, DOE, and other agencies."

From the investment side, Mulvihill says that he has seen more interest in theoretical and computational chemistry recently, but that not much of that interest is focused on safety or sustainability.

"Creating an end market for safer and sustainable chemistry and tools that are focused on making the prediction and identification of safer molecules faster and easier will help transition the industry towards safer chemistry"—for example, in the realm of predictive toxicology, he says. "There's a huge room for improvement here, and I think it could help accelerate the process of discovery and development of safer materials."

DISCUSSION

Analytical chemistry and theoretical and computational chemistry may represent special areas of opportunity for foundations where their funding can have a transformative impact. These fields received the least funding of any field throughout the study period. Existing federal funding mechanisms do not currently address these areas. Both fields have rich ties to sustainable chemistry, whether in the form of better fuel cells, CO₂ capture and conversion, safer chemicals or greener solvents. As such, they have the potential to inform and accelerate outcomes in other scientific areas, with potential catalytic impact on green and sustainable chemistry and UN SDGs.

Investment in machine learning and AI specific to the chemical sciences could have broad-reaching impacts and facilitate more efficient sustainable design, for example through the creation of predictive models.

Funding for green and sustainable chemistry applications must increase if we are to reach societal goals such as UN SDGs. Only 19% of the 238,300 grants funding basic research in the chemical sciences, industrial biotechnology, and chemical engineering in this study went to research related to UN SDGs. All funding for basic research should connect to UN SDGs if we are to make material progress toward these goals by 2030. Researchers must understand how they can align their research with green and sustainable chemistry, and funders must view their impact portfolios through a green and sustainable chemistry lens. To facilitate this new way of thinking, researchers and funders can apply a neural network approach to connect their fundamental research or research portfolio with SDGs. An effort to formalize such connections for reference by the scientific community will need to be undertaken in the future.

Cross-disciplinary collaboration and academiaindustry partnerships will be essential for reaching the UN SDGs. The ACS Campaign for a Sustainable Future has recently instituted two new grants to allow academics to gain industry experience, <u>one targeting established</u> <u>academic researchers</u> and the other, <u>early-career</u> <u>researchers</u>. More such targeted opportunities will be needed.

Transparency of health, safety, and environmental data will be critical to accelerate innovation and avoid regrettable substitutions. Openly accessible sources of data related to sustainability, health, safety, and other claims will be essential so that those claims can be verified.

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CONCLUSION

More funding for green and sustainable chemistry will be needed if we are to meet societal goals such as the UN SDGs by 2030. Analytical chemistry and theoretical and computational chemistry represent special areas of opportunity where additional funding could have a transformative impact. Researchers and funders must view their research and funding portfolios through the lens of green and sustainable chemistry so that efforts can be aligned. Funding agencies can collaborate and amplify the impact of investment by developing a common repository of experimental data, fostering interdisciplinary and academia-industry collaborations, and funding high-risk projects.

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APPENDIX: METHODS

TIME PERIOD

Awarded grants starting from the year 2013 through 2022 from all funding institutions were evaluated using the scientific research database Dimensions. The study chose to utilize "starting year" as a primary data point, as compared to "active year," which is a calculation that distributes the total awarded funds over the grant period.

BASIC RESEARCH

Dimensions does not identify basic research; therefore, a filter of terms was developed to exclude terms deemed to be outside the scope of interest. Terms used to exclude grants included: MRI (Major Research Instrumentation); SBIR; STTR; conference; workshop; symposium; symposia; scale up; scaleup. Additionally, ARPA-E was excluded as a funder since it is a major funding source consistent with advanced/applied research.

GREEN AND SUSTAINABLE CHEMISTRY

To narrow the scope of grants to green and sustainable chemistry, grants were selected that met the targeted field of research and at least one UN SDG.

Dimensions has integrated classification schemes for Fields of Research and UN Sustainable Development Goals (UN SDGs). The Fields of Research utilizes major fields and sub-fields from the Australian and New Zealand Standard Research Classification (ANZSRC 2020). These categories are built in Dimensions using emulations of the categorization systems led by machine learning.

Since green and sustainable chemistry is a broad field intersecting with many disciplines, it was decided that the grants would meet at least one of the following chemistry-related fields of research.

- Chemical sciences (ANZSRC 34)
- Analytical chemistry (ANZSRC 3401)
- Inorganic chemistry (ANZSRC 3402)
- Macromolecular and materials chemistry (ANZSRC 3403)
- Medicinal and biomolecular chemistry (ANZSRC 3404)
- Organic chemistry (ANZSC 3405)
- Physical chemistry (ANZSC 3406)
- Theoretical and computational chemistry (ANZSRC 2407)
- Industrial biotechnology (ANZSRC 3106)
- Chemical engineering (ANZSC 4004)

The grants also had to be recognized by Dimensions as meeting at least one of the UN SDGs.

DATA SETS

All data was exported in December 2023 with the exception of the data shown in Figure 1, which was exported in June 2023.

STUDY LIMITATIONS

- The methodology to identify grants according to UN SDGs was not within the scope of work, and there was insufficient data to assess the basis of the methodology. However, these grants were deemed to be consistent with sustainability, with perhaps an under-representation of 15% of grants. With limited understanding of the methodology, the ability to align grants with specific UN SDGs was not feasible.
- Keyword filters, utilized mainly to assess applications and more specific fields of research, have inherent biases which may affect the results. However, the primary fields of research and UN SDGs were a function of machine learning by Dimensions AI and would be expected to have greater reliability.



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