VIEWPOINT

Viewpoint: Chemistry for a Sustainable Future

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Chemistry *for a* SUSTAINABLE FUTURE

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Education and basic research in energy, green chemistry, and the environment can play pivotal roles in the quest for sustainability.

"Sustainability—the ability to provide a healthy, satisfying, and just life for all people on earth, now and for generations to come, while enhancing the health of ecosystems and the ability of other species to survive in their natural environments" (*1*).

In 1987, a UN report defined sustainable development as "development that meets the needs of the present without compromising the ability of future generations to meet their own needs" (*2*). This report is often recognized as the genesis of the modern sustainability movement. However, the concept of sustainability appears in historical records and ancient proverbs throughout the world and has an extensive history (*3*). As the challenge of living in harmony with the earth becomes increasingly difficult (*4*), more than ever, society needs education and high-quality, cutting-edge research to meet this challenge.

Society currently has a nonsustainable dependence on a finite supply of fossil-fuel-based hydrocarbons used in almost every synthetic material in the economy. The finite, nonsustainable supply of fossil fuels also serves as the main source of energy. The price of oil continues to rise while, at the same time, the countries that produce these vital fuels struggle with unstable social and political conditions. Finally, and perhaps most importantly, the growth in energy demand is projected to continue, and the cumulative impact of burning fossil fuels to meet this demand raises serious concerns.

Our nonsustainable use of materials and energy also harms the health and well-being of society and ecosystems. For example, CO_2, a byproduct of the combustion of fossil fuels, harms the environment by stimulating global climate change and potentially disastrous global warming. Specific challenges related to the chemical industry for achieving a sustainable society were identified in the National Academy of Sciences (NAS) workshop report *Grand Challenges for Sustainability in the Chemical Industry* (*5*). The question now becomes, given societal needs in the 21st century and beyond, what science and technology innovations do we need to achieve the goal of a sustainable future?

Chemistry, a branch of science that deals with the structure, composition, energetics, properties, and reactive characteristics of substances at atomic, molecular, and nanometer-length scales, is uniquely situated to contribute in positive and meaningful ways to sustainable well-being. Chemists are uniquely qualified to provide a molecular-level approach to and understanding of sustainability. Indeed, concepts that implicitly embed a sustainable philosophy, such as "atom economy" and "one-pot synthesis", have been goals in organic transformations for some time (*6*). A significant future challenge is to find molecular solutions to pressing sustainability issues as well as proactive solutions that prevent future problems. Many important and stimulating chemical research activities are encompassed by sustainability. Chemists who make contributions to these areas will have a positive impact on the quality of life that will help ensure a sustainable future for society.

During a recent workshop sponsored by the U.S. National Science Foundation (NSF), a diverse group of senior chemistry investigators with a wide range of expertise discussed four areas of sustainability (*7*). These areas—energy, green chemistry and processing, the environment, and education—present daunting issues. They are areas in which basic chemistry research and educational initiatives can play a pivotal role in driving innovations that will help achieve a sustainable future. Workshop participants considered advances in five enabling areas: nanoscience, bioprocesses, catalysis, measurement science, and cyberscience. This viewpoint article provides a broad overview of the issues discussed.

Research in energy

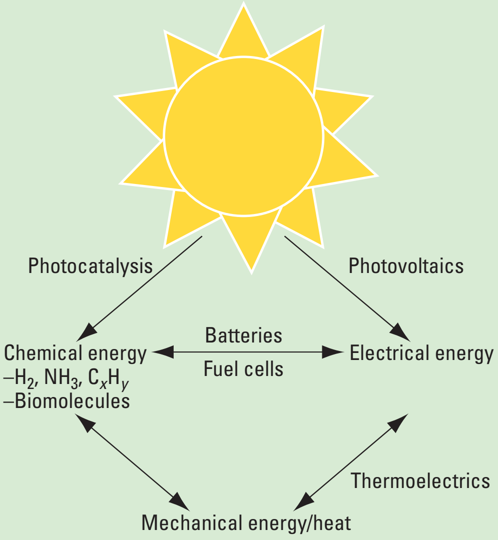
Grand challenge and the need for change. The significant environmental consequences of the use of carbon-based fuels and the decrease in their availability demand new approaches to energy and energy conversion. Chemists have played important roles in shaping or developing new methods of energy conversion (Grätzel cells, polymer electrolyte membrane fuel cells, new electrodes for lithium-ion batteries, and the emerging use of bioderived fuels like biodiesel). However, present energy needs require further innovation and dramatic changes. A sustainable future calls for a carbon-neutral economy that will use solar energy or alternative feedstocks, or both.

The role of chemistry and the advances needed. Chemistry is a central science in energy conversion, storage, and utilization. Most of our widely used forms of energy come from combustion of fossil fuels that are clearly not sustainable. Society requires new energy sources that can be sustainably created, stored, interconverted, and used. Figure 1 illustrates modes of energy conversion. Chemistry plays a crucial role in enabling many, if not all, of these transformations. Solar light can be used to create chemical feedstocks or to create electricity in a solar cell. Fuel cells convert chemical feedstocks into electricity, and batteries can be used to store the electrical energy produced. Chemical reactions convert commodity materials into more readily utilized fuels. Combustion reactions convert chemical energy into mechanical energy, whereas electrochemical reactions convert chemicals directly into electrical energy. All of these reactions also produce heat, and thermoelectrical materials can be used to convert heat to electricity.

FIGURE 1

Key energy currencies used by society

The connections between these energy forms are already well established and widely used, such as the conversions between different forms of chemical energy that are at the heart of the petroleum industry, the conversion of chemical to mechanical and electrical energy accomplished through combustion, and the interconversion of chemical and electrical energy with batteries. Technology is still needed in these areas as well as in the direct conversion of light energy to electricity with photovoltaics and of heat into electrical energy with thermoelectric devices. In all cases, chemical innovation is essential to accomplish stepwise changes in capability and efficiency.



Advances are needed in at least three key areas. First, the harvesting of sunlight and the conversion of this energy into more readily usable chemical or electrical energy need to be further developed. Solar energy is by far the largest exploitable energy source of the future. However, to be valuable to society, it must be harvested and converted to a useful form. Solar harvesting and conversion to electrical power can be accomplished by photovoltaics. New, low-cost materials that efficiently harvest sunlight and separate charge for photoelectrochemical and photovoltaic applications are critically needed. Storage can, for example, be accomplished in batteries or in chemical bonds. The rate at which consumers can deliver gasoline to their automobiles underscores the utility of storing energy from the sun in chemical bonds. Chemical feedstocks represent a desirable means for storing energy derived from the sun, because of their high volumetric and gravimetric energy densities, ease of storage and transport, and ease of rapid continuous or transient energy extraction. However, conversion of solar energy into useful feedstocks, such as the splitting of water into O_2 and H_2, represents a formidable challenge that has not been met after decades of research. Achieving this and related transformations is difficult and will require new or more efficient methods to activate inert molecules (N_2, CO_2, H_2O) and convert them photochemically into fuel stocks. In addition, chemists need a much deeper fundamental understanding of coupled, multielectron processes, including the kinetics of these reactions and the ability to control or direct the flow of electrons and energy in the system or device.

Second, improvements in the conversion of chemical into electrical energy are needed. Advances in this conversion require significant improvements in fuel cells and batteries. The development of fuel cells must be coupled with parallel efforts to produce and store the fuels needed to power these devices. New, sustainable electrode materials, membranes, and electrolytes are critically needed.

Third, more energy-efficient chemical transformations are needed. Advances also require new catalytic processes that allow efficient conversion of inert molecules, such as N_2, into enabling fuel stocks, such as NH_3, and that allow more ready commercialization of the chemistry of complicated chemical transformations with thermodynamics that are close to equilibrium. In some cases, the catalysis should be coupled with solar harvesting. Advances require improvements in materials and control that allow extraction of chemical energy by the operation of chemical reactors and combustors near equilibrium.

Research in green chemistry and processing

Grand challenge and the need to change. A sustainable future will require materials processing practices that use alternative and renewable feedstocks more efficiently, with fewer unwanted byproducts. Materials processing at present uses chemicals and materials synthesized from nonrenewable feedstocks, such as petroleum-derived molecules, that will begin to grow scarce in this century. A further problem comes from the products and byproducts of materials processing. Covalent bonds used to assemble products must be degraded before reuse. Conversions also require quantities of reagents and accessory compounds (chiral auxiliaries, protecting groups, etc.). Manufacturers must retrieve and dispose of such byproducts or risk polluting the environment with them.

Thermodynamic, rather than kinetic, processes control most carbon–carbon bond formation reactions that lead to undesirable byproducts and nonselective chemistry. To discover and optimize these reactions becomes a time-consuming process. Chemists must prepare and screen numerous candidate materials and use specialized macroreactors for each synthetic step. Each unit operation advances the synthesis by a single step. Chemists must also tailor organic solvents for each reaction type. Final-

FIGURE 2

Converting current practices to more sustainable ones

Current chemical practices	New paradigms in sustainable chemistry
Chemicals and materials synthesized from petroleum-derived molecules	Tailorable (e.g., genetically engineered) renewable feedstocks supply the building blocks for material synthesis Thermoprocessible plastics produced by simple modifications of oxygenated biomaterials
Products are assembled by covalent bonds that must be degraded prior to reutilization	Materials held together by noncovalent forces that can be disassembled under specific conditions
Conversions require stoichiometric quantities of reagents Accessory compounds (e.g., chiral auxiliaries, protecting groups) are often required Most carbon–carbon bond formation is under thermodynamic, rather than kinetic, control	Reactions promoted by highly selective and active catalysts
Reactions carried out in a variety of volatile organic solvents tailored for each reaction type	A single solvent (e.g., near-critical water) that allows tunable properties for multiple types of chemical reactions
Reaction discovery and process optimization are often slow processes	In situ spectroscopy for real-time monitoring of reactions over timescales from nanoseconds to hours during the discovery phase Higher level at which computations can be used to predict new catalytic systems
A large number of candidate materials are prepared and screened with respect to their properties	Accurate computational approaches to predicting the properties of novel materials reduce development effort
Specialized macroreactors are usually used for each synthetic step	The future chemical plant will consist of modular microreactors that can be rapidly assembled in multiple combinations to create new processes
Each unit operation advances the synthesis by a single step	Multiple reactions carried out in a single vessel promoted by compatible catalysts
Product separation and purification are often difficult and energy-intensive	Highly selective, nanomaterials-based separations methods avoid the need for distillation, extraction, crystallization, and chromatography

ly, product separation and purification frequently remain difficult and energy-intensive.

The role of chemistry and advances needed. Change will come about when chemists have the tools to use renewable resources with few byproducts produced by simpler, less energy-intensive, and more efficient processes to power our society. A sustainable future will come about when chemists can control and monitor chemical reactions more effectively.

An ideological shift is required in the chemistry community as a whole, from current chemical practices to new paradigms in sustainability chemistry. The basic concepts of these paradigm shifts—the conversion of old practices to new ones—are presented in Figure 2. These new practices include the use of renewable feedstocks, green solvents, module microreactors, and multiple reactions in a single vessel as well as finding highly selective reaction pathways.

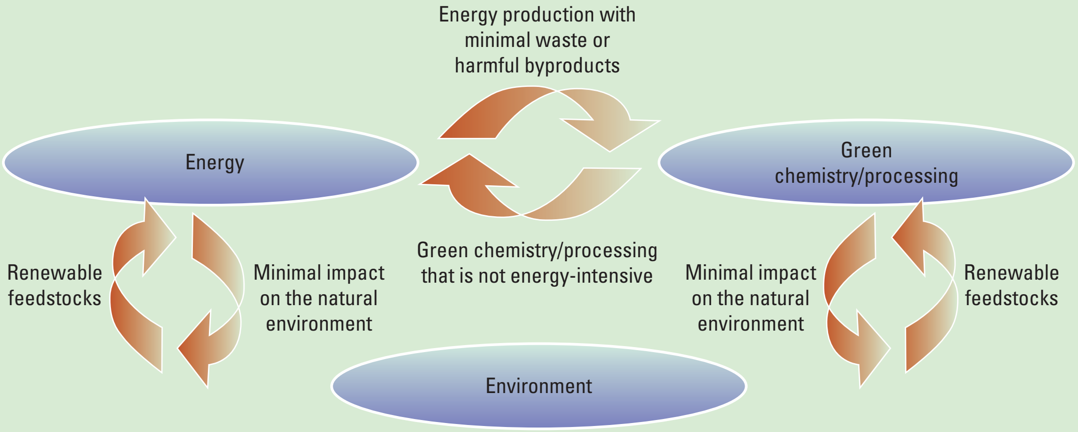
Research in environmental molecular science

Grand challenge and the need to change. Research in energy production and strategies for minimizing waste in chemical processing all revolve around the environmental impact of these processes (see Figure 3). The environment is a complex system. One of the greatest challenges in fully understanding the environment and environmental consequences of human activity comes from the molecular complexity of the natural and human-impacted environment (*8*, *9*). Chemists must ask: given the level of complexity, can we identify the main contributors to a complex system? Knowledge of the contributors will at least help chemists begin to better understand the

FIGURE 3

Sustainable chemistry and the environment

Chemistry advances in sustainability research address the importance of the environment. Understanding the natural and human-impacted environment on a molecular level is another key component of sustainability research.



system and also, just as importantly, help chemists form useful questions about what they do not understand. Second, chemists must find useful strategies for cleaning the environment. A sustainable society needs technologies to recycle and safely degrade pollutants, safely entrain radioactive waste, and provide clean water globally, as well as strategies for advancing our understanding of chemical processes in natural and engineered waters.

Chemists will need to understand reactive transport that involves different environmental compartments (atmosphere, soil, water), different actors (microbial, physical, chemical), and different—sometimes vastly different—timescales. Progress in chemical characterization must continue, and chemists need new approaches for understanding the most significant variables. Perhaps chemists will require a new combinatorial approach for evaluating effects of many variables, to complement "one-at-a-time" mechanistic studies.

The role of chemistry and advances needed. Recent advances in chemistry allow a more detailed molecular and elemental understanding of the components of air, water, and soil. For example, a molecular-level understanding of dissolved organic matter in aqueous systems is beginning to emerge, and recent analytical techniques allow chemists to measure the size and chemical composition of individual atmospheric particles that are known to play a role in health and climate. Scientists now have a molecular-level understanding of the important chemical reactions that take place on polar stratospheric clouds during ozone depletion. These advances have increased our understanding of the earth's systems.

An integral part of sustainable chemistry is the prediction of how chemical components interact with and affect the biospheres and ecospheres. A proactive approach to this goal requires fundamental advances in understanding the structure and reactivity of the complex chemical matrices responsible for transformation and phase-change reactions occurring in the natural environment, and consideration of the coupled effects of atmospheric, aqueous, soil, and biochemical processes. However, despite recent advances, our understanding of the impact of humans on the environment is clearly still limited.

Some of the most pressing new environmental challenges come from increasing CO_2 levels in the atmosphere. Chemists need a better understanding of ways to sequester CO_2, convert it to useful chemical building blocks, and minimize its unwanted production in chemical processes. In general, chemists will need to predict the potential for dangerous accumulations of harmful compounds such as CO_2 in a proactive way.

Education

Grand challenge and the need for change. Many chemists are working in the areas of energy, green chemistry and processing, and environment, and most chemists would recognize the concept of sustainability in chemistry as something important. However, most chemistry educators do not include these concepts in the classroom. To create a citizenry that is competent to make technical judgments, our society needs to teach sustainability issues throughout the education system. Universities will need to incorporate concepts of green chemistry in the undergraduate curriculum. The University of Oregon is a good example of an existing undergraduate program that involves green chemistry.

The role of chemistry and advances needed. Chemists working in sustainable chemistry need to educate the industrial and academic communities and convince them of the importance of addressing sustainability. Chemists working in sustainable chemistry must help chemistry students understand sustainability concepts so that the future workforce will see sustainability as a necessary issue in process development. The public must see the importance and urgency of sustainability in chemically related areas (the biggest of which is energy consumption). To accomplish these aims, the chemistry community should take several steps in the teaching of sustainability issues. Advances needed to create a sustainable world will involve workforce training, public education, and global involvement.

Research in enabling areas and technologies

Several areas will be key in advancing the sustainability research themes of energy, green chemistry and processing, and environment. Enabling research areas and technologies include nanoscience, bioprocesses, catalysis, measurement science, and cyberscience. How these enabling areas provide the science and technology innovations required for the different sustainability research areas is discussed below.

Nanoscience. Nanoscience is a means of discovering new materials for sustainability research that offers some of the most exciting possibilities. Nanomaterials often yield new properties (e.g., efficient multiple-exciton generation) that can be exploited for applications in sustainability. Tunability is an important property of nanomaterials. Optical, electrical, toxicological, and magnetic properties of nanomaterials can now be tuned by controlling their size, phase, shape, and surface properties. Other important attributes of nanomaterials include large surface areas that can be functionalized at the molecular level, new combinations of photon penetration depth with modified carrier diffusion lengths, improved light harvesting, and band-gap manipulation. Suspensions or thin films of the nanomaterials can be made transparent to visible light, inhibiting light scattering and allowing more efficient phototransformations. This research could improve photochemistry useful for sustainability research—for example, can solids, dispersed as nanoparticles, be used for more efficient photochemistry? Opportunities exist for researchers to further explore the interface of biology with nanomaterials and thereby develop rules for compatibility or structure–property relationships, or both.

The use of porous nanomaterials as "solid-solvent" cages in chemical synthesis could reduce the massive amounts of solvent that are currently consumed and may help identify "green" scalable synthetic methods. Chemists could design materials on the nanoscale for rapid disassembly. Can we fabricate semiconductor devices that disintegrate? Can we harness self-assembly and use those devices to enable disassembly? Can methods be found for element recovery and recycling through assembly and disassembly? All of these questions represent interesting and exciting opportunities raised by the potential of nanoscience.

Bioprocesses. Recent key advances in bioprocesses have contributed to chemistry advances in sustainability. Bioprocesses try to mimic or even use environmental materials to increase efficiency and decrease hazardous waste in the chemical process. The genome sequence explosion has increased knowledge about bioprocesses. That knowledge is helping in the application of nanoscience. Plants are known to synthesize nanoparticles, and the process can be controlled by genetic manipulations.

Bioprocesses offer the chance to change from a petroleum feedstock source to a renewable stream (*10*). The challenge is to identify bioprocess routes to new chemical building blocks on a much shorter timescale. A fast screening approach would facilitate progress in exploring a broad range of new methods for identifying chemical building blocks.

New bioprocess discoveries are now being exploited by industry. The establishment of commercial plants that produce 1,3-propanediol and polylactic acid has shown that biorenewable materials can be manufactured on an economically competitive basis. Recent research has shown that certain bacteria grow conductive wires that can be connected to external conductors for use as fuel cells and has demonstrated the feasibility of an integrated biorefinery.

Catalysis. Today, challenges exist in creating alternative fuels, reducing harmful byproducts in manufacturing, cleaning up the environment and preventing future pollution, dealing with the causes of global warming, protecting citizens from the release of toxic substances and infectious agents, and creating safe pharmaceuticals. Catalysts increase the rate of a desirable chemical reaction and are needed to meet these challenges, but their complexity and diversity demand a revolution in the way catalysts are designed and used. Challenges to catalysis research include discovering materials that harvest, store, and use energy and can effectively be used to clean water, air, and soil.

Measurement science. Chemistry relevant to sustainability issues often takes place in very complex environments. A necessary and promising area of enabling research involves process-measurement science. In particular, process measurement may help improve the efficiency of chemical reactions and avoid the production of waste byproducts by carefully monitoring reaction products. Advances in measurement science have driven many recent advances in the energy field. For example, improvements in our ability to characterize a material structurally, both in the laboratory and under conditions relevant to its use, whether in catalysis, in a lithium battery, or in a fuel cell, have arisen from advances in measurement science. The chemical and molecular nature of the natural and human-impacted environment also need to be accounted for. This entails detailed measurements of soil, water, and air.

For each of the sustainability research themes—energy, green chemistry and processing, and environment—the ability must be developed to make measurements in a multidimensional parameter space that includes varying timescales, length scales, chemical resolution, concentration resolution, and surface versus subsurface versus bulk measurements. Furthermore, these measurements need to be made under what have been termed operando conditions, as in situ, or field, measurements. These terms can be summed up as "point-of-use" measurements.

Cyberscience. Sustainability science, as well as the chemistry that will lead to a sustainable earth, is both data-intensive and data-driven. Sustainability research now produces such massive amounts of data that a new infrastructure must manage data, promote access to data, and encourage further discovery and strategies for acute and long-term problem solving related to energy, green processing, and environmental chemistry. Advanced tools for cyber-enabled chemistry will lead to better and more efficient data management, mining, capture, processing, and presentation.

Advanced cyberscience enhances understanding of chemical kinetics from the molecular to the field scale and addresses the immense timescales of geological (and hence geochemical) processes. Advanced cyberscience should also aid in the design and discovery of catalysts for alternative fuels and help reduce energy consumption in many industrial processes. All these data-intensive (and necessary) undertakings will accelerate with the proper investment in cyberscience and cyberinfrastructure.

In addition, advanced capabilities in high-end simulations have been key for several developments. Theory and computer simulations of processes at the molecular scale, as well as the ability to link simulations across multiple length scales and timescales, are emerging as essential partners with experiment in enabling understanding and design of materials and devices. For instance, simulation and experiment have successfully partnered in the design of lithium-battery electrode materials (*11*), and simulation has provided valuable guidance in the selection of catalysts for nitrogen activation (*12*). Although these examples illustrate creative applications of tools available today, methodological advances are needed to address chemical and materials challenges associated with energy, green chemistry, and environmental problems.

Future challenges and needs

Issues related to sustainability are vast and complex, and many individuals in a wide range of technical fields will ultimately need to work together to tackle them. Furthermore, complex economic, political, and human-dimension aspects need to be addressed (*13*). Basic research in science and engineering, in general—and, in some cases, chemistry, in particular—can play a pivotal role in driving the science and technology innovations needed to achieve a sustainable future. Initiatives in chemistry-related sustainability issues already exist—for example, the Green Chemistry Institute of the American Chemical Society (*14*), the European Technology Platform for Sustainable Chemistry (SusChem; *15*), and the International Union of Pure and Applied Chemistry's green chemistry initiative (*16*). A goal of this article is to inspire even more chemists to take on sustainability challenges, questions, and issues and to make advances that will positively impact society and influence fields that include pharmaceuticals, biomaterials, and agrochemicals. Because it is ultimately up to the public to support these initiatives and changes, it is important to remember that education on all levels is essential for creating a sustainable society. Many problems in sustainability are molecular in nature; therefore, chemists can play an important role in both sustainability research and education.

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