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Sustainable Chemistry: A Future Guiding Principle

Klaus Kümmerer*



Klaus Kümmerer
 Professor of Sustainable Chemistry
 and Material Resources
 Director, Institute of Sustainable
 and Environmental Chemistry
 Scientific Director, Research Hub,
 International Sustainable Chem-
 istry Collaborative Centre (ISC3)
 Leuphana University of Lüneburg

The discovery of a glacier mummy (the iceman “Oezi”) with a copper axe showed us that humankind converted considerable amounts of chemical substances into new ones already in the prehistoric and pre-fossil ages. The use of this new material had significant impact on society, culture, and trading. More than 150 years ago, the ever-increasing creation and usage of new chemicals and materials with rapidly growing diversity and quantity began. Right from the start of this revolution, its downside was the pollution of the environment, as well as health issues and other threats. Today this is an increasing global issue that results from the intended use of specific products. The technical and economical limits of product-integrated environment protection, effluent treatment, as well as the limits of ecosystems and risk assessment are increasingly visible. However, it is becoming even more apparent that limitations in terms of the availability of resources are also a consequence of the success of chemical science and chemical industries.

Chemistry is currently faced with one of the biggest challenges in its history. The main reaction to this is a search for how new resources can be utilized in the synthesis of (new) compounds. Another important approach in this context is green chemistry. However, some important questions still remain: Can you already classify a product as green if

just one of the Twelve Principles (Table 1) is fulfilled, for example, by using renewable feedstocks? Or must all Twelve Principles be fulfilled? How should they be weighted against each other? And what if a chemical or material meets all the Twelve Principles but is simply not needed?

Table 1: The Twelve Principles of Green Chemistry.^[a]

1	Prevent waste
2	Atom economy
3	Less hazardous chemical syntheses
4	Designing safer chemicals
5	Safer solvents and auxiliaries
6	Design for energy efficiency
7	Use of renewable feedstocks
8	Reduce derivatives
9	Catalysis
10	Design for degradation
11	Real-time analysis for pollution prevention
12	Inherently safer chemistry for accident prevention

[a] See P. T. Anastas, J. C. Warner, *Green Chemistry: Theory and Practice*, Oxford University Press, New York, 1998.

The increasing use of biomass and other resources for materials (e.g., palm oil, metals) and energetic purposes (e.g., bioethanol, biodiesel, or electronics) often result in tremendous negative economical, ecological, social, and political consequences. The amounts needed for a complete bioeconomy or *Energiewende* (energy revolution) at the present level of product and energy consumption will most likely not be available.

The application of composite materials should, for example, contribute to reducing the fuel consumption and related CO₂ emissions of cars. However,

wouldn't the energy demand thereby just be transferred to other sectors such as the provision of resources or recycling? Shouldn't we first reflect on mobility and then ask what and how chemistry could contribute in a sustainable manner?

Chemical substances have to be synthesized and purified in expensive procedures before they can be used for the manufacture of advanced materials and products. In order to generate the desired product properties, the manufacturing process itself, however, often involves dilution or mixing at the atomic or molecular level, that is, the deliberate contamination of the chemicals that have already been purified in a high-energy process. In many cases, and at the latest at the end of the lifecycle of a product, additional mixing of chemical products takes place. Before or during recycling, extensive efforts are then needed to again separate the constituents, regain them, and purify them again, if at all possible. The diversity of constituents and building blocks on the atomic and molecular levels is increasing, as is the diversity and amount of the materials resulting from their combinations. This complicates recycling or even renders it impossible.

According to the First Law of Thermodynamics, we won't win anything in the long run. We can only break even. The Second Law says that only under perfect conditions we won't lose anything. The Third Law says that we will never reach perfect conditions. In other words, we cannot completely avoid losses. Ther-

[*] Prof. Dr. K. Kümmerer
 Institut für Nachhaltige Chemie
 und Umweltchemie
 and International Sustainable Chemistry
 Collaboration Centre
 Leuphana Universität Lüneburg
 Universitätsallee 1 C.13 (Germany)
 E-mail: Klaus.Kuemmerer@uni-
 leuphana.de

thermodynamics also tells us that the less we want to lose, the more energy we have to invest, and that more entropy will occur elsewhere. If we had endless energy we would also generate endless entropy. Therefore, upcycling, infinite recycling, or a circular economy without unwanted effects will not be possible.

An increase of entropy does not only result in an increase of energy that we cannot use, but also in an increase in the dissipative loss of useful materials, such as the presence of metals in waste and in low concentrations nearly everywhere in the environment. The same holds for organic chemicals, such as persistent organic pollutants (POPs) and micropollutants, and materials such as plastics in the aquatic environment.

However, if we act wisely, we can reduce the losses to the lowest possible level. For this purpose, substance, material, and product flows should be as homogeneous as possible, and should also be of low spatial and temporal scales and with low dynamics. The more heterogeneous such flows are, the more energy and technological processes are needed to separate the components again. New products generally contain more new components than older ones. If innovation cycles are becoming shorter, or the concentrations or total amounts of specific constituents are too low, it becomes increasingly challenging to adapt or develop appropriate treatment and recycling technologies.

All stakeholders, and especially chemists, should therefore initially ask themselves if nonchemical alternatives for a specifically required function or service are possible and if they are more sustainable. Only if a thorough analysis shows that a chemical solution will be needed, should we then assess which chemical product can deliver the required function and service in the most sustainable manner over its entire lifecycle in the given context. Reduction as a goal for chemical products is a guarantee the sustainable use of resources, technology, and products and is a recipe for the safe future of chemistry.

This new self-understanding is a hallmark of a sustainable chemistry and key

to a true sustainable contribution of chemistry to the challenges ahead, thereby securing its own future viability. At the same time, it is the biggest challenge, as our self-understanding as chemists is based on the creation of ever-new chemicals and materials.

Chemistry is sustainable if it contributes in a sustainable manner to sustainability. A more precise definition of sustainable chemistry is not possible. Chemistry and its products are so manifold and diverse that a specific facet will either not be met at all, or not correctly, or only incompletely. Sustainable chemistry is simultaneously both a path and a goal. It is not a new subdiscipline of chemistry, but a guiding principle. In May 2016, sustainable chemistry was acknowledged by the UN as one of the most important approaches for sound chemicals management. Accordingly, the UN asked the member states to explore the opportunities provided by sustainable chemistry. However, sustainable chemistry is much more.

Sustainable chemistry starts from the function and service that is needed in a specific context, for example, mobility or housing. It then uses the knowledge of all chemical subdisciplines along the entire lifecycles of chemical products, goes far beyond the operational supply and value chains, and takes into account all stakeholders and their interactions. This extended view of sustainable chemistry focuses on service (“chemistry for what and for whom”) as the basis of added value rather than focusing on a specific compound or product. Examples include consulting based on the above-mentioned broader understanding of chemistry, data management, and provision of (specific) knowledge, chemical leasing (where customers pay in terms of what is achieved by the chemical product, rather than for the products themselves, the company delivering the chemical product is still the owner and takes it back after it is not needed anymore. Sustainable chemistry offers many opportunities for new businesses as well as advantages for manufacturers. For instance, an investment in facilities for production expansion may no longer be needed, or the need and therefore dependence on raw materials can be

reduced thanks to chemical leasing, consulting, or digitalization. If a manufacturer wants to take back their products at the end of their lifecycle, they will design them accordingly to allow for an effective and efficient recollection, dismantling, recycling, or further use (including the component parts) with a minimal energy consumption. This also results in better access to resources and additional know-how.

Adaptation of reactivity and lifetimes to usage and fate of chemicals, materials, and products along the different stages of their lifecycles is therefore also part of sustainable chemistry. Longevity and durability of products or the high stability of chemicals might be recommendable in some cases, however in a different context, it is not sustainable (for example POPs, aquatic and atmospheric micropollutants, and plastics in the oceans). Therefore it will be advantageous to plan reactivity, kinetics, and thermodynamics along all stages of the lifecycle of a product and to design them accordingly on all levels: At which points of its lifecycle and to which extend should a molecule or material be (or not be) reactive? What are the relevant timescales? Sustainable chemistry is the chemistry of the future, and is therefore not just the science and industry of creating and manufacturing even more new molecules, materials, and other products, but it is also the science and technology behind the design for sustainable disassembling (retrosynthesis, retroengineering), or complete natural degradation at the end of the product life. It is thus essential for the design of substance, material, and product flows of reduced quantity, diversity, and dynamics. Only chemists can achieve this goal, which requires all their knowledge and creativity.

Sustainable chemistry is the timely and unique opportunity for a new success story of chemistry in a postfossil and sustainable new world. For its successful and global implementation, all stakeholders need to contribute: enterprises of all sizes, the users of the chemical products, authorities, civil society, but most importantly well-educated chemists who can develop inspiring ideas to meet the challenges of the future.