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## The periodic table of the elements of green and sustainable chemistry

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Achieving a sustainable future will only be possible through the intersection of the best science and technology in combination with the societal, economic, policy, cultural, moral, and ethical ecosystem. Green chemistry and green engineering provide the scientific and technological foundation of the elements of green and sustainable chemistry while the other elements, relating to humanitarian aims, enabling system conditions, and noble goals, provide the imperative context. This alternative periodic table, strives to outline the range of aspects and tools that are available and needed to accomplish the daunting and necessary tasks of moving toward a sustainable tomorrow.

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### 1. Introduction

Without the innovations of chemistry, sustainable development will be impossible to achieve. If the chemistry that humans use to pursue these innovations continues to be, itself, unsustainable, sustainable development will be equally impossible, particularly as global population, and subsequently societal needs, continues to increase. It is only through the combination of chemical innovations conducted in a sustainable way that progress toward the sustainable development goals (SDGs)<sup>1</sup> can be achieved. Green chemistry has often been known as “the chemistry of sustainability”.<sup>2–4</sup> Sustainable chemistry is a term of more recent vintage that, in its most genuine usage, refers to a broader ecosystem beyond the science that includes education, economics, policies, management and other efforts that enable the science to be implemented and make a positive impact.<sup>5</sup> In this paper, we attempt to lay out a cohesive framework, “the periodic table of the elements of green and sustainable chemistry” (Fig. 1) that elucidates the various figurative aspects of the efforts to pursue chemistry that is directionally and qualitatively consistent with the pursuit of sustainability goals.

The tabular presentation of a complex topic is more than a familiar format for chemists during the sesquicentennial of Mendeleev’s original publication. The metaphor of the

elements and their relationship to molecules and materials is particularly appropriate when recognizing that just as elements can have multiple valence states and bonding can involve non-obvious molecular orbital interactions; so can the nature and interactions between these figurative elements of green and sustainable chemistry be complex and non-intuitive.

At the “heart” of this table are the “scientific and technological elements” which consist of the principles of green chemistry and green engineering;<sup>6,7</sup> a reflection of the fact that the fundamental science is at the heart of the chemical enterprise.<sup>8</sup> However, knowing that the science and engineering cannot operate alone, the area where the Main Group Elements would mostly reside are the conceptual frameworks and the economic and policy drivers that enable the greater enterprise. The group to the far left of the table are the “humanitarian elements” that emphasize the role that chemistry plays in meeting the essential needs of humanity and the biosphere. The group at the rightmost side of the table comprises the “noble elements” that identify the noble and aspirational elements of a vision of a sustainable civilization.

The table is meant to be an inclusive enumeration of the tools, strategies, efforts, and goals of chemistry and its enabling interconnections that work toward achieving a more sustainable civilization. Just as new elements have been discovered throughout the past 150 years, this table too will hopefully evolve and grow adding new dimensions and new possibilities.

### 2. Humanitarian

The UN Global Chemicals Outlook<sup>9</sup> predicts that the value of the chemical industry will double from US\$5 trillion by 2030. This will bring benefits as chemical technologies are used to

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wellness. Chemistry can be designed to ensure that the nature of the material and energy basis of our society not merely accomplishes the goals of addressing problems after the fact but to avoid the problems and promote wellness by design.

### 2.3 11, access to safe and reliable water (SW)

One of the essential materials of life is water and access to it for drinking, sanitation, and hygiene is necessary for life, health, and well-being.<sup>14</sup> Chemistry has been critical in historical approaches to water disinfection and improving water quality from removal of harmful contaminants to addressing odor and taste concerns. Chemistry will be required to realize the future methods, process, and materials that enable healthful drinking water without the unintended consequences of harmful disinfection by-products. Equally important is the imperative of sanitation to avoid the spread of disease by exposure to pathogens. These services must be supplied in ways that are mindful of equity, safety, and dignity.<sup>15,16</sup> The water infrastructure and treatment needed to enable adequate potable (and non-potable) water will be dependent on chemicals and chemistry to ensure appropriate water quantity and quality for the intended use, be it drinking, sanitation, hygiene or another use.

### 2.4 19, chemistry for benign food production and nutrition (Bf)

While the great increases in the efficiency of food production have been astounding and life-saving, there have been unintended consequences for the over-use of fertilizers and the use of pesticides and herbicides that harm beneficial insects and plants and damage the ecosystem.<sup>17</sup>

Chemical alternatives, as well as non-chemical alternatives, are being developed and need to be implemented at scale. These range from targeted bio-pesticides<sup>18</sup> to herbicides that focus on specific pests and plants<sup>19</sup> to pesticides designed to degrade rapidly into non-toxic degradation products.<sup>20</sup> Integrated pest management systems have been shown to be efficacious and economically practical without the environmental damage.<sup>21</sup>

There is also significant and ongoing progress towards alternative protein and nutrition sources ranging from plant-based “meats”<sup>22</sup> to insect-derived products<sup>23</sup> to algal based foodstuffs.<sup>24</sup> Efforts to enhance the nutritional value of food, rather than emphasis on calories, will continue to make significant contributions towards the implementation of chemistry to provide more optimal food sources with lower environmental impact.

### 2.5 37, ensure environmental justice, security, and equitable opportunities (J)

Proximity to chemical manufacturing, processing and use has historically come with disproportionate risk to the surrounding communities and ecosystems;<sup>25</sup> this includes the exportation of banned chemicals and hazardous waste to communities with few other economic opportunities.<sup>26</sup>

Individuals should have the right to live in homes and communities that are not placed at increased risk due to

transport or production of chemicals or inadequate protection of facilities. Use of highly hazardous chemicals increases vulnerability to accidents, natural disasters, or intentional acts of violence and terror. Adopting chemistries that are inherently benign is the most effective means of ensuring that communities are not placed at undue risk from the chemical enterprise. Case studies have shown that there are safer alternatives to toxic gases, VOCs, pesticides, and cleaning chemicals implicated in previous incidents.<sup>27</sup>

There should be no disadvantageous circumstances for individuals or communities living or working near chemical facilities. This is inclusive of legal emissions as well as unintentional chemical releases. Through the development of green and sustainable chemistry as well as community engagement, the historic adverse impacts of the chemical enterprise can instead provide desirable economic and safe opportunities in communities that have tended to be predominantly underserved and disenfranchised.

### 2.6 55, chemistry to preserve natural carbon and other biogeochemical cycles (Pc)

The integrated systems that are the basis of the planet's natural biogeochemical cycles, from carbon to nitrogen to water and beyond, are chemical cycles and chemical processes that are impacted by the human interferences and interactions with these cycles.<sup>28</sup> Human chemistry must be designed such that there will be no perturbation of the natural biogeochemical cycles and their interlinkages. Through thoughtful consideration of human material and energy utilization, there can be a preservation of the critical natural cycles essential to the preservation of life and all of its diversity on the planet.

### 2.7 73, no chemicals of war or oppression (Wo)

The history of the intentional use of weaponized chemicals is recognized as uncivilized and the continuation of the universal rejection of this practice is essential to a civilized society.<sup>29</sup> Likewise, the use of chemicals for carrying out the death penalty or for the oppression of individuals through chemical lobotomies or chemical castration must not happen. Designing, making, and utilizing chemicals for the purpose of mental or physical control over individuals is inconsistent with the peaceful uses of chemistry.

### 2.8 4, design to avoid dependency (Dd)

Some molecules can be addictive to humans. They can result in physical and neurological changes that result in dependency and its resulting impairment. Chemists have the duty to work at the highest levels on knowledge and awareness of the mechanisms of dependency in order to ensure that the molecules that are created do not result in human dependency and addiction.

Economic dependency is a separate yet important issue. Molecules should not be designed to be essential and inseparable to livelihood and wellness and embedded in systems

that provide critical items like food, clean water, and medicine.

Chemical dependency is not limited to the human species but rather can also impact other living things both animal and plant. Dependency needs to be understood such that design for variety and resilience is pursued preferably.

### 2.9 12, ensure access to material resources for future generations (Fg)

The basic elements will largely not be created nor destroyed – with the exception of radioactive decay and escape of helium from our atmosphere. However, the ability to access resources that are fundamental to the chemical and material infrastructure of our society and economy can be greatly impacted and diminished through irresponsible use. The combustion of valuable fossil fuels, the dissipation of phosphorus, and the diffusion of rare earth elements will make the resource base of the future more difficult to access for future generations.

### 2.10 20, transparency for chemical communication (Tc)

The potential benefits and the potential harms that can be provided by chemistry are too immense and powerful to be cloaked in the darkness of jargon. Yet, as chemistry continues to evolve and become more sophisticated, the opacity of the science to the general public increases as well. The responsibility of molecular scientists – and scientists generally – is not merely to discover, invent, and understand, but rather to effectively convey that understanding as clearly and transparently as possible.<sup>30</sup> To be clear, this is not the same as ‘as clearly and transparently as convenient’. The task of communication is not a secondary task but rather one of equal status in the scientific pursuit.

The lack of value placed on communication has resulted in alienation of the public from science and fear by the public of science.<sup>31</sup> The failure of scientists to effectively communicate has historically not merely damaged the scientific endeavor, it allows for anti-scientific rhetoric to fill the communication void. Of equal importance is the need for chemists to take an active role in raising awareness and providing education and training to enhance the benefits of this clear communication being received by an informed and increasingly sophisticated audience. The practice of green and sustainable chemistry depends on training at all levels, from K-12 to university and professional. Beyond the technical competency in chemistry required to maintain continuous innovation, it will be important to push at the conventional boundaries of the discipline. Educators can bridge core chemistry concepts with elements of green engineering, industrial ecology, toxicology, bioethics, public policy and other adjacent fields so that students will be well equipped for systems thinking as well as lifecycle, circular or cyclical strategies for chemical design.

### 2.11 38, chemistry for sustainable building and buildings (Cs)

The structures that are used to house people and their activities should be designed, constructed, and maintained to provide resilient protection while being conducive to health

and wellness of the occupants and the surrounding ecosystems. From the molecular basis of the materials throughout their life cycle to the systems to provide the requisite water, climate control, and lighting, chemistry has a significant role to play in efficiently providing safe indoor environments for humans and their activities while considering the surrounding landscape. Further, buildings can be designed to be modular providing for future adaptations, deconstruction and reuse to avoid end of life material waste.

Provision of shelter depends on a wide range of chemistries including composition of structural and insulating materials, components of electrical and lighting technology, heating and cooling systems, water handling, and integration of buildings with the surrounding landscape. These services must be provided without damaging human health or environmental systems. For example, chemistry has a role to play in minimizing the climate impacts of concrete production, which account for as much of 5% of current global emissions.<sup>32</sup> Building materials and furniture should be designed to prevent chronic exposure to harmful chemicals, as has been experienced in formaldehyde-based resins and other releases of volatiles leading to “sick building syndrome”.<sup>33</sup>

### 2.12 56, an individual’s molecular code belongs to that individual (Ic)

Every individual possesses the unique molecular code that is the underlying basis of their individuality and their identity. Further, this code has the power and potential for understanding health and wellness in a fundamental way, at the molecular scale.<sup>34</sup> While this molecular code may contain information and functionality that can result in value, every individual is sovereign over their code and this sovereignty cannot be taken from them by others. As the ability to understand, manipulate, and utilize the various levels of this biological code increases, it will be ever more essential to guarantee that control of this code remains with the individual.

### 2.13 74, molecular codes of nature belong to the world (Nc)

No human wrote any of the genetic codes of Nature and no human or group of humans can own it. Humans played no role in the billions of years of the design of genomes, bio/geo material structure, natural transformations and self-assembly. The inventions of Nature belong to Nature. The codes of Nature belong to Nature. The act of a human recognizing its brilliance and deeming it a discovery is not justification to claiming ownership and control and in any way limiting access to this brilliance by everyone.<sup>35</sup>

### 2.14 Green chemistry and green engineering

In this section we group the principles of green chemistry and green engineering according to desirable environmental outcomes. It is important to consider that any individual technology or strategy should be used thoughtfully in the context of the broader lifecycle of a chemical, chemical process, or final product. The subsequent grouping of enabling systems conditions includes discussion of metrics and tools that can be

used to prioritize “green” strategies and minimize the potential for environmental tradeoffs.

### 3. Prevent waste

Regardless of its nature, waste consumes resources, time, effort, and money both when it is created and then when it is handled and managed at end of life, with hazardous waste requiring even greater investments for monitoring and control.<sup>36</sup> As has been stated on numerous occasions, creating, handling, storing, and disposing of waste is necessarily an expense and does not add value in terms of innovation or performance. In processes of production, therefore, waste is always undesirable in all its forms.

Ideally, molecules, products, processes and systems would be designed to not create waste. That is, we should aim to eliminate the concept of waste by designing the outputs to be feedstocks elsewhere mimicking natural systems. Whether the waste is material, energy, space, time or the derivative of all of these, money, there are design strategies that can and are being implemented in green chemistry and engineering to eliminate the concept of waste.

#### 3.1 21, waste material utilization and valorization (Wu)

Waste is a human-centered concept. In Nature there is, for all practical purposes, no waste. In Nature, organisms and geosystems evolve to utilize the “waste” of one process to nourish, sustain, and strengthen another. While the history of human-designed chemical systems has been linear (*e.g.*, take-make-waste), there is a recognition that genuine elegance requires the building of circular systems where materials and energy flow in cycles as they do in Nature. This would require the developing the tools, techniques, and approaches for “designing waste” such that the “waste” itself is considered an additional product of the system.

These approaches of chemical waste valorization have found large-scale application in a variety of settings from individual product manufacturing processes to entire mega-scale factories to urban and regional networks.<sup>37</sup> Transforming waste into a value-added product is a science in its infancy and it will need to develop considerably in sophistication and scale in order to displace the wasteful linear processes that have historically dominated.

#### 3.2 39, “one-pot” synthesis (Op)

When chemical transformations have taken place historically, they have often required many steps, especially for complex molecules such as those in the field of pharmaceuticals. Each time there is a multi-step synthesis, there is the need for separation, isolation, and purification that results in loss of material, increased energy usage, and time lost.<sup>38</sup> “One-pot” synthesis, by contrast, refers to transformations carried out in a single reaction vessel without isolation. Designing a process this way result in significant efficiencies and waste reduction.<sup>38</sup> The challenge is to avoid tradeoffs such as

increased usage of toxic substances or decreased product quality. When done correctly, decreased steps and decreased reaction vessels can provide significant benefits.

#### 3.3 57, process intensification (Pi)

Traditional methods of chemical manufacture have intrinsic inefficiencies that result in wastes of materials, energy, time, and space. This occurs when an overall process is split into large numbers of ‘unit processes’ of reaction, separation, and purification. When these steps can be combined the benefits are not only waste reduction but also lower capital and operating costs and increased inherent safety. The concept of having small continuous-flow ‘reactors’ that can achieve scale-out by increasing the number, so-called “numbering up”, can have advantages over traditional “scaling up” of bulk processes.<sup>39,40</sup> Microreactor technology aids in multicomponent reactions, or reaction telescoping, in which multiple chemical steps may be carried out within a single reactor network.<sup>41</sup>

#### 3.4 57, self-separation (Ss)

The chemicals and materials enterprise is one of the great consumers of energy in industry. One very large piece of this energy consumption is the operation of separations.<sup>42</sup> Separations includes many elements of isolation, purification, and some kinds of cleaning. In addition to the energy that is input into the traditional separation systems, the embedded energy that is contained within the solvents that have often been used in separation systems is also very significant.

The development of systems that can be designed to facilitate “self-separation” can decrease energy and material usage when done properly.<sup>43</sup> Designing a molecular product to separate from its reaction matrix or enabling an impurity generated in a process to self-separate due to intrinsic factors can have sustainability advantages.

## 4. Molecular transformation

The modern miracle of chemical enterprise is the ability to transform the materials that occur naturally in the world into new materials with new properties and performance that would not otherwise exist. History has shown there are thoughtful and wise ways to engage in molecular transformation and there are methods that are profoundly toxic, wasteful, and depleting. The new emerging synthetic methods that have been demonstrated in the field of green chemistry come from thoughtful life-cycle design and often use Nature and biological systems as an inspiration, mentor, and guide.<sup>44</sup> Through this type of thoughtful design, we move from a narrow definition of mere efficiency to one of holistic productivity.

#### 4.1 22, molecular self-assembly (Sa)

The process of intentional bond-making has been one of the most important accomplishments of chemistry.<sup>45</sup> Historically,

this process has often been forced through the use of energy or reactive reagents to occur at the time, place, and rate that is desired. The more complex the molecule, the more steps and energy that has often been employed.

Looking at natural and biological systems, there are many examples where complex molecules with extensive stereochemistry and intricate ring systems are realized through molecular self-assembly that takes place upon appropriate stimulus.<sup>46</sup> This can be achieved in human-designed synthesis as well. It is, of course, always important to not merely design a self-assembling molecule by shifting the energy and reagent inputs to another part of the product life-cycle such as its precursors.

#### 4.2 40, integrated processes (Ip)

Long chains of unit reaction processes can have significant disadvantages for energy and material waste due to the separation, isolation, and purification steps usually encountered after each step.<sup>47</sup> These separations are amongst the most energy-intensive aspects of a process. In addition, there are almost always material losses due to transfer between unit processes. By designing processes to be integrated to the highest feasible degree there can be significant advantages not only for energy and material efficiencies, but also for the time that is required to transfer between vessels and the reduced worker exposure that can be obtained.

Integrating not only individual processes, but numerous processes can also be valuable to accomplish goals such as utilization of waste heat/material from one process as a feedstock for another.

#### 4.3 58, additive synthesis (As)

In an addition reaction, all atoms of the reactants are incorporated into the final product whereas elimination and substitution reactions inherently generate waste as part of the nature of the reaction.<sup>48</sup> The use of addition reactions can allow for significant decreases in the waste generated intrinsic to the synthetic method. By building up a molecule atom by atom or fragment by fragment one uses only what is necessary to construct the target. Addition reactions must be used thoughtfully to avoid shifting the burden of waste from one step to another step or another part of a process. The additive concept translates beyond the molecular scale to materials and manufacturing applications where environmental benefits are similarly significant.<sup>49</sup>

#### 4.4 76, non-covalent derivatives/weak force transformation (W)

Chemists have spent more than two centuries pursuing mastery of bond-making, with great success. However, it is also true that Nature accomplishes much of its performance and functional modifications, not through covalent bonds but rather through weak-force interactions.<sup>50</sup> These weak forces engage at the time and place necessary to impart the properties temporally as needed. Weak forces are also used to guide synthetic pathways in Nature.

While humans have been increasingly aware of the essential importance of weak forces, there has not been the pursuit of mastering these powerful tools such that they can be used as design levers to create the kind of functionality that is desired.

## 5. Less hazardous synthesis

While efficiency has historically served as a proxy for sustainable practices in the chemical enterprise, it is imperative that the goal of reducing the quantity of material and energy consumed is closely coupled with considerations related to the nature of that material and energy. Using less may not have the beneficial effects of reducing the overall hazard of the synthetic process depending on the nature of the feedstocks, reagents, and auxiliary chemicals.<sup>51</sup> It is imperative that these inputs and outputs, in addition to the intended product, are as inherently benign as possible. Further, the conditions under which synthetic processes are carried out should also be considered when pursuing the goal of a more sustainable chemical enterprise.<sup>52</sup> This offers benefits from environmental and human health perspectives in addition to a reduction in vulnerability to chemical accidents and sabotage.<sup>27</sup>

#### 5.1 23, reduce use of hazardous materials (Ru)

The use of hazards – physical (*e.g.*, corrosivity, reactivity, explosivity flammability), toxicological (carcinogenicity, reproductive and developmental including endocrine disruption, neurological), or global (*e.g.*, ozone depletion, GHG's) – can be minimized or eliminated throughout the entire life-cycle of a chemical process.<sup>6</sup> Utilization of hazardous chemicals can be avoided through substitution of alternatives that have been designed for reduced hazard or, at a minimum, assessed and understood to have reduced hazard by comparison to what it is replacing.

Throughout processes, the feedstocks, reagents, solvents, catalysts and other substances can be replaced such that negative environmental and human health consequences can be minimized.

#### 5.2 41, *in situ* generation and consumption of hazardous materials (Gc)

Reactivity is an essential part of chemical transformations and is also closely associated with the hazardous nature of many substances. One strategy that can be employed to avoid exposures of workers or nearby communities to toxic/reactive reagents, is to generate and consume them in the processes without any significant accumulation of these substances.<sup>53</sup> Through '*in situ*' generation, the substance needs only to be generated in minuscule quantities for the short time it is needed before it is consumed that reaction.

#### 5.3 59, C–H bond functionalization (Ch)

Substitution and elimination reactions are inherently inefficient synthetic transformations at the molecular level. While these types of reaction provide access to countless molecules, they generate stoichiometric amounts of a "leaving group" that

must be separated and recovered or treated as waste. In organic chemistry, one of the most useful alternatives is catalytic C–H bond activation. Ongoing research is aimed at improving selectivity and performance of systems that enable C–H functionalization in a highly controlled manner.<sup>54</sup>

#### 5.4 77, inherent safety and security (Is)

Chemists and chemical engineers know the properties, structures, and conditions that underlie explosivity, flammability, and corrosivity. Designing molecules such they are not capable of ignition, combustion, or explosion is something that is within the skillset of chemistry today.

While safety has been a concern of the chemical enterprise for much of its history, this has often been accomplished through protection from the consequences of these physical hazards when they occur rather than through molecular design for reduction of intrinsic hazard.<sup>27</sup> These design tools can protect from accidents as well as terrorism and sabotage vulnerability.

## 6. Molecular design

The basis of our society and economy are synthetic chemicals and materials. While there have been significant advances in toxicology associated with identifying, and in some instances predicting, industrial chemicals that are likely to cause harm to human and ecosystem health, the gains in informing the *a priori* design of chemicals with reduced hazard to humans and the environment have been elusive.<sup>55</sup> To realize the goal of designing chemicals that are safe and functionally relevant, there is a need to create an interdisciplinary body of knowledge that sits at the nexus of computational chemistry, mechanistic toxicology, and big data analytics among others. It is only when we change the inherent nature of the chemicals and materials that are foundational to quality of life that we can truly advance towards a sustainable future that is no longer reliant on costly regulatory and technological controls of circumstances in which hazardous chemicals can be used and managed.

#### 6.1 24, design guidelines (Dg)

Design is intentional. If a chemical contains a hazard that is not intended, it is a design flaw. Yet, many of our made-made chemicals contain hazards to humans or the biosphere by accident or lack of thoughtful design.

As we understand the underlying basis of hazard to human health and the environment at the molecular level, we can design to avoid it. As we understand the properties which enable chemical accidents and other adverse consequences, we can and must design to avoid these outcomes where possible.<sup>56</sup>

#### 6.2 42, computational models (Cm)

With increasingly deeper molecular-level understanding of the nature of chemical hazard comes increased potential for the

use of computational models to assess, predict, and design out hazards from the chemicals we use and produce. The wide range of physical/chemical properties that are the underlying basis for toxic mechanisms of action, exposure pathways, transport and fate, *etc.*, can be evaluated *in silico* with greater accuracy and the insights derived from these evaluations can be used to avoid the adverse consequences that have marked the less-desirable aspects of the history of the chemical enterprise.<sup>57</sup>

#### 6.3 60, bioavailability/ADME (Ba)

At the foundation of protecting living things from toxicological impacts is the concept of ADME (absorption, distribution, metabolism, excretion). By understanding the molecular parameters that control the stages of ADME, substances can reduce a chemical's bioavailability—its ability to access a biological system. The insights from pharmaceutical research in trying to maximize bioavailability have provided intellectual tools that can be used in all aspects of the chemical enterprise in thoughtful design for hazard reduction.<sup>58</sup>

#### 6.4 78, high throughput screening (empirical/*in vivo*/*in vitro*) (Ts)

Empirical testing of the toxicity of a chemical is an essential part of the deep understanding of the potential consequences of a chemical. As we move away from animal testing due to ethical and financial drivers, the development of bioassays is increasingly important. The bioassays emerging not only cover a large number of biological processes and toxicological endpoints, but also can be done within a high throughput framework. Through these high-throughput screening assays, there can be extensive amounts of data generated providing insights into the concerns that may be associated with a chemical or alternatively, inform safer design of future chemicals.<sup>59</sup>

## 7. Solvents and auxiliary chemicals

The cost, environmental impact, and safety of a chemical process is often driven by the solvents and other auxiliary chemicals.<sup>60</sup> It is interesting to note that the amount of solvent and auxiliary chemicals used often exceeds raw materials, reagents, and products, particularly in the case of separation and purification processes.<sup>61</sup> Once again, while quantity of these chemicals it is an important consideration from a perspective of material and energy efficiency, it is the nature of our historic solvents that has posed the greatest challenge to the environment and human health. Conventional solvents have generally been volatile, increasing likely exposures; hydrophobic, serving as long term sources of concern in environmental systems; and toxic to ecosystems and humans, particularly a concern for chemical workers. Just as we are aspiring to design safer chemical products, the same effort and attention should applied to the design of safer solvents or solvent-free processes.<sup>62</sup> This can be accomplished by reducing inherent hazard as well as minimizing exposure potential.<sup>63,64</sup>

### 7.1 25, aqueous and biobased solvents (Aq)

Water is the original solvent: the solvent of life. And yet, the long history of the chemical enterprise largely eschewed water as a solvent. As petrochemical processes came to be dominant, it was considered to be logical that organic solvents would be most compatible with hydrocarbon-based transformations. Research launched in the 20th Century but accelerating in the 21st has shown that water can be not only a possible but also desirable solvent for many chemical processes where it was once thought not possible.<sup>65</sup> Water has been shown in cases to accelerate reaction rates, enhance selectivity, and bring benefits of non-toxicity, non-flammability, low cost, and ready availability in most instances. While there may be circumstances where water has environmental drawbacks, for example in energy requirements for recyclability, separation of products, or waste treatment, overall water can be a preferable solvent for many chemical processes.

Similarly, biomass shows increasing promise for replacing fossil resources in the production of solvents. Recently, bio-based derivatives have been either used directly as green solvents or as key precursors to innovative solvents that are potentially less toxic and more bio-compatible.<sup>66</sup>

### 7.2 43, ionic liquids/non-volatile solvents (Il)

When salts can be designed to perturb their crystal structure adequately such that they are a liquid at room temperature, they are known as room temperature ionic liquids (RT-IL). These liquids have been demonstrated to be effective solvents in a wide range of applications all while having negligible vapor pressure.<sup>67</sup> This is important as lack of vapor pressure avoids one of the most concerning routes of exposure for most volatile solvents, that of respiration. Another major concern with traditional solvents is their direct impact on the atmosphere, for example *via* photochemical processes. With RT-IL, this would be virtually impossible, however it should be recognized that indirect impacts from RT-IL raw materials or manufacturing processes could still be significant.<sup>68</sup>

While the lack of vapor pressure is an elegant attribute for this class of solvents, it is also critical that these solvents are designed for reduced toxicity as well.<sup>69</sup>

### 7.3 61, sub- and super-critical fluids (Sc)

There are compressible gases that at a certain temperature and under a certain pressure, collectively their critical point, become fluids that are neither gas nor liquid but rather a "supercritical fluid". These fluids have been known for centuries but ongoing research is creating new opportunities for their application as solvents.<sup>70</sup> Carbon dioxide is the most highly studied of these and has been demonstrated at large scale to be a useful solvent for everything from synthesis to extraction, cleaning, and analysis.<sup>71,72</sup>

The green advantages of these supercritical fluids are numerous including lack of toxicity for water and carbon dioxide, lack of flammability, tunability, and the possibility of 'infinite recycl-

ability' by cycling pressure. (Note: The use of carbon dioxide as a solvent does not require the generation of new CO<sub>2</sub> and therefore does not contribute to greenhouse gas emissions.)

### 7.4 79, "smart" solvents (obedient, tunable) (S)

The ability to make a solvent respond to stimuli and change its properties under new conditions can be extremely consequential. Historically, solvents were energy consuming because solubility was controlled almost exclusively through heating and cooling. With next generation solvents that have been demonstrated and developed, solvents can be controlled by factors such as pressure or pH.

These new so-called obedient solvents open up possibilities for niche and industrial uses that change the energy profiles for many chemical processes.<sup>73</sup>

## 8. Energy

The chemical sector consumes approximately 20% of total industrial energy consumption in the U.S., and contributes in similar proportions to U.S. greenhouse gas emissions.<sup>74</sup> Given the reliance on fossil fuel resources and the associated greenhouse gas emissions, there is a clear indication that, at a minimum, the chemical enterprise should strive to be as energy efficient as possible, normalizing to chemical function rather than mass in the assessment.<sup>75</sup> Gain in efficiency can be realized by considering both the quantity and quality of energy inputs as well as waste energy utilization. Of course, the chemical sector has a significant role to play in changing the nature of our energy feedstocks towards ones that are renewable, and developing materials that can enhance energy generation, storage, and transmission to enable the use of these renewable energy sources.<sup>76</sup>

### 8.1 26, energy and material efficient synthesis and processing (Ee)

Synthesizing, transforming, and manufacturing of raw materials into the desired chemical products requires the input of energy to drive the reaction. The form of this energy, in addition to the amount, has a significant impact of the environmental cost of carrying out the reaction. There have been recent advances to reduce the overall energy demand, and subsequent environmental and economic impacts, of chemical production by exploring different means of energy delivery including mechano-,<sup>77</sup> electro-,<sup>78</sup> photo-,<sup>79</sup> and electro-magnetic<sup>62</sup> chemical driven transformations.

The synthesis, transformation and manufacture of chemical products almost always involves separations in the form of removal of contaminants (purification), retrieving the desired molecules (isolation), removal of extraneous/undesirable materials (cleaning), or breaking a complex mixture into its components, including the removal of water (separations). While these operations have historically been extraordinarily material and energy intensive,<sup>42</sup> new approaches and new methods for the wide range of separations need to be devel-

oped and utilized to make these necessary processes more effective, efficient, and sustainable.

### 8.2 44, renewable/carbon-free energy inputs (R)

As long as the chemical enterprise is among the largest energy consumers of the economy, there is an imperative to ensure that the energy consumed is renewable and minimal-carbon. In the past this was often limited to fortuitous alignment of economic incentives with local resources, *e.g.* siting operations to take advantage of hydropower or geothermal energy. Now the options are becoming less geographically limited with solar and wind energy more plentiful and increasingly integrated with energy grids. There remain challenges in meeting the unique demands of chemical manufacturing processes. Renewable energy systems must be further improved to deliver the scale and quality needed for chemical processing, refining, and distillation.<sup>80</sup>

### 8.3 62, energy storage and transmission materials (Es)

Even the most sustainable and renewable sources of energy risk going to waste when not utilized immediately if there is not adequate ability to store or transport this energy. Physical, mechanical, chemical and other methods of energy storage and transmission will require the underlying materials to be benign and Earth abundant. Battery technologies, hydrogen storage, *etc.*, will only be as sustainable as the materials are throughout their life-cycles.<sup>81</sup>

### 8.4 80, waste energy utilization and valorization (V)

While much attention is often paid to the amount of waste materials that fill up landfills around the world or that make their way to become ocean contaminants, there is less attention to waste energy generation. Energy waste in the form of heat, light, vibration, noise, *etc.*, has a cost due to the impacts of energy generation for which there is no return as well as the impacts of the waste energy on the systems around it (*e.g.*, warming, wear and tear, mechanical erosion). The ability to capture this waste energy and find value-added uses is an important part of any design strategies for a sustainable product process, or system.<sup>82</sup>

## 9. Renewable feedstocks

Fossil fuel is the basis of the chemical, material and energy foundation of the global economy. Fossil fuel feedstocks are used to generate electricity, to produce transportation fuels, and to produce a wide range of consumer goods, such as plastics, healthcare and drug products, and agrichemicals. These reserves are finite and pose additional challenges related to geopolitics and physical accessibility.

Given this context, there has been emerging and important efforts to increase the use of biobased feedstocks for energy, chemicals, and materials production. Using renewable feedstocks from agricultural, forestry and aquatic resources, particularly nonfood, residues, and waste streams

from processing these materials, will be essential to developing changing the material and energy basis of our economy and society.<sup>83</sup> However, this must be implemented in a context of competition with food, land and water use, as well as benign and efficient downstream processing for recovery of the full value of the feedstock. This will require advances in our synthetic transformation portfolio and changes to our current chemical production infrastructure (*e.g.*, solvent selection, separation processes) while unlocking new functionality and performance from these feedstocks that is not available in petroleum-based inputs. Moving to renewable feedstocks is an imperative for the advancement of a more sustainable future.

### 9.1 27, integrated biorefinery (Ib)

While matter is neither created nor destroyed, the molecular conversion of natural resources through industrialized processes has the ability transform these resources from benefits into burdens. The conversion of energy dense hydrocarbons to heat-trapping greenhouse gasses is the most known example but the concept extends to water resources, mineral resources, biodiversity resources, water resources, soil resources, *etc.* In the absence of the ability to fully renew and restore, there can be no license for our chemical enterprise to access and transform the parts of the geosphere and biosphere that cannot be replaced.

Perhaps the most materially efficient technological process in history is the refinery. The modern petrochemical refinery has lessons for the bio-based chemical economy that has not reached the same level of efficiency. Being able to retrieve value from all extractable fractions from high volume low value to low volume high value in an integrated biorefinery will be an important piece of realizing the goal of a bio-based economy.<sup>84</sup> This effort requires not only advances in extraction through green solvents but the ability to tune the quality (*e.g.*, purity) of the extract, be it from lignocellulose,<sup>85</sup> agricultural or other waste streams,<sup>37</sup> algae biomass,<sup>86</sup> or other renewable sources.

### 9.2 45, carbon dioxide and other C1 feedstocks (C)

Carbon has been lusted over in its diamond form. Carbon has driven economies in its coal form. Carbon has emerged as a 21st Century energy source in its methane form. Carbon is essential to the biosphere and threatens climate stability in its carbon dioxide form. Carbon is deadly in its carbon monoxide form. The emergence of C1 chemistry is the essential manipulation of one-carbon building blocks to transform them from recalcitrant to useful, from destructive to value-adding, from challenge to an opportunity.<sup>87</sup>

Learning to sustainably access the promise of carbon dioxide and other C1 molecules as a feedstock is one of the great tasks of green and sustainable chemistry.<sup>88–90</sup>

### 9.3 63, synthetic biology (Sb)

New genomes are no longer science fiction. The ability to design and control biological organisms and processes is well

on its way and has the potential to become one of the most powerful tools to benefit the move toward a sustainable world. It also has the potential to cause almost unimaginable harm. Thoughtful development, use and implementation of synthetic biology processes must proceed within a sustainability construct.<sup>91</sup> Long-term implication of use and misuse must be considered and built in prior to implementation. The impact of synthetic biology will be felt by this world in the coming decades and it is essential that these impacts be positive and not follow the errors of previous technological advances of realizing a specific utility coupled with myriad unintended consequences.

#### 9.4 81, biologically-enabled transformation (Bt)

Nature is the original chemist carrying out an inconceivable numbers chemical transformations each second with a volume that dwarfs the combined output of every chemical company and an elegance that puts the occupants of the best chemistry departments to shame. Capturing and harnessing the power of biological processes to carry out chemical transformations can be a powerful strategy for a sustainable economy.<sup>92</sup> Oriented toward renewable, bio-based feedstocks, these processes (*e.g.*, fermentation) can be utilized for production of materials in a manner that is supportive of and conducive to life.

## 10. Catalysis

There are few areas of chemistry that exemplify sustainability better than catalysis. Catalysis allows for increasing the rate of a transformation, increased efficiency, use of less feedstock, enhanced product quality, lower waste and lower emissions while at the same time increasing the profitability of a process/product.<sup>93</sup> Virtually every major petrochemical, specialty chemical, or pharmaceutical company would not be economically viable without the use of catalysis. The blend of environmental benefit and economic returns *via* catalysis makes it amongst the most obvious and powerful tools to advance sustainability through chemistry.

#### 10.1 28, enzymes (E)

Enzymes are often viewed the pinnacle of what catalysis strives to be. They carry out conversion of chemicals with an elegance and selectivity that most chemists would only dream of. Yet the limitations of enzymatic catalysis are something that needs to be understood; useful technologies require tolerance of a wide range of temperature, pressure, pH and concentration levels. The development of manufacturing methods that exploit the advantages of enzymes will be an important contribution to green and sustainable chemistry manufacturing.<sup>94</sup>

#### 10.2 46, earth abundant metal catalysis (Ac)

The recent history of metal catalysis is that often some of the most toxic and/or precious metals were developed and used as catalysts and targeted for research and study. These include

osmium, mercury, chromium, platinum, palladium, gold, iridium and others. The cost and sustainability impacts of this approach are significant. While it must be noted that there exist excellent recovery schemes, each of these have costs and risks that should be minimized.

The exploitation of Earth-abundant metals (*e.g.*, iron, copper) that are neither scarce nor depleting is an active area of development that will be important to achieve the necessary advantages of metal catalysis without the same associated historic impacts.<sup>95</sup>

#### 10.3 64, heterogeneous catalysis (Ht)

Heterogeneous implies that something is not uniform in nature and contains a few or many different components, or substances that make up one whole or mixture. In chemistry, it can also mean something is comprised of the same substance only in different phases (gas, liquid, solid). For example, ice water is heterogeneous because it is comprised of liquid water and solid water. In sustainability, heterogeneity can confer some desirable properties. In consideration of a catalyst, heterogeneous catalysts confer many advantages compared to homogeneous catalysts including better stability, ease of handling, separation, and simplified recycling of the catalyst.<sup>96</sup>

#### 10.4 82, homogeneous catalysis (Hm)

When something is the same throughout and consists of all the same parts it is homogeneous. In chemistry, this means that it is a pure element, or a compound or mixture that contains the same composition throughout and in the same state of matter (solid, liquid, and gas). Homogeneous catalysts are important to green and sustainable chemistry due to ease in characterizing how they function; they are typically straightforward to modify for optimized performance or lower environmental impacts.<sup>97</sup> Homogeneous catalysts are amenable to interesting strategies such as controlled phase transfer or changes in solubility aiding recovery and reuse. The boundary between homogeneous and heterogeneous catalysis can be blurred by immobilization or compartmentalization techniques. In any case, the technologies are a powerful tool for aligning performance, economic, and sustainability aims for a chemical process.<sup>93</sup>

## 11. Degradation

Persistent substances may remain in the natural and man-made environments for an indefinite time. These compounds may accumulate to reach levels that are harmful to health, environment and natural resources.<sup>98</sup> Such contamination may be poorly reversible or even irreversible, and could render natural resources such as soil and water unusable far into the future.<sup>99</sup> As such, there is a need to design chemicals and materials, particularly those that are intentionally or unintentionally distributed in the environment, that are stable during their useful life, and then completely degrade once they are no longer functionally necessary. Designing for degradation is

necessary but not sufficient to realize the goals of green and sustainable chemistry; the subsequent degradation products should, themselves, be non-persistent and benign to human health and the environment.<sup>100</sup>

### 11.1 29, benign metabolites (Bm)

Metabolites are small molecules that are by-products of metabolism or degradation of larger molecules in a living organism. Metabolites can be formed during physiological metabolism in humans, during plant metabolism, or in other living organisms. Many of these metabolites have specific functions within the organism that help to regulate various processes.<sup>101</sup> However, some can cause adverse health effects and are toxic to the environment. Benign metabolites refer to the metabolites that are non-toxic to an organism or the environment. This thinking is important in sustainability practices as design must account for product breakdown and not just the product itself in order to mitigate toxicity in humans and ecotoxicity. Benign parent compounds can break down into very harmful metabolites. This may be especially relevant to biologically active chemicals such as pharmaceutical<sup>102</sup> and herbicides/pesticides<sup>103</sup> that could be better designed to ensure degradation in the environment would produce benign metabolites.

### 11.2 47, molecular degradation triggers (Md)

Molecular degradation triggers are events that help to promote degradation and break down of chemicals and molecules.<sup>20</sup> These could include molecule modification, UV light triggers, or any number of different triggering events. Today there are many stable compounds that persist in the environment for lengthy periods of time. Triggers could help to mitigate the presence of these harmful, persistent molecules and could be key in sustainability efforts. Molecular degradation triggers can help to form benign by-products following the end of life of chemicals and products.

### 11.3 65, degradable polymers and other materials (Dp)

Polymers should not be (effectively) immortal. Yet, many approach that level of persistence when compared to the human time-scale. This has resulted in well-known concerns for plastics in landfills and in the oceans.<sup>104</sup> It also is of concern for lesser-known issues such as the potential impacts of all of the micro- and/or water soluble synthetic plastics that due to their persistence are being integrated into ecosystems and the biosphere. Polymers can be designed such that their entire lifetime is approximately the same as their useful lifetime.<sup>105</sup> Enduring and persisting beyond intended use serves little purpose and has been the cause of serious problems.

### 11.4 83, prediction and design tools (Pd)

Designing next generation chemicals and materials will require next generation prediction and design tools.<sup>106</sup> Analytical understanding and computational models continue to be more powerful allowing increased insights to go beyond simply predicting potential adverse impacts towards informing

design. This is critical because predicting that something may be harmful without a mechanistic basis for that model outcome does not provide sufficient and necessary guidance to a chemist on how to redesign the molecule to preserve function while minimizing or eliminating the hazards.<sup>107</sup>

## 12. Measurement and awareness

In order to know whether an action or invention is positive or negative for the world, there needs to be some kind of feedback from the system.<sup>108</sup> In the absence of this feedback, there is little more than insufficient guesses and suppositions. However, the way that we choose to measure the performance and impact of our products, processes, and systems will often have a profound impact on the understanding that we take away from these measurements. If we are operating in multi-dimensional systems like those involved with sustainability, we will need measurement systems that are as multi-dimensional if we wish to gain insight from them. Traditional, limited measurements such as efficiency measures will be insufficient for this complex system. Additionally, our measurement systems have often been retrospective tools that would give us reports on what happened in the past sometimes with long enough lag times that the information itself is irrelevant. We now have tools and computational abilities that can provide real-time insights and awareness that allow for relevant action.

### 12.1 30, sensors (Sn)

Chemical sensors and chemo-electronic sensors can provide a level of detection and real-time awareness that will be critical to a sustainable society.<sup>109</sup> With applications ranging from air and water quality to health indicators to environmental ecosystems shift, the development of ubiquitous, integrated sensors can provide data that inform insights into planetary and human health. These same sensors can inform and empower more efficient use of materials and energy in manufacturing and consumer use. Sensor technology can provide a consciousness about factors and dynamics that were once thought unknowable.

### 12.2 48, in-process control and optimization (Co)

In manufacturing processes and operations, the way to verify smooth operation was through periodic analysis that require extractive testing and analysis of the product. This required time and labor and resulted in waste of materials and energy. Often, product that did not meet specifications (so-called off-spec) would need to be discarded as waste, frequently in large quantities. It is now possible and important that future processes and even operations beyond manufacturing utilize in-process control and optimization through the use of real-time sensors and analysis.<sup>110</sup> In this way, there is the ability to sense off-spec material before it is formed in significant quantities and to make the appropriate corrections *in situ*. This becomes especially vital when pursuing the goal of process integration.

### 12.3 66, exposome (Ex)

The exposome refers to everything an individual is exposed to starting from the time before they are born through end of life.<sup>111</sup> Each of these exposures can accumulate, compound, and interact with each other and effect one's health. Exposures include anything from one's environment, diet, work place, and lifestyle and can affect health in a number of facets and ways. One component of the exposome is an individual's unique physiological characteristics and genetics, which can play a major role in how an individual will react to an exposure. In terms of sustainability it becomes important to consider the potential exposures in designing any product or chemical.<sup>112</sup> By better understanding the exposome we can design more sustainable and safer products and many of the harmful exposures to human health can be minimized.

### 12.4 84, green analytical chemistry (Ga)

Analysis of the air, water, and land to detect pollution was historically conducted with field sampling protocols that require extensive effort to be brought to a laboratory where extensive work-up generated large volumes of solvents and waste. The processes of measurement and analysis of an environmental problem often contributed to other environmental problems. With the use of real-time, in-field analysis the necessary measurements can be taken without the wasted time, material and energy. This "green analytical chemistry" has been extended to a wide-range of analytical techniques beyond environment analysis reducing the quantity of materials needed and waste generated.<sup>113</sup>

## 13. Enabling systems conditions – conceptual frameworks

Conceptual frameworks provide a basis for considering the role of the chemical enterprise in advancing sustainability and the associated complexities. Such frameworks provide a means to understand the relevant concepts as well as their relationships to one another. Frameworks of this nature help to inform the overarching design of the role of chemicals and chemistry in contributing to the goals of a sustainable future.

### 13.1 5, biomimicry (B)

Nature has a 3.5 billion-year head start on designing products, processes, and systems and it shows. Nature is indescribably brilliant in its ability to produce the widest range of chemicals and materials using locally available starting materials, usually at ambient temperatures and pressures, completely eliminating the concept of waste, and doing it in a way that is conducive to life. In the face of this ingenuity, the only wise and sustainable strategy is to take Nature as a mentor and a guide in designing human made products and systems.<sup>114</sup> The lessons to be learned are limitless and the benefits to be had, essential.

### 13.2 13, circular economy (Ce)

Circular economy refers to closing the material loop. This means working to keep resources in use for as long as possible and requires both the producer and consumer to be aware of how they are utilizing resources.<sup>115</sup> It can help to ensure waste and resources, at any point from production to end of life of a final product are reused, repaired, or recycled in some capacity. This helps to decrease waste and becomes especially important in sustainability efforts, helping companies to reduce waste, save money, and work to ensure there is not depletion of finite resources. The concept of circular economy should be considered in all phases of the product life cycle and can not only help to save resources, but also decrease the amount of toxic waste output.

### 13.3 31, benign by design (Bd)

"Performance" of a product, process, or system, has been a concept that has been narrowly defined in terms of how well something achieves a very specific goal. Perhaps it's a dye being a particular shade of blue or a lubricant being able to reduce friction. While performance has been focused on the desirable qualities, this has often come with undesirable or adverse unintended consequences.

Benign-by-design builds all factors into the definition of performance such that inherent safety is also included along with function.<sup>7</sup>

### 13.4 49, industrial ecology (Ie)

Industrial ecology aspires to manage material and energy flows in the same way that an ecosystem performs, with the aims of ultimately decreasing environmental stress and improving resource efficiency.<sup>116</sup> Considering industrial processes as a closed loop as much as possible creates the opportunity to decrease inputs through the reuse of outputs either within a facility or between different organization. By viewing waste as a resource – by closing these material and energy loops – waste and resource depletion caused by industry can be minimized. Industrial ecology helps to find solutions to environmental problems by identifying problem areas in business and industry and can aid in improved sustainability practices.

### 13.5 67, trans-generational design (Tg)

It has been shown that exposure to a chemical by one generation can have deleterious effects on the future generations, even without direct exposure themselves.<sup>117</sup> This is especially relevant to chemicals that interfere with the body's hormonal systems leading to a variety of adverse health effects including reductions in sperm counts as well as tumors, birth defects, and other developmental disorders.<sup>118</sup> In this way, the chemistry we practice and the chemicals we produce today can have lasting and debilitating effects on future generations. This emerging knowledge carries an enormous burden of responsibility to be accountable not only to today's population but to those not yet born.

### 13.6 85, bio-based economy (Be)

Bio-based economy refers to the innovation in utilization of biomass to sustainably make bio-based products such as chemicals, materials, fuel and energy. It is an attempt to move away from reliance on depleting resources and rely on renewable, bio-based feedstocks. Traditionally, chemicals have been made from petroleum feedstocks.<sup>119</sup> Although chemical production only accounts for 5%–7% of petroleum consumption,<sup>120</sup> petroleum sources represent over 98% of chemical feedstocks.<sup>121</sup> The advantages for moving to renewable feedstocks include an opportunity for innovation and a chance to take advantage of nature's ability to perform exquisitely selective chemistry. Petrochemical feedstocks provide very simple hydrocarbons, which chemists have learned to make more complex. Natural feedstocks are inherently different. They are complex molecules, and chemists are still developing elegant ways to efficiently transform them into useful products.

## 14. Enabling systems conditions – economics and market forces

While the current global economic systems and market forces tend to drive perverse incentives that have resulted in the design and evolution of our existing chemical infrastructure, these same powerful drivers can be harnessed to encourage behavior that is aligned with the goals of a sustainable future. As profit is the almighty motivator, it is imperative that we move to a system whereby externalities are internalized through costs and whereby benefits beyond financial gains can be systematically and rigorously factored into decision making. We must align environmental, social, and economic goals if we want to design a future that does not continue on our current unsustainable path.

### 14.1 6, life cycle cost-benefit analysis (Cb)

Cost-benefit analysis is a decision-making process that helps to identify, and quantify, the costs and benefits associated with all potential scenarios or options. It is a systematic approach to estimating the strengths and weaknesses of alternatives used to make decisions between alternatives. Opportunity cost, the benefit missed by choosing one option over the other, is often also factored into the analysis. It can be used to compare intangible items, such as ecosystems services or the benefit of choosing an option that confers less environmental and negative health impact over a more detrimental option.<sup>122</sup> In sustainability practices cost-benefit analysis can help to identify options that may confer more favorable environmental conditions, while also minimizing costs over the entire life cycle. It is important to consider the full life cycle in this type of analysis as costs may be higher upfront for greater benefits later on.

### 14.2 14, full cost accounting (Fc)

Full cost accounting allows for the implementation of environmental, health, and social assets to be considered in the econ-

omic costs and benefits of decision making.<sup>123</sup> It allows for complete end-to-end cost analysis of producing products or services. The goal is not necessarily to monetize their value, but rather to better understand their impact on an ecosystem and society, and potential ability to create value. Full cost accounting can help in sustainability by identifying areas where reducing environment impact could create value and confer monetary and non-monetary benefits that can be translated into economic terms.<sup>123</sup> It allows for better management of the natural and social resources in our world today and a way to achieve more sustainable outcomes.

### 14.3 32, harm charge/carbon tax (Hc)

Carbon tax is a tax placed on the burning of fossil fuels, or carbon-based fuels, and corresponds to greenhouse gas emissions.<sup>124</sup> The fee is either placed on the producers or passed along to the consumers for the carbon emissions produced from burning of fuel. It can be implemented in a number of different facets such as through costs associated with home heating, flights, and shipping capacities. A harm charge is a similar concept only less specific. It places a charge on any practice harmful to the environment or human health such as a chemical spill, using non-sustainable products, or water pollution. The charges or taxes are utilized in order to serve as a disincentive to practices harmful to the climate, the environment, and human health, helping to shift thinking towards more sustainable practices. Further, the revenue generated from these charges can be used to invest in sustainability practices elsewhere in the system.

### 14.4 50, depletion charge (Dc)

Similar to harm charge, depletion charge presents an opportunity to internalize an externality. In this case, the externality is the consumption of finite resources. Depletion charge presents an opportunity to incrementally increase the economic cost associated with the use of a finite resource by factoring in scarcity.<sup>125</sup> That is, using the next amount of a finite resource would be increasingly expensive to disincentivize its ongoing use. This incremental charge does not need to be linear, and could itself increase with ongoing use of the finite resource rapidly leading to a price that is cost prohibitive rendering that finite resource economically infeasible.

### 14.5 68, sustained research funding (Rf)

Scientific investigations, studies, and breakthroughs will be necessary to move away from the unsustainable trajectory that we are on. These investigations, in many cases, may require sustained efforts either due to the difficulty of the challenge or the inherent nature of longitudinal insights.<sup>126</sup> These research efforts are particularly fragile to disruptions caused by the unpredictable modalities of research funding schemes whether in the public or private sector. The imperative of sustained, predictable funding support will be an essential element of achieving the kinds of insights and inventions necessary for sustainable prosperity.

## 14.6 86, capital investment (Ci)

The chemicals and material manufacturing infrastructure that makes everything from building materials to wind turbines is very capital intensive. Current schemes for capital investment, (e.g., venture, private equity) have the common goal of getting targeted returns while minimizing risk. This model significantly favors incrementalism which is far easier to understand and analyze what the risk profile might be for technological investments. It also favors low capital-intensive projects such as software and “app” projects and disfavors projects such as large-scale infrastructure and manufacturing. Achieving sustainability goals necessitates transformative technologies and dramatically reconstituted sustainable infrastructure at unprecedented scale requiring wise, patient capital at a significantly increased level.

## 15. Enabling systems conditions – metrics

For metrics to be useful in sustainability, they must have attributes that reflect sustainability itself. They must be both quantitative and qualitative.<sup>127</sup> They must be relevant across time scales and able

$$F = \text{Function/kg of chemical}$$

to combine both reductionism and integrative systems thinking. Too often traditional metrics that have determined the cost or benefit of our product or processes have looked at only one aspect of the overall system.<sup>108</sup> These reductionist metrics are flawed in terms of limiting our purview, our design space, and our innovation. Further, they have been inadvertently enabling of unsustainable technologies and policies. Broad thinking is developing on how to enhance the old metrics with new systems indicators that are a reflection of the magnitude and directionality needed for sustainable design and decision-making. These multi-dimensional ‘vector metrics’ will be essential in setting the course for sustainability in the future.

### 15.1 7, atom economy (Ae)

Measuring the efficiency of chemical reactions is necessary to compare alternative synthetic routes to products in terms of environmental and economic costs. Percentage yield has historically served this function, as it compares the (predicted) theoretical and actual product quantity. However, a high yield is not sufficient to identify environmentally-preferable synthetic routes because there can be significant waste generated in a reaction that produces close the predicted amount of product. As such, we need an additional metric, atom economy, to measure how much of the reactant atoms actually form the final product<sup>128</sup> whereby:

$$\% \text{Atom economy} = \frac{\text{molar mass of product}}{\text{molar mass of all reactants}} \times 100\%$$

This is effectively guiding a chemist to pursue pollution prevention at the molecular scale. In principle, the higher the

atom economy, the lower the amount of waste product formed, so considering both the yield and the atom economy can help in designing a green chemical process. In practice, other components of a reaction that do not appear in the balanced chemical equation, such as solvents or separations, may have a larger impact on waste generation. The metrics discussed below can provide additional guidance.

### 15.2 15, E-factor (Ef)

The amount of waste produced in the manufacture of a chemical product or a product of any kind should be minimized. While one would intuit that this measure was always part of manufacturing efficiency, it was not. The introduction of the calculation of the *E*-factor<sup>51</sup> took the original form of:

$$E \text{ factor} = \text{kg waste/kg product}$$

and can be adjusted to include a variety of aspects of the manufacturing process. *E*-Factor provides information that was historically neglected but is critical to moving towards more efficient and effective chemical production.

### 15.3 33, F-factor (Ff)

Virtually, no one ever bought a chemical. They bought function or performance. They wanted the service the chemical provided. With that realization, a metric, *F* factor, has been developed to recognize and quantify the desire to get maximum function with the minimal amount of chemical used.<sup>75</sup>

This approach has been expanded in the discussions of the chemical equivalent of Moore's Law.<sup>129</sup>

The desire is for the value of *F* to be as large as possible by increasing the functional performance and/or decreasing the amount used to achieve some functional performance. This drives the system towards ideality where you get all of the function of a chemical or product without the existence a chemical or a product; the chemical analogy of getting the function of the telephone without the need for telephone wires on every street.

### 15.4 51, qualitative metrics (QI)

While most of traditional assessment is based around quantitative metrics, qualitative metrics may be equally necessary in providing understanding related to sustainability,<sup>130</sup> especially in the early design phases. The nature and the character of aspects of green and sustainable chemistry are not always reductionist exercises.<sup>131</sup> The renewability of a feedstock, the toxicity of a molecule, the environmental justice implications of a factory siting, market acceptance of an energy technology *etc.*, may all have qualitative aspects that are critically important. While qualitative metrics may be less rigorous and involve integrative systems thinking that is outside traditional analytical frameworks, it is possible that they are more closely linked to the interconnected nature of sustainability systems and goals as outlined in the sustainable development goals.<sup>3</sup>

### 15.5 69, quantitative metrics (Qn)

One of the most active areas in analytical tools related to green chemistry and engineering is that is quantifiable metrics.<sup>132</sup> There are important measures of (process) mass intensity ((P) MI),<sup>133</sup> reaction mass efficiency (RME),<sup>134</sup> carbon efficiency (CE), innovative green aspiration level (iGAL)<sup>135</sup> and others. These quantifiable metrics can be useful and informative in answering specific questions of efficiency and informing potential downstream environmental impact (through tools such as life cycle assessment, section 17.3) when a reductionist analysis is necessary to inform improvement. It is as important to know what data or information the quantifiable metrics are providing as it is to understand what questions they aren't addressing. The strengths of quantifiable metrics are essential and their weaknesses must be equally respected.

### 15.6 87, chemical body burden (Bb)

Chemical body burden refers to the measurement or load of chemicals in the body.<sup>136</sup> This load can be detected through blood, urine, breast milk sampling or any number of biomonitoring activities. Chemicals in the body could have numerous harmful effects and could weaken the immune system making the body more susceptible to disease.<sup>137</sup> The burden may be due to bioaccumulation through various mechanisms of exposure. Understanding the amount and types of chemicals in the body can help to better inform what chemicals are in the environment. Chemical body burden is important to sustainability because it can make known the chemicals with the greatest bioaccumulation in nature and greatest exposures to humans, helping to inform future design of chemicals and products that avoid these unintentional impacts.

## 16. Enabling systems conditions – policies and regulations

The landscape of technologies in the chemical enterprise is not merely shaped by scientific and engineering solutions alone but rather in combination with the environment of regulation, policies, and laws that construct the social context in which they operate.<sup>138,139</sup> Policies and regulations can accelerate or retard sustainability solutions and they can protect or help displace entrenched unsustainable technologies. The development of regulations and policy that will empower and enable green chemistry and green engineering to succeed in society will be necessary to remove the obstacles and inertia that keep the *status quo* in place.<sup>60,140</sup>

### 16.1 8, extended producer responsibility (Pr)

Extended producer responsibility refers to the responsibility a producer holds to design their product in a way that reduces negative environmental and health impact.<sup>141</sup> It also places end-of-life management on the producer and not the consumer.<sup>142</sup> This is especially important to sustainability. If the producers, who are responsible for what the environment and

the population is exposed to are not held responsible for ensuring their products are healthy and environmentally friendly, it becomes a problem of remedy rather than stopping it at the source. Extended producer responsibility helps to manage and mitigate end-of-life waste and all pollution generated from products at all stages of its life cycle.

### 16.2 16, property-based regulation (Pb)

The history of chemical regulation is to construct lists of chemicals that are considered too hazardous or too risky and impose some types of controls on them. Chemical-by-chemical regulation is slow, costly, inefficient, and inadequate.<sup>143</sup> The nature of the concern for a chemical is not based on its chemical name but rather on its combination of properties. Some combinations of properties may lead a chemical to be bioavailable, others to be persistent, still others to be reactive or explosive.<sup>58,144</sup> Since it is the combination of these properties that cause the concern, it is the properties that should be the basis of regulation. In this way, the chemicals of concern can be addressed proactively while providing certainty to the regulated community and critical guidance to the molecular designers of future products.

### 16.3 34, chemical transparency (Ct)

Chemical transparency refers to the disclosure of all chemicals and ingredients in all products. This is becoming exceedingly important among consumers.<sup>145</sup> Consumers want to know what is in their chemical products and as part of their decision to trust the brands they use.<sup>146</sup> This pressure from consumers and government can help to hold manufacturers accountable and aid in the development of safer, more benign chemicals, and continually move toward developing more sustainable products.<sup>147</sup> Not only does this let consumers have the choice to choose safer, more environmentally friendly products, but it also allows for easier and better exchange of practices among different companies. There are significant efforts underway to standardize the reporting of chemical ingredients in a variety of products to aid in data collection and product comparison.

### 16.4 52, chemical leasing (Cl)

Virtually no one ever bought a chemical. They bought function. The bought performance. There is very little value to the ownership of the vast majority of chemicals unless they are used for their intended purpose. And yet, because of the traditional sell/own business model, the waste that results from over-purchasing is significant and systemic. Further, the system is constantly driving towards selling more chemical to make more profit driving towards designed obsolescence and short-term use. The chemical leasing model is one where the “sellers” supply the service or function rather than selling a chemical.<sup>148</sup> In this model, instead of selling as much chemical as possible (resulting in excess and waste), the motivation is to use as little of a chemical to accomplish the desired service as the same profit can be generated from delivering much less product.<sup>148</sup> Chemical leasing is a business model whose effectiveness has been demonstrated at large scale and has extensive potential to be expanded.<sup>149</sup>

### 16.5 70, self-enforcing regulations (Se)

The idea that regulations and laws to protect the environment and human health can be effectively enforced by government inspectors and officials has been belied by experience.<sup>150</sup> This historical model has demonstrated over the past half-century that most of the damage is not detected and when it is detected it is at a timeframe that is inadequate to prevent the often tragic, consequences. With the advent of sensors, real-time in-process controls, big-data analysis, and machine-learning, it is now possible to rethink models for enforcement. Instead of sampling hazardous waste sites for laboratory analysis to determine levels of contamination, there are now possibilities for integrated, networked monitoring systems. New processes can be designed such that they only can function as long as emissions are below certain levels for various contaminants. The emerging field of self-enforcing regulations can also build in predictability and reduced economic and time burden for the regulated community while ensuring enhanced effectiveness in achieving the goals of the regulation.

### 16.6 88, innovation ecosystem – translation from lab to commerce (I)

In order for a discovery or innovation to have an impact on the world, it virtually always needs to be enabled by an innovation ecosystem that incorporates the essential enabling elements.<sup>151</sup> These include support for basic research and development and that R&D needs to be commercialized through thoughtful and risk-taking investment. These roles can be filled by various actors ranging from public sector government agencies to private sector investors.<sup>152</sup> Appropriate and just intellectual property considerations need to be supported by governance and returns on investment need to be realized through adequate financial systems. With key roles and responsibilities assured, the innovation ecosystem can be used to bring about the transformative innovations in the chemical enterprise that are needed to advance sustainability.<sup>153</sup>

## 17. Enabling systems conditions – tools

Increasing the development of tools to enable green chemistry and green engineering has expedited the adoption of more sustainable choices in the selection and innovation of products and processes. These often-quantitative resources allow chemists, engineers, and other professionals to pursue the incorporation of green chemistry into a wider range of products and processes with greater confidence in their decision-making and more credibility in building the business case for implementing these innovations.

### 17.1 9, epidemiological analysis and ecosystem health (Ea)

Epidemiological analysis refers to the understanding and analysis of how different populations are effected by various risk-factors, disease and other health outcomes.<sup>154</sup> Ecosystem

health refers to the health or condition of the environment and all living organisms in that environment. That is, its susceptibility/resiliency to natural disaster and ability to sustain life defined by a number of indicators unique to the ecosystem.<sup>155</sup> In conjunction, these two concepts define the health of an area and all the living organisms within it. These concepts are key to sustainability because they define the success of sustainability practices. If something is being carried out in an unsustainable way it will be directly reflected in the health of the population and environment.

### 17.2 17, alternatives assessment (Aa)

Alternatives assessment is a technique aimed at minimizing harm by assessing all options and solutions and understanding the consequences of each.<sup>156</sup> They help to characterize hazard based on health and environmental information. It is often utilized in risk assessment and as a decision-making approach. One common application is a chemical alternatives assessment in order to aid in choosing the safer chemical over a more hazardous one with the aim of avoiding regrettable substitution.

### 17.3 35, life cycle assessment (Lc)

Life cycle assessment determines the total environmental impact of a product from beginning to end of life, or cradle-to-grave.<sup>157</sup> This is done through accounting for all material and energy-related inputs and outputs throughout the life of a product.<sup>157</sup> It helps to measure all steps of production and use, and their subsequent environmental and health implications. Life cycle assessment provides a producer information for all direct and indirect environmental impacts associated with their products and processes, illuminating areas for improved design choices or making decisions between one chemical product or process and another.<sup>158</sup>

### 17.4 53, solvent selection screens (So)

Solvents are often critical to a chemical process as a medium in which to dissolve solutes and form solutions. They are also often the deciding aspect in the cost and environmental impact of a chemical process.<sup>159</sup> However, when it comes to choosing the right solvent there are often many options, all which have different properties and different environmental impacts. A solvent selection tool identifies different solvent options using a variety of statistical, regression, and structure/property-based strategies, and then provides comparisons through various graphical outputs and shortlists.<sup>160</sup> It allows the user to apply filters that select for certain properties and pick the best possible solvent for the situation. It also can aid in sustainability through improving industrial process and aiding in the evaluation of solvents in regard to their environmental and health impact.<sup>161</sup>

### 17.5 71, chemical footprinting (Cf)

Chemical footprinting allows for comprehensive, full life cycle management of chemicals being used by companies today. It gives companies the tools and ability to better understand what chemicals are in their products and a metric to better

manage the safety and environmental impact of those chemicals.<sup>162</sup> This benchmarking tool is important in sustainability practices because it helps to create a common standard for all to follow, while also reducing chemical risk, identifying areas for improvement, and measuring the progress being made.

### 17.6 89, education in toxicology and systems thinking (Et)

In most professions, the people that create something have responsibility for the implications of what they create. This is not true in the field of chemistry. All chemists need to understand the consequences to the world and its inhabitants of what they create and study. Yet, virtually no education programs for chemists include the requirement of training in molecular toxicology or systems thinking. The basic principles of chemical dose-response, bioavailability, bioaccumulation, and biomagnification need to be understood by chemists as well as the molecular level understanding of the fundamentals of acute and chronic toxicity, carcinogenicity, and endocrine disruption, among all relevant human health endpoints.<sup>163,164</sup>

Many of the innovations necessary to realize green and sustainable chemistry, it is necessary to consider a broad array of issues that often involve systems of systems, such as the vital role and value of ecological systems and services and the life cycle impacts and benefits of an engineered system, from its raw materials to end of life.<sup>108</sup> Although chemists have a long history of thinking in complex systems, there is a need to extend this type of thinking to include the regulatory environment, economic drivers, and social behavior. For example, the systems thinking within green and sustainable chemistry should also include acknowledging who have been disadvantaged through environmental justice and understanding the role of economic incentives and policy instruments to align socioeconomic behavior with environmental goals.<sup>165</sup> Finally, there is an urgent need to effectively communicate not only the innovation(s), but the contextualizing system in which it will be implemented.

## 18. Noble goals

There are some concepts that are transcendent. These considerations rise above the immediate economic or political concerns of the day. Noble elements are those they are grounded in moral imperatives that are shared across cultures and across time. These elements find their basis in values, justice and trans-generational equity. Chemistry can impact all of these issues either positively or negatively and therefore they must consciously enter into our decision-making and our designs.

### 18.1 2, hippocratic oath for chemistry (Ho)

First, do no harm. The products that are made and the processes that make them and the resources that they come from will do no harm to the planet, both the biosphere that occupies it and the geosphere that sustains all living things. There will be no harm to those workers obtaining the feed-

stocks and transforming them, to the consumers using them, to the communities and populations, human and non-human alike, that may be exposed to them.<sup>166</sup> There will be as much thought and care put into the consequences of chemistry as there is into the design and invention of the chemistry.

### 18.2 10, design for posterity (P)

We borrow this planet and everything that is in it from the future. We own nothing. We owe everything. Our debt is repaid through the care exhibited by thoughtful use and design. Perpetuating flawed unsustainable systems based on limited knowledge or short-sighted perspectives is design for the past which simply enshrines ignorance and errors.

Constant change to reflect the highest levels of awareness that can lead to a more sustainable world is the path toward being respected by the future and ensuring that there will be a future to be respected by.

### 18.3 18, life-compatible products & processes (Lp)

Nature is conducive to life. We are part of Nature and must assume our role as being conducive to life. The chemistry we discover and the chemicals we introduce into the world must reflect this role. The idea of legally acceptable toxicity and poisoning, socially acceptable degradation of ecosystems, and tolerable rates of species extinctions are frameworks that are flawed, illogical and incompatible with our role in Nature.

### 18.4 36, zero waste (Z)

Waste is a man-made concept. In Nature outside of man, there is no waste. Evolutionary brilliance ensures that the waste from one organism will be utilized at high value to another organism. Waste in our chemical and material world is simply a material or energy for which a valuable use has not be discovered or implemented. While we will never defeat thermodynamics in attaining perfect cycles and entropy will always win, the cycles and systems that can be constructed can strive for continuously moving toward the perfect goal of zero waste.

### 18.5 54, chemistry is equitable and fully inclusive (Fi)

The natural laws of chemistry have no predisposition to any gender, race, creed, religion, nationality, ability, nor orientation. Yet the participation within the chemical enterprise has historically been dominated by a small demographic sliver of the population. The science and application of chemistry can only benefit by a maximum breadth of perspectives, skills, experiences, cognitive approaches, and values of a diverse community with a culture of inclusion. No endeavor, scientific or otherwise, can be 100% effective if it excludes so much of its talent. It would be as absurd to limit participants of a scientific field to individuals of a certain height or weight as it would be to limit them by their gender or ethnic background.

Full inclusion of all groups in the chemical enterprise should be pursued as a pathway to genuine excellence and not merely the narrow historical definitions of excellence as posited by those who have historically dominated the field.

### 18.6 72, benefits distributed equitably (De)

The benefits of chemistry are immense and have revolutionized the quality and length of human life. But not for everyone. The benefits of chemistry and chemicals are not distributed equally. Large percentages of the population have borne the burdens of a chemical-intensive society where the smallest percentage of the population has received benefits with virtually no burden.

### 18.7 90, extraordinary chemical knowledge comes with extraordinary responsibility (K)

A diminishingly small percentage of the population has the knowledge and understanding of how to manipulate matter at the molecular level. Those possessing this knowledge came to it through a confluence of the gift of sufficient intellectual capacity and the good fortune of having access to some type of educational framework not of their making. The power of chemistry is daunting and world-changing. It impacts societies, oceans, and atmospheres.

With these two gifts comes a responsibility to use the power of molecular manipulation for good and not ill. To build and not destroy. To heal and not to harm.

## 19. Conclusion

To attain the full the power and potential of chemistry to improve the world, it needs to begin with the fundamental science of green chemistry and green engineering. This requires not only implementing all of the tools, frameworks and perspectives contained in the elements of sustainable chemistry, but also developing predictive tools to inform the design of more sustainable products, processes, and systems. You cannot achieve sustainable chemistry without green chemistry. Green chemistry will not be implemented at scale without the other elements of sustainable chemistry. Like all human endeavors and actions, all of these efforts in chemistry need to take place within an ethical, humanitarian, and moral framework. Just like the countless possible substances of the known universe are comprised of the known elements of the Periodic Table, there are countless possible paths to a sustainable future when employing the elements of sustainable chemistry.

## Conflicts of interest

There are no conflicts to declare.

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