Foundations of Chemistry
https://doi.org/10.1007/s10698-025-09536-2

The concept of 'nature' in chemistry in a digital and ecological age

Christian Schnurr[1,2]

Accepted: 11 February 2025

Abstract
The chemical understanding of 'nature' is a naturalistic one where 'nature'—understood as the chemical dynamics that guide material change—coincides with chemical reality and possibility. A naturalistic chemist considers all chemical substances equally 'natural', and more importantly also all possible substances. I characterize the first point as the 'monistic' and the second as the 'potentialistic' understanding of 'nature' in chemistry. I argue that this notion of 'nature' is ecologically vacuous and lies at the heart of the ecological havoc that modern chemistry is causing. Not only because of these ecological concerns but also because of the increasing digitization of chemistry is the chemical self-image as a 'synthesis science' at a crossroads. In the digital age, I claim, chemistry is increasingly becoming a 'simulation science'. I evaluate these developments from an ecological perspective. In a recourse of ecological visions of chemistry, I outline possibilities of synergies between an ecological and a digital transformation of chemistry.

Keywords Nature · Natural-artificial · Unnatural · Ecology · Chemical space · Digitization

Introduction. Chemists struggling with 'nature'

Ironically, the concept of 'nature' has a difficult standing in the natural sciences. Already at the times of their origin in the early modern period, the term 'nature' was contentious and has been criticized by important figures such as Robert Boyle and Johann Christoph Sturm for being too prejudiced and equivocal (Spaemann 2012). Boyle pleaded for replacing the term 'nature' with less ambiguous words or, if unavoidable, at least specifying which particular sense of 'nature' is meant (Boyle 1996). Indeed, this critique seems to have borne fruit. Three-and-a-half centuries later the natural sciences are doing surprisingly well in describing natural phenomena without referring much to terms such as 'nature' or 'natural' in their theoretical frameworks. Wherever necessary, more technical terms such as 'earth system' or 'sustainability' have taken their place.

✉ Christian Schnurr
christian.schnurr@uni-a.de

1 Environmental Science Center, University of Augsburg, Augsburg, Germany

2 Chair of Analytical Food Chemistry, Technical University of Munich, Munich, Germany

Published online: 14 March 2025

While the sciences have effectively phased out the term 'nature' from their methodological and theoretical discussions, the general public seems to be hooked on the concept more than ever. This is mirrored in advertisement language, where 'nature' and 'natural' are, for decades, among the most common words in advertisement slogans (Slogometer 2024). In Europe, a third of all newly launched food and drinks products advertise with a 'natural claim' (Schofield 2019). Political demands, aesthetic imaginaries, and religious undertones mix effortlessly in a concept that time and time again unsettles, confuses, and enrages (some of) the chemistry community which finds itself on the 'other side' of nature, being associated with the 'artificial', the 'unnatural', the 'impure'.

Chemists (or those who claim to speak for chemistry) are usually quite clumsy, or even polemic when complaining about the colloquial use of 'nature'. The common language distinction between 'natural' and 'chemical' substances is countered with the platitude that "all substances are chemical" (Markl 1992; Kennedy 2021). Products claiming to be "free of chemicals" are ridiculed, and confronted with the equally cheap slogan "everything is chemistry" (Goldberg and Chemjobber 2014; Goldberg et al. 2016). The preference for natural products is branded as 'chemophobia', an exaggerated fear of chemistry, based on a lack of scientific knowledge, and only to be solved by better educating the masses (Gribble 2013; Kennedy 2018). In fact, many of these arguments are brought forward with exactly the kind of linguistic and philosophical imprecision that, in the same breath, the general public is accused of displaying.[1] Empirical studies show that chemists overestimate how negative the public image of chemistry actually is (Rip 2006; Royal Society of Chemistry 2015; Hampel 2017). This phenomenon has itself been termed 'chemophobia-phobia' – the exaggerated fear of chemists that the public might be afraid of chemistry (Rozendaal 1981, Lorch 2015, cf. Schnurr 2025a). In many ways, the misrepresentation and disregard that the chemistry community holds against the public expression of concern regarding the risks of chemistry is at the root of public mistrust (cf. Wynne 2001).[2]

Successful mediation of the debate about 'chemistry and nature' requires transdisciplinary communication and disciplinary reflection. While I have outlined some approaches to the former in a previous article (Schnurr 2022), I want to engage here in the latter by clarifying what 'nature' actually means for a chemist. So far, this question has been addressed only in a few publications, most directly in Joachim Schummer's article *The Notion of Nature* in Chemistry (2003), and Roland A. Fischer's chapter *Natürlich, naturidentisch,* künstlich (1996). The collected volumes *Chemie und Geisteswissenschaften* (1992), *Natürlich, technisch, chemisch* (1996), and the works of Bernadette Bensaude-Vincent (2005, 2008a) provide a larger interdisciplinary framework around the topic 'chemistry and nature'. In this article, I build on this groundwork by critically examining the predominantly 'naturalistic' notion of 'nature' in chemistry from an ecological perspective. I will argue that the self-image of chemistry as a synthesis science is ecologically vacuous and therefore at the core of chemistry's unsound relationship to the ecological world. The current trend towards the digitization of chemistry is, in that regard, a chance to 'update' that self-image. Incorporating ecological thought into digital chemistry projects and involving

[1] A typical logical fallacy in the 'chemophobia'-literature is the inference that, because everything in nature has a chemical dimension to it, chemistry in its entirety can be considered 'natural'. Typical straw man arguments imply that the public is unaware of the hazards that natural substances pose, or that the disapproval of synthetic substances is primarily a form of fear (instead of a form of political criticism).

[2] I attempt a more constructive criticism of the everyday language dichotomy between 'chemistry' and 'nature' (e.g. as employed in advertisement) in a forthcoming article (Schnurr 2025b).

digital methods in sustainable chemistry projects are important pillars of making chemistry less unsustainable in the twenty-first century.

The article progresses in six steps. First, I describe the naturalistic understanding of 'nature' in chemistry, including its conceptual origins. Second, I characterize it as 'monistic' and 'potentialistic'. In the third step, I engage deeper with the potentialistic aspect in the context of the 'chemical space' concept. Fourth, I outline the self-image of chemistry as a synthesis science and show how the digitization of chemistry interacts with that self-image. In the fifth step, I assess these considerations from an ecological point of view, before, in the sixth step, I provide an outlook of how the digitization of chemistry can work hand-in-hand with ecological concerns.

'Nature' in chemistry

There is no 'official' definition of 'nature' in chemistry (e.g. by an authority like the International Union of Pure and Applied Chemistry (IUPAC)) for reasons stated above and below. However, there are a few publications (named above) that explicitly deal with the subject. They are the result of designated reflection on the topic (e.g. based on conferences on 'chemistry and nature'), are peer-reviewed, and, in my experience, represent the opinion of a large number of chemists. The view expressed in them is that all chemical substances, whether of biological or synthetic origin, are equally 'natural'. I call this the '*naturalistic*' understanding of 'nature' in chemistry. (I adopt the term 'naturalistic' from philosophers Peter Janich (1996) and Gregor Schiemann (2005), referencing the philosophical branch of naturalism which rejects the existence of non-natural entities and argues that reality is exhausted in 'nature'). As we will see, this is not the only concept of 'nature' in chemistry (however, the dominating one), but it is the one strongest at rift with ecological concerns. Therefore, I will analyze the naturalistic understanding of 'nature' in chemistry in detail here, point out the problems attached to it, and argue for strengthening an ecological perspective.

Conceptual origins

The naturalistic understanding of 'nature' in the natural sciences arose with the scientific revolution in the sixteenth and seventeenth centuries. While the word 'revolution' has gained some criticism from historians of science, who point out the many continuities with previous (medieval) knowledge systems (Principe 2011), the scientific revolution indeed led to important changes in the concept of 'nature', which I want to briefly outline here.

Breaking with the scholastic tradition of the Middle Ages (which combined antique Greek philosophy and theological thought), a new method of knowledge discovery formed around seminal works in astronomy, and physics, e.g. Copernicus' *De revolutionibus* (1543), Bacon's *Novum organon* (1620), Galileo's *Discorsi* (1638), Boyle's *New Experiments* (1660) and Newton's *Principa* (1687), to name just a few. The concepts of empirical observation, experiment, mathematization, and natural laws became the methodological centers of the modern sciences (Peuker 2016). With this came a turn away from the Aristotelian philosophy of nature. This is probably best exemplified in the discussion of locomotion: The Aristotelian idea of 'natural motions' – i.e. heavy things (stones, water) moving downward towards the earth, light things (fire, air) moving upward away from the earth – held a distinction between ‘natural’ and ‘forced’/‘violent’/ ‘unnatural’ motion (Aristotle 1922, Bodnar 2023). This distinction was overcome with Galilean and later Newtonian mechanics, where the trajectories of spatially moving objects were formulated within mathematically expressed laws of nature (Principe 2011). A stone thrown upwards was now seen as following its ‘natural’ (lawful) course of movement. This lawfulness was emphasized by the fact that such an experiment could be reliably reproduced. The distinction between ‘natural’ and ‘unnatural’ locomotion was overcome by conceptualizing the ‘forced’, artificially-induced motion as an experimental-technical action outlining the law-like condition of nature (Hoyningen-Huene 1989; Janich 1996). If extended to material change in general this perspective holds that both natural changes and the human capacities to change nature are constrained by the same general dynamics phrased as laws of matter (Schummer 2003). With this, the ‘natural’ and the ‘technical’ not only ceased to stand in antithesis, but they entered a dialectic relationship: The technical experiment became the focal point of generating knowledge about ‘nature’; at the same time, the technical realm submitted to the boundaries of natural laws and acknowledged them as its premise (Cassirer 1985).

The naturalistic understanding of ‘nature’ in chemistry

These developments (I showed mere snippets of them) are the conceptual origins of chemists today rejecting the everyday language distinction between ‘natural’ and ‘artificial’ substances. Let us look at how this is expressed by contemporary chemists, taking the example of chemistry professor Roland A. Fischer (1996, my translation, also in following quotes) who reflected on the ‘natural’ and the ‘artificial’: “These words are no *termini technici* in chemistry, like ‘element’ or ‘compound’. The current theoretical framework of chemistry does not distinguish between ‘natural’ and ‘artificial’ chemistry.” Fischer goes on to beautifully describe his own experience as an inorganic and metalorganic chemist where not so much the success but rather the failure of experiments regularly reminds him of the ‘natural’ premises and limitations of his work. “Oscillating between success and failure, between chemical events that are perceived as possible and as impossible, an aspect of the reality of nature reveals itself to me” (Fischer 1996). It is the law-like and often unexpected ‘invisible hand’ of what is ‘naturally (im)possible’ that leaves him with the impression that amid all these deliberate, artificial interventions into matter, that are the daily bread of the chemist, there is “a certain ‘naturalness’” (Fischer 1996) at play. What he experiences is the methodological irony of the natural sciences: ‘nature’ unveils itself in the technical apparatus; the laboratory is the birthplace of knowledge of ‘nature’.

While Fischer gives good insight into the perspective of a practicing chemist, philosopher of chemistry Joachim Schummer has provided the theoretical account. In *The Notion of Nature in Chemistry* (2003) Schummer argues for a “dynamic” understanding of ‘nature’. “[N]ature is the total of subtle forces, virtues, or tendencies of matter”, and more specifically “nature in chemistry is […] the chemical dynamics among all possible substances, their specific reactivities and changeabilities” (Schummer 2003). Schummer leaves it open “how chemical dynamics is to be interpreted theoretically” (Schummer 2003), for example avoids the question of whether chemical dynamics are ‘law-like’ or not (probably because the concept of natural laws is still controversially debated in the philosophy of chemistry)[3] and only briefly refers to the Greek origin 'δύναμις' (dynamis) meaning "potentiality, force, or tendency" (Schummer 2003). But even without a theoretical interpretation of 'chemical dynamics' it becomes clear that Schummer's notion of 'nature' is 'naturalistic' in the sense outlined above: he proposes to "use the term 'nature' for the object chemists have actually studied whenever they were pursuing chemical knowledge" (Schummer 2003). 'Nature' in that sense becomes synonymous with "chemical reality and possibility" (Schummer 2003).

This has two important consequences that I will address under the headwords of 'monism' and 'potentialism'.

Monism. 'Nature' without an opposite

The naturalistic understanding of 'nature' is monistic insofar as there is no meaningful opposite of 'naturalness'. If, to the naturalistic chemist, 'nature' is synonymous with "chemical reality and possibility" then "'unnatural' simply means chemically impossible" (Schummer 2003). This is also what Fischer described from the viewpoint of the practicing chemist. "A chemist cannot make chemical impossibilities possible" (Fischer 1996). 'Nature' sets boundaries to what is chemically achievable, but, by the same token, everything that is chemically achievable is 'natural'. This is fundamentally different from the everyday language understanding of 'nature' which is typically a dyadic one. There, 'nature' is used as a complementary term opposed to realms of human practice (e.g. nature and technology, nature and art, nature and human spirit) (Spaemann 2012; Martin 2022). In the case of chemical substances, such dyadic understandings draw a distinction between 'natural' and 'artificial' substances along the lines of human material history, technological creativity, or ecological compatibleness (more of that later). From a naturalistic perspective, on the contrary, only 'impossible' substances (e.g. a double-bounded hydrogen atom) would be 'unnatural'. This understanding is prominently featured in the epigraph that Fischer chose for his chapter: "Only miracles are really 'artificial', since they are impossible" (Stanislaw Lem, cited in Fischer 1996). With such limitations – perhaps the wine that Jesus made out of water in the Gospel of John is truly 'unnatural'? – any practically meaningful opposite of chemical 'naturalness' vanishes. As Janich (1996, my translation) sums up the monistic aspect of the naturalistic understanding of 'nature': "Everything is natural".

Potentialism. 'Possible nature'

The second noteworthy aspect of the naturalistic understanding of 'nature' is that it is potentialistic. It also considers *possible* events and outcomes 'natural'. More precisely, it considers *all* possible events and outcomes 'natural'. We have seen this in Fischer (1996) for whom the authority of 'nature' lies in what is possible and what is not, making – conversely – every possible chemical event and outcome 'natural'. Similarly, Schummer (2003) adds that 'nature' is not just "chemical reality" but also chemical "possibility".

[3] Less elaborated accounts of the naturalistic approach are quicker to phrase it like this: "All reactions during artificial synthesis take place following the laws of chemical combination which are laws of nature. No law of nature is being violated during artificial organic synthesis" (Nidiry 2021).

Such potentialistic understanding of 'nature' is not just a chemical issue but a general one of the natural sciences, as Peuker (2016, my translation, also in following quotes) points out: "The modern, mathematically formulated concept of the law of nature confirms what was already inherent in the concept of experiment: the object of the natural sciences is not only the actually existing nature, but also the possible nature." This has been generally discussed by philosophers and sociologists of science (Böhme et al. 1978; van Daele 1987). For chemistry, however, the concept of 'possible nature' takes on a very specific form. To understand this, I will briefly introduce the concept of 'chemical space'.

Chemical space

'Chemical space' is a concept that gained popularity around the turn of the millennium. The term 'space' has to be understood in an abstract sense (e.g. similar to a Euclidian space), as a set of objects – in this case, chemical species – with a notion of 'nearness' (or distance) among them. This nearness can be based on structural similarity, synthetic reachability, or other descriptors of chemical species. In that sense, substances of a specific substance group (e.g. prenylated flavonoids or para-substituted benzenes) are (always only under a specific perspective) close to each other in chemical space (Restrepo 2022).

The chemical space as a whole is understood as the entire set of chemical species. A few cases should be differentiated here. The *potential* chemical space comprises *all possible* chemical species. In the most basic sense, this would mean just any random ensemble of atoms held together by chemical bonds. Schummer (1996, my translation, also in following quotes) has called this 'a priori possible substances'. Mathematical chemist Guillermo Restrepo (2022) has provided a respective calculation, based on the estimated number of atoms in the universe. A much smaller number would be that of all '*theoretically* possible substances', as Schummer (1996) calls those substances whose experimental realization seems feasible based on chemical theory. A modest subgroup of that would be the 'Weininger number' 10^{200} which chemoinformatician Davin Weininger hypothesized to be the number of possible substances consisting of C, N, O, P, S, and halogens, with a molecular weight less than 1000 dalton (Restrepo 2022).

The upper bounds of the potential chemical space are so high that all the matter in the universe would not suffice to create one molecule of each chemical species at the same time (one would need to synthesize them one after the other). And even if that would succeed, the respective information generated would transgress the upper limit of how much information is storable in the physical universe (10^{123} bits; Bekenstein bond) (Restrepo 2022). The potential chemical space is so large that any attempt to actually materially produce a subset of it is necessarily limited to miniature fractions. This means that the *actual* chemical space at a given time is always just a shadow of the theoretically possible chemical space.

This is even more remarkable considering that the actual chemical space – all chemical species that have been described at a certain point in time – has expanded rapidly over the last two hundred years. Starting with the advent of organic synthesis at the beginning of the nineteenth century, chemists increased the portfolio of known substances at an exponential rate, doubling its size roughly every 16 years (Restrepo 2022). While organic chemistry was initially concerned with substances derived from plants and animals, already by the year 1830 substances of synthetic origin outnumbered those of biological origin (Ramberg 2022). In 1869, the year that Mendeleev published his first draft of the periodic system, the total number of known chemical substances was 11,000 (Restrepo 2020). Growing through different periods – Llanos et al. (2019) differ between a proto-organic (1800–1860), organic (1860–1980), and organometallic (1980–present) regime – the corpus of known chemical substances has reached an enormous size. In the year 2024, the actual chemical space – all chemical species described since 1800 – comprised roughly 20 million chemical species, more than 90% of them synthesized (and not of biological origin) (Restrepo 2022).

Note that 20 million is a rather conservative estimation based on Restrepo (2022). Digital databases like Reaxys (Elsevier) or the CAS Registry (American Chemical Society) give even higher numbers of "179 million organic, inorganic and organometallic substances" (Reaxys 2024) or "219 million organic substances, alloys, coordination compounds, minerals, mixtures, polymers, and salts disclosed in publications since the early 1800s" (Chemical Abstract Service 2024). However, these databases also include so-called 'prophetic substances'. These are chemical compounds listed in the embodiments of patents that have not actually been synthesized but whose *synthesizability* is held out in prospect by the procedure laid out in the patent. This is not some rare exception but rather a common example of how fluid the borders between the potential and the actual chemical space are.

Similar to 'prophetic substances', chemical vendors have started in recent years to offer large digital catalogs of 'make-on-demand' substances. These are substances that have never actually been produced and are not available 'in-stock' but are *very likely synthesizable* from in-stock substances (Irwin et al. 2020). The development of digital make-on-demand libraries has expanded the amount of commercially available molecules since 2016 from 3.5 million to over 29 billion compounds (Lyu et al. 2023). In just a few years, the "purchasable chemical space" has become predominantly populated with 'possible' chemical species. Today, more than 99.9% of the world's catalog molecules have never actually existed so far but are merely digital representations (Irwin et al. 2020).

The (ontological) status of these compounds is an interesting question for the philosophy of chemistry. Sometimes called "tangible molecules" (Tingle et al. 2023), these compounds are not just theoretically possible but readily accessible in practice. Their synthesis success rate is > 85% "which is about the same success rate as for supposedly in-stock compounds", and it typically takes only 6 weeks to actually produce them (Irwin et al. 2020). I suggest understanding the "tangible chemical space" as a subgroup of the 'theoretically possible chemical space', with additional practical criteria: the experimental realization of its constituents is not only feasible based on chemical theory (Schummer's criterium for 'theoretically possible') but also held out in prospect by the current constitution of the practical domain of substance production (e.g. technical capabilities of vendors, size of in-stock libraries for educts, the corpus of reliable synthesis methods, …).[4]

The self-image of chemistry

Several points have become clear. The digitization of chemistry is rapidly unfolding. The enormous size of the potential chemical space dwarfs the actual chemical space. The digitization of chemistry is not a mere 'side project' but is becoming a central platform for deciding on which substances are being produced in practice. Potential and actual chemical

[4] I specify it as "current" because what is "tangible" varies over time.

space are tightly interwoven, they mutually inform each other, and the boundaries frequently get malleable, e.g. in the case of ‘prophetic’ or ‘tangible’ substances. In the exploration of chemical space, substances of biological origin (“natural substances” in everyday language) play a marginal role. They make up less than 10% of the actual chemical space and a minimal fraction of the potential chemical space.

In a way, the concept of (potential) chemical space is the epitome of the naturalistic understanding of ‘nature’. To the naturalistic chemist, not just all substances of the actual chemical space are equally ‘natural’ (what I called ‘monism’), but also all substances of the potential chemical space (what I called ‘potentialism’). More importantly, the concept of chemical space (maybe for the first time in modern chemistry) gives chemists the possibility to envisage ‘nature’ *as a whole*. A grand, holistic view on ‘nature’ has typically been associated with physics. One may think of the famous quote attributed to Rutherford that “all science is either physics or stamp collection”.[5] Chemistry with its numerous exceptions and individual cases, its pragmatic, often rule-based (and not law-based) approach to the material world (Ruthenberg 1994), seems to rather describe individual phenomena of ‘nature’ than its entirety. Traditionally, a universalistic approach to (naturalistic) ‘nature’ has been associated with physics. Since its origins, physicists have tried to find unifying theories for phenomena of astronomical magnitude and microscopic minuteness. Nowadays, the dream of describing ‘nature’ as a whole is aspired in physics in the search for a “world formula” (or “theory of everything”) – a complete quantum theory including general relativity, which would offer a single theoretical framework for all physical phenomena, from the Big Bang to subatomic particles. The chemical space concept now offers similar visions of grandness to chemistry. However, a major difference is that the approach of physics is “bathogenous” (from Greek bathús, ‘deep’), as Liegener and Del Re called it. “[T]he ultimate goal is to proceed to ‘deeper’ and ‘deeper’ levels of reality, so as to show that all phenomena are the result of the interaction of a few elementary particles, indeed are manifestations of a single unified field” (Liegener and Del Re 1987). Chemistry, on the other hand, has a “horizontal” approach, which “consists in the ordering of facts into categories, omission of irrelevant concepts and introduction of operative ones” (Liegener and Del Re 1987). The chemical space concept now offers a chance for chemistry to be “on par with physics” (Schummer 2003) by assessing ‘nature’ in its totality (and not just snippets of it) while at the same time staying true to its “horizontal” approach, “floating at a certain level” (Liegener and Del Re 1987) of engagement with the material world (namely the molecular level). However, there are principal limitations (discussed above) to how comprehensively chemistry can fulfill its aim of exploring the entire potential chemical space. Rather than ‘realizing’ (synthesizing) the entire potential chemical space, “[t]he charm of chemistry lies in finding a minimal set of features characterizing the extension of the space and its diversity” (Restrepo 2022). Ironically, at the exact moment that chemistry has ‘finally’ found a framework for engaging with ‘nature’ as a whole, the vastness of chemical space also ‘puts it in its place’, leaving only the humbler option of searching for a much smaller ‘representative’ subset, that Restrepo (2022) calls “interesting chemical space”.

Physics’ grand endeavor to apprehend ‘nature’ as a whole has had the welcome side effect that many physicists developed an interest in philosophy. Will the debates about chemical space do the same to chemistry? Necessarily, chemical space projects

[5] Mentioned in Restrepo (2022). The quote goes back to physicist John Desmond Bernal mentioning in *The Social Function of Science* (1939) that “Rutherford used to divide science into physics and stamp collecting”.

incite metachemical questions about the overarching aims of chemistry. Restrepo (2022) begins his article about the vastness of chemical space with such a reflection: "Chemistry is about producing new substances and innovative methods to procure them. It is about documenting such a material enterprise for the sake of reproducibility and, above all, of expanding chemical knowledge." In the first sentence, one can already see how strongly the concept of chemical space touches upon the self-image of chemistry as a synthesis science. At least since Marcellin Berthelot's famous maxim "chemistry creates its own object", knowledge creation in chemistry has been understood as intricately interwoven with synthesizing (new) substances (Ruthenberg 2024). To the chemist, analyzing something includes synthesizing it. "Chemists are laboratory workers, they are learning about matter through making materials", is how Bernadette Bensaude-Vincent quotes Gaston Bachelard's account of this self-identity. "Knowing through making, making things and making them pure, as artefacts, is the chemist's approach to nature" (Bensaude-Vincent 2008b). By producing new substances, chemists are changing the material world. Chemistry continuously expands its own subject area. Ruthenberg (2024) has discussed this in reference to Michael Heidelberger's expression "Erweiterung der Wirklichkeit im Experiment" (experimental expansion of reality). Schummer (1997) similarly uses the expression "Stoffliche Weltveränderung der Chemie" (substance-ial world change of chemistry). In their epistemological pursuit, chemists go to enormous lengths. Schummer (2004) has pointed out that "the great majority of synthetic research is performed to improve the synthetic abilities of chemistry itself", meaning most substances are synthesized in order to have better means for synthesizing other substances. "[P]roducing new substances is actually an end in itself for the whole field" (Schummer 2004).

How does the concept of chemical space relate to the self-image of chemistry as a synthesis science? In one way it reinforces this self-image by providing the ultimate prospect of all possible substances that can be synthesized. In another, it dampens it by putting up principal limitations to the synthetic regime. Synthesizing the whole potential chemical space seems like a hopeless endeavor. Probably the most important point is that the ties between actually synthesizing and digitally modeling chemical substances are growing closer. To use drug discovery as an example: The question of which substances are suitable drug candidates is answered based on computational screenings of make-on-demand libraries using molecular docking simulations (Lyu et al. 2023). Decisions about actual syntheses are made based on digital models. These simulations are, in turn, not exclusively digital endeavors but informed (and validated) by actual syntheses and property (e.g. bioactivity) tests. "[C]hemical space [is] not an abstract mathematical structure, but a space constructed from concrete chemical experiences" (Schummer 1996). If, in the end, a molecule turns out to be a promising drug candidate, this information will again feed the information landscape of the chemical space. Substantial changes in the shape of the chemical space for drug discovery might eventually change fundamental assumptions about what a good drug candidate even looks like. This again leads to different decisions of which drugs are actually produced. To sum it up: In the digital age of chemistry, both are increasingly intertwined: what Schummer (1996) called the "systematization of the possible based on the factual" and the "systematization of the factual based on the possible". Chemistry – while remaining a synthesis science – is increasingly becoming a simulation science.

An ecological critique

In recent years, historians of science, science and technology studies (STS) scholars and (more rarely) philosophers of chemistry have increasingly worked towards deconstructing the image of chemistry as a 'neutral', 'non-political', 'purely scientific' endeavor. Not only do chemical scientists, institutions, and companies exhibit political influence, and not only are chemical products central to political projects (be it a war, or a healthcare campaign), but even "the ways in which we know and represent the world […] are inseparable from the ways in which we choose to live", as Nieto-Galan (2019) claims in *The Politics of Chemistry*:

"[C]hemistry, just like any other human activity, must be deeply embedded in the social practices that shape its identity (being a chemist), norms (nomenclature, academic disciplines), conventions (research funds, grants), discourses (public addresses, publications), instruments (labs, experimental culture) and institutions (universities, research centers, academies). Therefore, 'doing' chemistry merges into 'doing' politics" (Nieto-Galan 2019).

I want to add to this list that also notions of 'nature', be it the naturalistic one that chemists predominantly hold, or the one used in everyday language, are not as apolitical as is (sometimes explicitly, more often implicitly) assumed.[6] The synthetic paradigm of chemistry – generating thousands of new substances every day, mainly for the sake of enhancing said paradigm even further – is tightly woven into its self-image as a synthesis science. This paradigm only seems reasonable, even desirable (and, hence, remains widely unquestioned by chemists) based on a naturalistic understanding of 'nature'. The high appreciation of the synthetic domain is inseparably connected to a monistic understanding of 'nature' that is indifferent towards the biological or synthetic origin of a substance. The aspiration to widen the pallet of existing substances further and further rests on the potentialistic idea that 'nature' is expandable. Only if 'nature' is understood as the sum of all possible substances, does the exploration of chemical space and its astronomical possibilities (most of which will never see the light of day) seem like the ultimate fulfillment of the chemical enterprise.

This synthetic paradigm is not just a private self-image of individual chemists but is embraced and reinforced by official institutions. As a part of the US-American National Research Council, the Committee on Challenges for the Chemical Sciences in the 21st Century (2003) wrote in their periodical report on the status of chemistry: "The long-term goal of the basic science in synthesis is to develop the ability to create all the substances and organized chemical systems and transformations that are possible under the limits of natural laws […]. The importance of such an extension of Nature is […] part of the basic science of chemistry itself."

The naturalistic understanding of 'nature' in chemistry is in stark contrast with the everyday language understanding of 'nature', where it is primarily understood in ecological terms. Ecology offers the most connectable (and in that sense most successful) framework of thinking about 'nature' today. Across the board, in science, politics, economics, literature, advertisement, and everyday life, ecological ideas shape discussions about 'nature'. This success stems from the

[6] This insight, in general, is, of course, not new in the slightest. At least since Lynn White's influential paper *The Historical Roots of Our Ecologic Crisis* (1967) questioning notions of 'nature' with regards to their cultural and political context is more than common in the (environmental) humanities. I merely apply this to the debate about 'chemistry and nature'.

two-sidedness of the ecological understanding of 'nature': It is both a scientific and an ethical framework. From a scientific point of view, it conceives 'nature' as the entirety of several interconnected systems (cosmological system, earth system, biosphere, ecosystem, organisms) that influence each other via physical and metabolistic relationships, but in themselves function in a self-regulatory fashion. From an ethical point of view, the ecological understanding of 'nature' reveals the uniqueness, complexity, diversity, richness, autonomy, sensibility, and vulnerability of planetary life (Wirtz 1992; Rink et al. 2004; Soentgen 2020). By that, it offers both: a conceptual framework for understanding 'nature' and a relational framework for appreciating, caring for, and protecting 'nature'. Since it acknowledges both the ecological disposition of humans and the disruptive element that (certain) human actions pose on ecological relationships and material cycles, it does not make for the typical dualisms of 'nature-versus-culture'. At the same time, it offers a means of singling out anthropogenic material practices that disrupt the self-regulation of a system (earth system, an ecosystem, or the metabolism of an organism). It can therefore give guidance to political decisions about how to structure human material culture. The ecological perspective on 'nature' provides a holistic framework for human engagement with 'nature': it offers understanding, relation, and orientation.

From an ecological perspective, the naturalistic understanding of 'nature' that is predominant in chemistry is disconcerting. The monistic idea that all chemical substances are equally 'natural' is contrasted with the ecological insight that some substances align with the metabolism of organisms, ecosystems, and the earth system better than others. Chlorofluorocarbons that deplete atmospheric ozone, per- and polyfluoroalkyl substances that do not degrade in ecosystems, or chlorinated hydrocarbons that accumulate in organisms are examples of substances that can be called 'unnatural' from an ecological point of view. The potentialistic idea that 'nature' can be expanded is contrasted from an ecological perspective with an appreciation of the delicate attunement between the constituents of a system. The self-image of chemistry as a synthesis science and the accompanying growth regime is contrasted by the idea of planetary boundaries that safeguard the self-regulatory capacities of earth system and ecosystems (Persson et al. 2022).

The naturalistic understanding of 'nature' in chemistry does not allow for such considerations. It is ecologically vacuous. 'Nature', seen naturalistically as the entirety of possible chemical dynamics and outcomes, has no special place for substances of biological origin or in metabolic cycles. It is *an*ecological, one could say (as in *a*historical, or *a*political). The naturalistic understanding of 'nature' in chemistry does not stand in opposition to ecological thought but in complete disregard of it.

It is, therefore, not suited to offer conceptual, or even practical, guidance in times of an (among other factors) 'chemically-induced' global environmental crisis. Synthetic chemical substances, once they 'leave the laboratory', are central "agents of global change"; the production volume and diversity of synthetics that end up in the environment is increasing at rates greatly surpassing those of other drivers of global environmental change (Bernhardt et al. 2017). Scientific assessments and regulatory measurements are "falling woefully behind" in securing the safety of new compounds (Burton et al. 2017; Daley 2017). 80% of the substances registered as non-intermediates with above 1 tonne per year production in the European Union's REACH framework (Registration, Evaluation, Authorisation and Restriction of Chemicals), still had their risk assessment outstanding after 10 years of operating time of REACH (Persson et al. 2022).[7]

[7] I use REACH as a rather moderate example to stick to substances that are actually marketed. More general accounts of the same issue are often less informative, e.g. Gessner and Tlili (2016) use the CAS registry numbers and claim that of "over 100 million unique chemical substances, less than 0.36% […] are

A naturalistic chemist can worry about this, but – to phrase it pointedly – only if she starts thinking like an ecologist (or a biologist, or a toxicologist). If the naturalistic chemist wants to be concerned about the consequences of the synthetic growth regime of chemistry, she has to step outside of the dominant approach to 'nature' in chemistry and adopt the perspective of an ecologist (or an ethicist, or a political thinker).

This has been frequently expressed by the proponents cited above. Fischer (1996) said: "The science of chemistry, which I understand as the ever-growing sum of all material transformations and effects that are found to be possible, does not provide me, as a chemist, with answers to questions of values. [...] The path from what can be done to what ought to be done, the decision between what is to be desired and what is to be avoided, is precisely not a chemical question." Similarly, Peuker (2016) claims for the natural sciences, in general: "Science only shows a range of possibilities, but the concretization and realization of these possibilities lies outside the sciences in the decisions of politics and companies. This difference between science and its application is all too often overlooked, with the result that the negative consequences of the application of science are attributed to science itself." In Schummer (2003), we even find a positive spin on this: "[S]ince the dynamic notion [of 'nature'] includes no moral constraints about the chemical change of our material world, [...] such constraints must be found in a general moral discourse with reference to generally accepted values." And isn't that a good thing? Isn't chemistry doing exactly what it should by 'staying out of the way' of ethicists, politicians, and a democratic public who can freely decide which of the possibilities that the humble servant provides ought to be implemented? Would not everything else be an infringement of the functional differentiation that characterizes modern societies?

So, is it a problem that chemistry outsources its ecological concern? As indicated above, this does not necessarily mean outsourcing it to 'somebody else' (e.g. a politician, an ethics think tank ...); many chemists themselves engage in environmental thought and action, but do they really do this *as chemists* (or rather as ecological thinkers, as political lobbyists, as concerned citizens ...)? And when we think of the transition disciplines between chemistry and ecology – e.g. ecotoxicology, chemical ecology ... – which are so intimately concerned about the biosphere and the organisms in it; does not their concern stem from 'the ecological side' of their discipline and less from the 'chemical side'? Should chemists be as comfortable with the ecological vacuum inherent to their naturalistic understanding of 'nature' as in the quotes above?

Footnote 7 (continued)

regulated." Such claims need to figure in that the majority of novel substances is only produced in amounts high enough for chemical characterization and never has any economic or environmental relevance. The number of chemical substances (and mixtures) that have actually been registered for production and use is around 350.000 (Wang et al. 2020). Of these, around 6000 make up 99% of the entire chemical production volume (Bond and Garny 2019). Claiming equal relevance for all hundreds of millions of chemical species registered in databases weakens an argument that, in my opinion, is best phrased in general terms: The synthetic growth regime of chemistry is contributing to more and more substances 'pushing' into the market and therefore increases the pressure that overwhelms scientists and regulators involved in safety assessment.

I want to comment on this from different sides.

(1) Simply looking at how 'personal' chemists tend to take the everyday language dichotomy between 'nature' and 'chemistry',[8] one might ask if this is not a (subliminal) expression of discontent towards the ecological vacuum in their disciplinary self-image.

(2) The intensity with which (many) chemists feel like they must engage with the debates about 'nature and chemistry' indicates that they feel like they 'have something to say' about the topic. While not necessarily thinking much about the term 'nature' in their disciplinary work, chemists, I assume, would still feel bypassed if one were to leave them out of a discussion about the meaning of the term 'nature'.

(3) While chemists seem to be comfortable with the fact that their disciplinary self-image does not involve ecological values it is of course not free of values in general. The self-image of chemistry as a synthesis science is guided by epistemic values: chemists ought to do what they do (primarily: synthesize new substances) because it increases chemical knowledge or extends the means to do such (e.g. when new substances facilitate the synthesis of others). Cherishing these epistemic values is connected to a regime of continuous growth. More chemical substances means more chemical knowledge. The dialectical irony that underlies this growth regime has been pointed out by Schummer (1999, my emphasis): "The growth of chemical knowledge increases our *lack of knowledge*." By adding new substances to the material world, chemists continually change their object of knowledge and thereby not only produce more knowledge but also "nonknowledge" about the (relational) properties of the new (corpus of) substances. "Thus, in general, synthesizing new substances produces much more nonknowledge than knowledge" (Schummer 2001). Especially if "new substances leave […] the laboratories and become part of our material environment" this "tremendously increases its chemical complexity, *i.e.* its chemical incomprehensibility. Thus, in real life, chemically produced nonknowledge turns into increased unpredictability of environmental changes induced by the introduction of new substances" (Schummer 2001).

(4) According to Schummer, chemists are morally responsible "for all possible harms caused by their creations" (Schummer 2001).[9] "Even if synthetic chemists themselves neither introduce their new substances into the environment nor promote them for commercial usage, their first synthesis of a substance is the crucial causal step for its existence and possible harm caused by that. […] Therefore, chemical synthesis is not a morally neutral activity, as many chemists tend to see it" (Schummer 2001). In a world where ecological degradation is increasingly attributed to synthetic chemical products (Bernhardt et al. 2017; Persson et al. 2022), do chemists really want to wear ecological blinkers while trying to synthesize as many substances as possible as fast as possible?[10]

[8] Examples of chemists getting polemical towards the everyday language distinction of 'natural' and 'chemical' substances can be found in Markl (1992), Gribble (2013), Schummer (2017), Kennedy (2018, 2021).

[9] Schummer (2001) adds that this of course does not exclude others (company executives, politicians …) from being responsible too. Furthermore, being morally responsible does not equate to 'being guilty' in case of harm (but is a prerequisite for it). The former is a question of causation, the latter a question of moral judgment. (One can be deemed not guilty of causing harm if one had sufficiently good reasons for one's action. This does not change the fact that one was responsible for the outcomes.).

[10] For example, a thought experiment of how to accelerate the synthetic regime in order to produce all 10^{200} 'Weininger'-substances by the year 2050 is discussed in Restrepo (2022).

(5) A starting point for a disciplinary self-image that assumes responsibility for the global environmental changes that chemical innovation brings about is the conception of chemistry as a "technoscience". The groundwork for this has been laid (among others) by Bensaude-Vincent (2013) who distinguishes between a 'weak' and a 'strong' notion of (chemistry as) technoscience. The weak notion acknowledges that chemistry is best understood as an "alliance of modern science, technology, and industry" with a "dual face as pure and applied science". The strong version questions the notion of scientific 'purity' itself, challenging the idea that matters of fact are discerned from matters of interest, or that only the *applications* of science are to be considered value-sensitive (Bensaude-Vincent and Loeve 2018). The notion of technoscience "attract[s] attention to a regime of production of science in which research is conducted in a context of application, where the setting of research priorities mimics the dynamics of markets while the production of knowledge mimics the industrial production of commodities." By blurring the boundaries of when chemistry is 'applied' and when it is 'pure', where it is 'merely academic' and where it is 'chemistry in practice', the notion of chemistry as technoscience can inspire the inclusion of practical concern for the social and ecological impacts of chemical products. This would open up the question of whether non-epistemic values such as "social robustness, social & economic relevance and sensibility to environment" (Bensaude-Vincent 2013) have a place in the disciplinary self-image of chemistry.

An ecological vision?

Ecologist Barry Commoner (1971) once called the expansion of synthetic organic chemistry in the eighteenth and nineteenth centuries "probably the most rapid burst of creativity in human history." With regards to the environmental pollution that many synthetic organic substances brought about in the twentieth century, he commented: "Only later was the potentially fatal flaw in the scientific foundation of the new technology discovered. It was like a two-legged stool: well founded in physics and chemistry, but flawed by a missing third leg—the biology of the environment" (Commoner 1971, as cited in Reibstein 2017).

At least since the 1960s, chemistry has been in search of that missing leg. The conceptual and practical efforts undertaken in this direction have been enormous. The inclusion of ecological ideas into chemical research and production has historically progressed in several different frameworks. According to Marcin Krasnodębski (2022a, 2023, 2024), the main fields that formed were *environmental chemistry* (since the 1960/70s in the United States, e.g. Moore and Moore 1976; Bockriss 1978), *Ökologische Chemie* ('ecological chemistry', since the 1970s in West Germany, e.g. Korte 1980), *Sanfte Chemie* ('soft chemistry', in the 1980/90 s in West Germany, e.g. Gleich 1989; Fischer 1993), *green chemistry* (since 1987 in Italy, later France and since the 1990s in the United States, e.g. Garrett and DeVito 1996; Anastas and Williamson 1998), and *sustainable chemistry* (roots in the 1990s, a more explicit identity since the 2010s, e.g. Kümmerer et al. 2013). Some newer frameworks like one-world chemistry (Matlin et al. 2016) or circular chemistry (Keijer et al. 2019) have been criticized for "reinventing the wheel" (Krasnodębski 2022b).

These approaches share the inclusion of ecological thought into the domain of chemical synthesis and production, e.g. in principles like benign-by-design, atom economy, or a (chemical) industrial ecology. The different frameworks vary in how radical they are. Green chemistry has a rather narrow focus on more efficient and less hazardous synthetic processes. Sustainable chemistry has a broader understanding of transformation, including social and economic perspectives (e.g. leasing chemicals). Sanfte Chemie demanded an alternative way of doing science and an ethics toward inanimate matter (Krasnodębski 2023, 2024).

Yes, an ecological vision of chemistry is possible, in fact, it has been laid out by chemists for the last 50 years. At the beginning of this article, I pointed out that the naturalistic understanding is not the only notion of 'nature' in chemistry. Ecological ideas like 'nature does not waste anything' or 'everything in nature is connected' form the background of many principles of environmental, green, and sustainable chemistry, for example green chemistry principle 1 (waste prevention) or circular chemistry principle 2 (maximize atom circularity) (Keijer et al. 2019). An extensive list of these principles can be found in the literature cited above. This brief overview only wants to showcase that the incorporation of ecological thought into chemistry is an ongoing and evolving process. My suggestion, now, is to stronger 'think together' the ecological transformation of chemistry with the other 'megatrend' – the rapidly unfolding digitization of chemistry.

In many ways, the convergence of the ecological and the digital transformation of chemistry is already happening, sometimes referred to as the "twin transition" (Cefic and Arthur D. Little 2023). Across the board, in chemical production, research, and education, there is growing awareness of possible synergies between digital and sustainable chemistry. To name just three examples of this awareness: In a recent industry survey, 40% of chemical companies claimed that digitalization will help them fulfill their sustainability goals (Ernst & Young 2022). In academia, master programs such as *Sustainable Chemistry and Digital Processing* at the University of Applied Science in Krems, Austria, are popping up (imc 2024). Similarly, the German youth science organization, together with Evonik, organized a forum for its alumni called *Towards a Digital Green Chemistry* (Jugend Forscht 2019).

The digitization of chemistry is, of course, not a homogenous field. Research in digital chemistry centers around computational techniques such as molecular dynamics, density functional theory (DFT), Bayesian optimization, design of experiments (DoE), machine learning (ML), and artificial intelligence (AI) (Schilter et al. 2024). The industrial production of chemicals further involves technologies such as cloud computing, smart sensors, internet of things, blockchain, and robotics as central parts of its digital transformation (KPMG 2024).

There are numerous case studies for the successful implementation of digital methods for sustainability purposes in chemical research and production. One such case is the acceleration of materials discovery for carbon capture technologies. Here, DFT studies aid the development of metal–organic frameworks (MOFs) and catalysts for carbon dioxide capture and conversion to methanol (Ye et al. 2013, 2014; Pinheiro Araújo et al. 2022, 2023). The resulting 'renewable methanol' can serve as a recycled feedstock for the chemical industry, contributing to the aims of green/sustainable/circular chemistry (e.g., departure from fossil feedstocks, recycling of waste/emissions). Recently, the process of MOF discovery for carbon dioxide capture has been accelerated by AI-driven tools (Hardian et al. 2020; Gulbalkan et al. 2024). For example, a random forest ML model was able to assign the partial atomic charges in MOFs with similar accuracy and 40% faster than the DFT-based methods (Kancharlapalli et al. 2021). Similarly, in the field of material discovery for clean energy, there have been proposals for an AI-based autonomous materials discovery process. This involves chemical space being narrowed down to promising candidates for a given problem (e.g., materials for photovoltaics or energy storage) that are achievable by automated synthesis and whose automated performance evaluation, after synthesis, informs the screening process via feedback loops (Tabor et al. 2018).

While these case studies revolve around the development of materials for sustainability applications, the *in silico* design of chemical products, in general, offers opportunities for a more sustainable product design, regardless of the application. Because computational techniques allow for a deeper understanding of chemical processes and enable modeling real-world scenarios, they facilitate the minimization of physical experiments, thereby streamlining the discovery process and reducing resource consumption (Schilter et al. 2024). Furthermore, the implementation of green metrics (cf. Blömer et al. 2024) into the design process of a new chemical product can help to put the philosophy of green chemistry into practice.

Besides product development, the improvement of operational efficiency is another possible area where digital tools can help to reduce the environmental impact of chemical production. Two examples of this are the integration of AI-guided bioprocess modeling in biorefinery systems ('smart biorefineries') (Arias et al. 2023) and DoE optimization techniques for yield and purity enhancement in pharmaceutical and fine chemical industries (Zuin Zeidler 2024). Also, environmental impact analysis of chemical products can profit from the digital transformation of the chemistry sector (Elisa IndustrIQ 2023). An example from the industry would be the BASF (2023) supercomputer *Quriosity* which, among many things, simulates the impact of (potential) pesticides on groundwater.

In light of these examples, the question arises of how serious of a disruption the digitization of chemistry really is for the predominant synthetic regime. In many instances, one could probably best speak of a digitally-guided optimization of the status quo. Therefore, the aim of this section is not to foster optimism but rather *attentiveness* towards the possible synergies between a digital and an ecological transformation of chemistry. With the chemical industry rapidly adopting digital technologies ('chemistry 4.0'), there is an opportunity (but also a closing time window) for deciding how deep (or shallow) these synergies might be.

Furthermore, the article does not want to perpetuate the idealism of computer chemists of the second half of the twentieth century, who were dreaming of a "chemistry without substance" (or, at times, purposefully evoking these imaginaries to boost their discipline).[11] In fact, thinking of digitalization processes as dematerialization processes comes with its flaws. The digital industry consumes 5–9% of the world's total electricity and accounts for 2–3% of global carbon dioxide emissions, indicating, in the case of chemistry, the need to balance the potential of new digital technologies with their environmental impact. It becomes clear that, in many ways, the digital and the environmental transformation are not necessarily "twins" but also antagonists. One might also expect 'rebound effects' where chemical production increases its efficiency and, as a consequence, increases its size (Debref 2012). These uncertainties correspond to the larger question of whether the environmental/green/sustainable chemistry frameworks even "correctly identify what should be rectified (aren't the supposed shortcomings of science the shortcomings of the economic system in which this science is ingrained?)" (Krasnodębski 2022b). In my opinion, this question is best answered based on evidence of whether alternative, more sustainable chemical processes actually lead to a 'phase-out' of the original processes (or just add a separate sphere to the current production regime).

[11] Here, I refer to the upcoming work on the history of computational chemistry by historian of chemistry Marcus B. Carrier.

With regards to synergies between the digital and the ecological transformation of chemistry, one might speak of 'weak' and 'strong' versions. A 'weak' synergy would be a digitally guided optimization of the status quo of chemical production (e.g. optimizing fossil-based synthetic routes). A 'strong' synergy would be if digital progress incites a change in one of the foundational pillars of chemistry's unecological constitution. I want to outline some possibilities of how this could look like.[12]

Currently, oil and natural gas account for 99% of chemical feedstocks, the remainder coming from biomass and coal (Tickner et al. 2021). If digital processes were to facilitate the switch to renewable feedstocks a major pillar of modern chemistry would be challenged. Such digital methods for automated discovery and assessment of competitive sustainable reaction routes that are based on renewable or waste feedstocks have recently been reviewed by Weber et al. (2021). In general, evaluating routes in reaction networks based on sustainability metrics like environmental impact factor, atom economy, or energy requirements would be an effective way to examine chemical space for sustainable pathways (Jacob et al. 2017; Weber et al. 2021).

Besides reaction networks, also chemical end products are increasingly evaluated with digital methods. Quantitative Structure-Activity Relationship (QSAR) modeling is already a common computational technique for predicting chemical (eco)toxicity (Romano et al. 2022). The further development of predictive (eco)toxicology will determine how effective the ecological risk assessment of large numbers of substances can be. In the best case, one can hope for swifter safety assessments and regulatory procedures, maybe finally stepping up to the ever-growing number of novel substances pushing into the market and therefore building a counterpart to the growth regime of synthetic chemistry.

Environmentally-minded chemists have always been willing to explicitly introduce values into chemistry.[13] An early proponent once called the design of safe chemicals a "domestication of chemistry" (Krasnodębski 2022a), whereupon a colleague of his noticed how fitting this was – given that domestication means "to adapt to life in intimate association with, and to the advantage of, man" (Garrett 1996). The digitization of chemistry might give new life to the idea of 'domesticating chemistry'. Restrepo (2022) has argued that chemical space is too big anyways to "synthesize every possible substance" which is why the real task is to find a representative "interesting chemical space". Maybe not under the primacy of epistemic values, but under the primacy of "placing the well-being of humanity at the heart of chemistry" (Krasnodębski 2022b) an *ecologically-benign chemical space*, oriented on principles of ecological/green/sustainable chemistry, would currently be the most interesting chemical space to model and explore. Such an ecologically-benign chemical space could serve as a suitable prefiguration of how a 'domesticated chemistry' could look like.[14] Certainly, it would be a proper ('strong') symbiosis of ecological and digital chemistry because ideas of 'digitally domesticating' chemistry challenge the unlimited growth regime of synthetic chemistry. After all, the success of a sustainable transformation of chemistry relies not only on the question of what chemistry can do but also on what it can *stop* doing.

[12] Several more (practical) ideas are discussed in Fantke et al. (2021).

[13] Already Moore and Moore (1976) wrote that the scientific "segregation of 'is' from 'ought' is perhaps arbitrary, and even worse may reduce the benefits which scientific inquiry can provide.".

[14] To add an economic incentive, perhaps constituents of the ecologically-benign chemical space could enjoy preferential treatment in regulatory procedures.

The self-image of chemistry as a synthesis science has guided the field for more than two centuries. The ecological crisis marked the point of insight into the malalignment of the synthetic regime with ecological values. Will the digitization of chemistry mark the point where this insight is increasingly put into practice? At least, it offers a possibility to reflect anew on the ecological aspirations that are so inherent in the chemical tradition as well and develop them further.

Acknowledgements The article is based on a talk given at the 27th annual conference of the International Society for the Philosophy of Chemistry. I thank all participants for their helpful feedback, especially Hrvoj Vančik. I also owe tremendous thanks to Guillermo Restrepo for his extensive help on questions of chemical space. My special gratitude goes to Jens Soentgen, Uwe Voigt, Simone Müller, and Helmuth Trischler for feedback on the draft. I thank Floris Winckel, Ivano Basile, and Sena Bozdag for minor comments. I am grateful to two anonymous reviewers for the fruitful discussion.

Author contribution Christian Schnurr is responsible for Conceptualization, Methodology, Writing—Original Draft, and Writing—Review & Editing.

Funding Open Access funding enabled and organized by Projekt DEAL. This research was carried out as part of the International Doctorate Program "Rethinking Environment" located at the University of Augsburg and the Ludwig Maximilian University of Munich and funded by the Elite Network of Bavaria.

Data availability No datasets were generated or analysed during the current study.

Declarations

Conflict of interest The authors declare no competing interests.

References

Anastas, P.T., Williamson, T.C. (eds): Green chemistry: Designing chemistry for the environment. ACS Symposium Series, vol. 626. American Chemical Society, Washington, DC (1998)

Arias, A., Feijoo, G., Moreira, M.T.: How could Artificial Intelligence be used to increase the potential of biorefineries in the near future? A review. Environ. Technol. Innov. **32**, 103277 (2023). https://doi.org/10.1016/j.eti.2023.103277

Aristotle: De Caelo: Transl. by Stocks, J. L. Clarendon Press, Oxford (1922)

BASF: Quriosity: Computing power for complex modeling, virtual experiments and simulations. https://www.basf.com/be/en/who-we-are/innovation/how-we-innovate/our-RnD/Digitalization_in_R-D/supercomputer#content-728936049 (2023). Accessed 22 December 2024

Bensaude-Vincent, B.: Faut-il avoir peur de la chimie? Les Empêcheurs de penser en rond, Paris (2005)

Bensaude-Vincent, B.: The new identity of chemistry as biomimetic and nanoscience. In: Bertomeu-Sánchez, J.R., Burns, D.T., van Tiggelen, B. (eds.) Neighbours and Territories: The Evolving Identity of Chemistry, pp. 53–64. Louvain-la-Neuve, Mémosciences (2008)

Bensaude-Vincent, B.: Chemistry as a technoscience? In: Llored, J.-P. (ed.) The Philosophy of Chemistry: Practices, Methodologies, and Concepts, pp. 330–341. Cambridge Scholars Publishing, Newcastle upon Tyne (2013)

Bensaude-Vincent, B., Loeve, S.: Toward a philosophy of technosciences. In: Loeve, S., Guchet, X., Bensaude-Vincent, B. (eds.) French Philosophy of Technology: Classical Readings and Contemporary Approaches, pp. 169–186. Springer, Cham (2018)

Bensaude-Vincent, B.: Matière à penser. Presses universitaires de Paris Nanterre (2008a)

Bernhardt, E.S., Rosi, E.J., Gessner, M.O.: Synthetic chemicals as agents of global change. Front. Ecol. Environ. **15**(2), 84–90 (2017). https://doi.org/10.1002/fee.1450
Blömer, J., Maga, D., Röttgen, J., Wu, Z., Hiebel, M., Eilebrecht, S., Jentsch, S., Eggers, N.: Assessment of chemical products and processes: Green metrics and life cycle assessment – A comparison. Chemie Ingenieur Technik **96**(5), 561–574 (2024). https://doi.org/10.1002/cite.202300229
Böhme, G., van den Daele, W., Krohn, W.: Die Verwissenschaftlichung von Technologie. In: Böhme, G., van den Daele, W., Hohlfeld, R., Krohn, W., Schäfer, W., Spengler, T. (eds.) Starnberger Studien 1. Die gesellschaftliche Orientierung des wissenschaftlichen Fortschritts, pp. 339–376. Suhrkamp, Frankfurt (1978)
Bockriss, J.: Environmental Chemistry. Plenum Press, New York (1978)
Bodnar, I.: Aristotle's Natural Philosophy: The Stanford Encyclopedia of Philosophy. https://plato.stanford.edu/archives/sum2023/entries/aristotle-natphil/ (2023). Accessed 9 December 2024
Bond, G.G., Garny, V.: Inventory and evaluation of publicly available sources of information on hazards and risks of industrial chemicals. Toxicol. Ind. Health **35**(11–12), 738–751 (2019). https://doi.org/10.1177/0748233719893198
Boyle, R.: A Free Enquiry into the Vulgarly Received Notion of Nature. Cambridge University Press, Cambridge (1996)
Burton, G.A., Di Giulio, R., Costello, D., Rohr, J.R.: Slipping through the cracks: why is the U.S. environmental protection agency not funding extramural research on chemicals in our environment. Environ. Sci. Technol. **51**(2), 755–756 (2017). https://doi.org/10.1021/acs.est.6b05877
Cassirer, E.: Symbol, Technik, Sprache: Aufsätze aus den Jahren 1927–1933. Meiner, Hamburg (1985)
Cefic, A. D. Little: Digital Technologies for Sustainability in the European Chemical Industry. https://cefic.org/app/uploads/2023/04/ADL_CEFIC_Digital_technologies_for_sustainability_2023.pdf (2023). Accessed 10 February 2025
Chemical Abstract Service: CAS Registry. https://www.cas.org/cas-data/cas-registry (2024). Accessed 10 September 2023
Committee on Challenges for the Chemical Sciences in the 21st Century: Beyond the Molecular Frontier: Challenges for Chemistry and Chemical Engineering. The National Academies Press, Washington (2003)
Commoner, B.: The Closing Circle: Nature, Man, and Technology. Knopf, New York (1971)
Daley, J.: Science Is Falling Woefully Behind in Testing New Chemicals. https://www.smithsonianmag.com/smart-news/science-falling-woefully-behind-testing-new-chemicals-180962027/ (2017). Accessed 13 September 2023
Debref, R.: The paradoxes of environmental innovations: the case of green chemistry. J. Innov. Econ. Manag. **9**(1), 83–102 (2012). https://doi.org/10.3917/jie.009.0083
Elisa IndustrIQ: Digitalisation: The Key to Sustainability in Chemical Manufacturing. https://elisaindustriq.com/blog-chemical-digitalisation-the-key-to-sustainability-in-chemical-manufacturing/ (2023). Accessed 9 February 2025
Ernst & Young: Why the chemical industry is prioritizing digitalization. https://www.ey.com/en_gl/insights/advanced-manufacturing/why-the-chemical-industry-is-prioritizing-digitalization (2022). Accessed 22 December 2024
Fantke, P., Cinquemani, C., Yaseneva, P., de Mello, J., Schwabe, H., Ebeling, B., Lapkin, A.A.: Transition to sustainable chemistry through digitalization. Chem **7**(11), 2866–2882 (2021). https://doi.org/10.1016/j.chempr.2021.09.012
Fischer, R.A.: Natürlich, naturidentisch, künstlich: Beiträge zur Begriffsbestimmung aus der Sicht eines Chemikers. In: Janich, P., Rüchardt, C. (eds.) Natürlich, technisch, chemisch: Verhältnisse zur Natur am Beispiel der Chemie, pp. 121–136. De Gruyter, Berlin, New York (1996)
Fischer, H.: Plädoyer für eine Sanfte Chemie: Über den nachhaltigen Gebrauch der Stoffe. C.F. Müller, Ambik, Braunschweig (1993)
Garrett, R.L.: Pollution prevention, green chemistry, and the design of safer chemicals. In: Garrett, R.L., DeVito, S.C. (eds.) Designing safer chemicals: Green chemistry for pollution prevention. ACS Symposium Series, vol. 640, pp. 2–15. American Chemical Society, Washington, DC (1996)
Garrett, R.L., DeVito, S.C. (eds): Designing safer chemicals: Green chemistry for pollution prevention. ACS Symposium Series, vol. 640. American Chemical Society, Washington, DC (1996)
Gessner, M.O., Tlili, A.: Fostering integration of freshwater ecology with ecotoxicology. Freshw. Biol. **61**(12), 1991–2001 (2016). https://doi.org/10.1111/fwb.12852
Gleich, A. von: Der wissenschaftliche Umgang mit der Natur: Über die Vielfalt harter und sanfter Naturwissenschaften. Campus, Frankfurt (1989)
Goldberg, A., Roth, K., Chemjobber, C.J.: Chemiefreie Haushaltsprodukte. Chemie in Unserer Zeit **50**(2), 144–145 (2016). https://doi.org/10.1002/ciuz.201600750

Goldberg, A., Chemjobber, C.J.: A comprehensive overview of chemical-free consumer products. Nat. Chem. (6), http://blogs.nature.com/thescepticalchymist/ (2014)
Gribble, G.W.: Food chemistry and chemophobia. Food Secur. **5**(2), 177–187 (2013). https://doi.org/10.1007/s12571-013-0251-2
Gulbalkan, H.C., Aksu, G.O., Ercakir, G., Keskin, S.: Accelerated Discovery of Metal-Organic Frameworks for CO2 Capture by Artificial Intelligence. Ind. Eng. Chem. Res. **63**(1), 37–48 (2024). https://doi.org/10.1021/acs.iecr.3c03817
Hampel, J.: Ein notwendiges Übel? Chemie in der öffentlichen Wahrnehmung. In: Weitze, M.-D., Schummer, J., Geelhaar, T. (eds.) Zwischen Faszination und Verteufelung: Chemie in der Gesellschaft, pp. 55–72. Springer, Berlin, Heidelberg (2017)
Hardian, R., Liang, Z., Zhang, X., Szekely, G.: Artificial Intelligence: the silver bullet for sustainable materials development. Green Chem. **22**(21), 7521–7528 (2020). https://doi.org/10.1039/d0gc02956d
Hoyningen-Huene, P.: Naturbegriff - Wissensideal - experiment: Warum ist die neuzeitliche Naturwissenschaft technisch verwertbar? Zeitschrift Für Wissenschaftsforschung **5**, 43–55 (1989)
imc: Sustainable Chemistry and Digital Processing. https://www.imc.ac.at/en/study/master/science-technology/sustainable-chemistry-and-digital-processing/ (2024). Accessed 22 December 2024
Irwin, J.J., Tang, K.G., Young, J., Dandarchuluun, C., Wong, B.R., Khurelbaatar, M., Moroz, Y.S., Mayfield, J., Sayle, R.A.: ZINC20-a free ultralarge-scale chemical database for ligand discovery. J. Chem. Inf. Model. **60**(12), 6065–6073 (2020). https://doi.org/10.1021/acs.jcim.0c00675
Jacob, P.-M., Yamin, P., Perez-Storey, C., Hopgood, M., Lapkin, A.A.: Towards automation of chemical process route selection based on data mining. Green Chem. **19**(1), 140–152 (2017). https://doi.org/10.1039/c6gc02482c
Janich, P., Rüchardt, C. (eds.): Natürlich, technisch, chemisch: Verhältnisse zur Natur am Beispiel der Chemie. De Gruyter, Berlin, New York (1996)
Jugend Forscht: Towards a Digital Green Chemistry. https://www.jugend-forscht.de/alumni/alumni-veranstaltungen/perspektivforen/towards-a-digital-green-chemistry.html (2019). Accessed 22 December 2024
Kancharlapalli, S., Gopalan, A., Haranczyk, M., Snurr, R.Q.: Fast and accurate machine learning strategy for calculating partial atomic charges in metal-organic frameworks. J. Chem. Theory Comput. **17**(5), 3052–3064 (2021). https://doi.org/10.1021/acs.jctc.0c01229
Keijer, T., Bakker, V., Slootweg, J.C.: Circular chemistry to enable a circular economy. Nat. Chem. **11**(3), 190–195 (2019). https://doi.org/10.1038/s41557-019-0226-9
Kennedy, J.: Fighting Chemophobia: The story of how we became afraid of chemicals and what to do about it. CreateSpace (2018)
Kennedy, J.: Everything Is Natural: Exploring How Chemicals Are Natural, How Nature Is Chemical and Why That Should Excite Us. Royal Society of Chemistry, London (2021)
Korte, F.: Ökologische Chemie: Grundlagen und Konzepte für die ökologische Beurteilung von Chemikalien. Thieme, Stuttgart (1980)
KPMG: Chemical Consulting Insights. https://kpmg.com/de/en/home/insights/2024/08/chemicals-4-0-this-is-how-the-chemical-industry-drives-sustainability-and-digitalisation-forward.html (2024). Accessed 9 February 2025
Krasnodębski, M.: Lost green chemistries: history of forgotten environmental trajectories. Centaurus **64**(2), 509–536 (2022a). https://doi.org/10.1484/J.CNT.5.131246
Krasnodębski, M.: Reinventing the wheel: a critical look at one-world and circular chemistries. Stud. Hist. Philos. Sci. **96**, 112–120 (2022b). https://doi.org/10.1016/j.shpsa.2022.09.004
Krasnodębski, M.: An unlikely bifurcation: history of sustainable (but not Green) chemistry. Found Chem. **25**(3), 463–484 (2023). https://doi.org/10.1007/s10698-023-09474-x
Krasnodębski, M.: Beyond green chemistry: Radical environmental transformation through Sanfte Chemie (1985–1995). History Sci. **62**(2), 280–304 (2024). https://doi.org/10.1177/00732753231194801
Kümmerer, K., Amsel, A.-K., Bartkowiak, D., Bazzanella, A., Blum, C., Cinqueman, C.: Key Characteristics of Sustainable Chemistry. Towards a Common Understanding of Sustainable Chemistry. https://isc3.org/cms/wp-content/uploads/2022/06/ISC3_Sustainable_Chemistry_key_characteristics_20210113.pdf (2013). Accessed 22 December 2024
Liegener, C., Del Re, G.: Chemistry vs. physics, the reduction myth, and the unity of science. Zeitschrift für Allgemeine Wissenschaftstheorie **18**(1–2), 165–174 (1987). https://doi.org/10.1007/BF01801083
Llanos, E.J., Leal, W., Luu, D.H., Jost, J., Stadler, P.F., Restrepo, G.: Exploration of the chemical space and its three historical regimes. Proc. Natl. Acad. Sci. U.S.A. **116**(26), 12660–12665 (2019). https://doi.org/10.1073/pnas.1816039116

Lorch, M.: Chemophobia, a chemists' construct. https://www.rsc.org/news-events/opinions/2015/jul/chemophobia-mark-lorch/ (2015). Accessed 11 November 2024
Lyu, J., Irwin, J.J., Shoichet, B.K.: Modeling the expansion of virtual screening libraries. Nat. Chem. Biol. **19**(6), 712–718 (2023). https://doi.org/10.1038/s41589-022-01234-w
Markl, H.: Die Natürlichkeit der Chemie. In: Mittelstraß, J., Stock, G. (eds.) Chemie und Geisteswissenschaften: Versuch einer Annäherung. Akademie Verlag, Berlin (1992)
Martin, C.G.: Systematische Einleitung: Die ästhetische Einstellung zur Natur als Gegenstand der Naturästhetik. In: Martin, C.G. (ed) Naturästhetik im Zeitalter der ökologischen Krise, pp. 1–32. mentis, Paderborn (2022)
Matlin, S.A., Mehta, G., Hopf, H., Krief, A.: One-world chemistry and systems thinking. Nat. Chem. **8**(5), 393–398 (2016). https://doi.org/10.1038/nchem.2498
Mittelstraß, J., Stock, G. (eds.): Chemie und Geisteswissenschaften: Versuch einer Annäherung. Akademie Verlag, Berlin (1992)
Moore, J.W., Moore, E.A.: Environmental Chemistry. Academic Press, New York (1976)
Nidiry, E.S.J.: Pesticides: Myths and Facts. Notion Press, Chennai (2021)
Nieto-Galan, A.: The Politics of Chemistry: Science and Power in Twentieth-Century Spain. Cambridge University Press, Cambridge (2019)
Persson, L., Carney Almroth, B.M., Collins, C.D., Cornell, S., de Wit, C.A., Diamond, M.L., Fantke, P., Hassellöv, M., MacLeod, M., Ryberg, M.W., SøgaardJørgensen, P., Villarrubia-Gómez, P., Wang, Z., Hauschild, M.Z.: Outside the safe operating space of the planetary boundary for novel entities. Environ. Sci. Technol. **56**(3), 1510–1521 (2022). https://doi.org/10.1021/acs.est.1c04158
Peuker, B.: Das Naturbewusstsein der Naturwissenschaften. In: Rückert-John, J. (ed.) Gesellschaftliche Naturkonzeptionen: Ansätze verschiedener Wissenschaftsdisziplinen, pp. 149–171. Springer, Berlin (2016)
PinheiroAraújo, T., Morales-Vidal, J., Zou, T., García-Muelas, R., Willi, P.O., Engel, K.M., Safonova, O.V., Faust Akl, D., Krumeich, F., Grass, R.N., Mondelli, C., López, N., Pérez-Ramírez, J.: Flame spray pyrolysis as a synthesis platform to assess metal promotion in In_2O_3 -catalyzed CO_2 hydrogenation. Adv. Energy Mater. **20**, 20 (2022). https://doi.org/10.1002/aenm.202103707
PinheiroAraújo, T., Morales-Vidal, J., Zou, T., Agrachev, M., Verstraeten, S., Willi, P.O., Grass, R.N., Jeschke, G., Mitchell, S., López, N., Pérez-Ramírez, J.: Design of flame-made $ZnZrO_x$ catalysts for sustainable methanol synthesis from CO_2. Adv. Energy Mater. (2023). https://doi.org/10.1002/aenm.202204122
Principe, L.M.: The Scientific Revolution: A Very Short Introduction. Oxford University Press, Oxford (2011)
Ramberg, P.J.: Introduction: Creating Modern Chemistry. In: Ramberg, P.J. (ed.) A Cultural History of Chemistry in the Nineteenth Century, pp. 1–40. Bloomsbury, London (2022)
Reaxys: What chemistry content is in Reaxys? https://www.elsevier.com/promotions/reaxys-solution (2024). Accessed 18 December 2024
Reibstein, R.: A more ethical chemistry. Curr. Opin. Green Sustain. Chem. **8**, 36–44 (2017). https://doi.org/10.1016/j.cogsc.2017.09.004
Restrepo, G.: Das periodische system und die evolution des chemischen Raums. Nachr. Chem. **68**(11), 12–15 (2020). https://doi.org/10.1002/nadc.20204094740
Restrepo, G.: Chemical space: Limits, evolution and modelling of an object bigger than our universal library. Digital Discov. **1**(5), 568–585 (2022). https://doi.org/10.1039/D2DD00030J
Rink, D., Wächter, M., Potthast, T.: Naturverständnisse in der Nachhaltigkeitsdebatte: Grundlagen, Ambivalenzen und normative Implikationen. In: Rink, D. (ed.) Naturverständnisse in der Nachhaltigkeitsforschung, pp. 11–34. Frankfurt, Campus (2004)
Rip, A.: Folk theories of nanotechnologists. Sci. Cult. **15**(4), 349–365 (2006). https://doi.org/10.1080/09505430601022676
Romano, J.D., Hao, Y., Moore, J.H.: Improving QSAR modeling for predictive toxicology using publicly aggregated semantic graph data and graph neural networks. Pac. Symp. Biocomput. **27**, 187–198 (2022)
Royal Society of Chemistry: Public Attitudes to Chemistry. Royal Society of Chemistry, London (2015)
Rozendaal, S.: Chemici Bang Voor Chemie NRC Handelsblad **11**(277), 11 (1981)
Ruthenberg, K.: Metachemistry. De Gruyter, Berlin/Boston (2024)
Ruthenberg, K.: Die Regelhaftigkeit der allgemeinen Chemie. In: Janich, P. (ed) Philosophische Perspektiven der Chemie: 1. Erlenmeyer-Kolloquium der Philosophie der Chemie, pp. 65–82. BI-Wissenschaftsverlag, Mannheim, Leipzig, Wien, Zürich (1994)

Schiemann, G.: Natur, Technik, Geist: Kontexte der Natur nach Aristoteles und Descartes in lebensweltlicher und subjektiver Erfahrung. Quellen und Studien zur Philosophie, vol. 68. De Gruyter, Berlin, New York (2005)
Schilter, O., Schwaller, P., Laino, T.: Balancing computational chemistry's potential with its environmental impact. Green Chem. **26**(15), 8669–8679 (2024). https://doi.org/10.1039/D4GC01745E
Schnurr, C.: Ist das natürlich oder ist da Chemie drin?" Ansätze zu einer transdisziplinären Verständigung über die,(Un-)Natürlichkeit' der Chemie. GAIA – Ecol. Perspect. Sci. Soc. **31**(2), 94–102 (2022)
Schnurr, C.: Vom stoff zur praxis. Naturphilosophie der chemiekritik. In: Krebs, A., Gasser, G., Weichlein, R. (eds.) Ethik und Ästhetik der Natur. Überlegungen im Anschluss an das Weltbild der Igel. Schwabe, Basel (2025)
Schnurr, C.: Das Bild der Chemie in der Öffentlichkeit. Und das Bild der Öffentlichkeit in der Chemie: Plädoyer für mehr Chemiekritik. In: Rehn-Taube, S. (ed) Chemie: Ausstellungskatalog, forthcoming. Deutsches Museum, München (2025a)
Schummer, J.: Realismus und Chemie: Philosophische Untersuchungen der Wissenschaft von den Stoffen. Königshausen & Neumann, Würzburg (1996)
Schummer, J.: Die stoffliche weltveränderung der chemie: philosophische herausforderungen. In: Hubig, C. (ed.) Cognitio Humana: Dynamik des Wissens und der Werte, pp. 429–436. Akademie Verlag, Berlin (1997)
Schummer, J.: Coping with the growth of chemical knowledge: Challenges for chemistry documentation. Educ. Work. Chemists Educación Quimica **10**(2), 92–101 (1999)
Schummer, J.: Ethics of chemical synthesis HYLE. Int. J. Philos. Chem. **7**(2), 103–124 (2001)
Schummer, J.: The notion of nature in chemistry. Stud. History Philos. Sci. Part A **34**(4), 705–736 (2003). https://doi.org/10.1016/S0039-3681(03)00050-5
Schummer, J.: Why Do Chemists Perform Experiments? In: Sobczyńska, D., Zeidler, P., Zielonacka-Lis, E. (eds.) Chemistry in the philosophical melting pot. Dia-Logos, vol. 5, pp. 395–410. Peter Lang, Frankfurt am Main (2004)
Schummer, J.: Einführung. In: Weitze, M.-D., Schummer, J., Geelhaar, T. (eds.) Zwischen Faszination und Verteufelung: Chemie in der Gesellschaft, pp. 1–6. Springer, Berlin, Heidelberg (2017)
Slogometer: Natur, Natürlich. https://www.slogans.de/slogometer (2024)
Soentgen, J.: Der Ökologische Naturbegriff. In: Heichele, T. (ed.) Mensch - Natur - Technik: Philosophie für das Anthropozän, pp. 115–130. Aschendorff Verlag, Münster (2020)
Schofield, E.: The evolution of 'clean' in food and drink. Mintel Global New Product Database (2019)
Spaemann, R.: Philosophische Essays. Reclam, Stuttgart (2012)
Tabor, D.P., Roch, L.M., Saikin, S.K., Kreisbeck, C., Sheberla, D., Montoya, J.H., Dwaraknath, S., Aykol, M., Ortiz, C., Tribukait, H., Amador-Bedolla, C., Brabec, C.J., Maruyama, B., Persson, K.A., Aspuru-Guzik, A.: Accelerating the discovery of materials for clean energy in the era of smart automation. Nat. Rev. Mater. **3**(5), 5–20 (2018). https://doi.org/10.1038/s41578-018-0005-z
Tickner, J., Geiser, K., Baima, S.: Transitioning the chemical industry: The Case for addressing the climate, toxics, and plastics crises. Environ. Sci. Policy Sustain. Dev. **63**(6), 4–15 (2021). https://doi.org/10.1080/00139157.2021.1979857
Tingle, B.I., Tang, K.G., Castanon, M., Gutierrez, J.J., Khurelbaatar, M., Dandarchuluun, C., Moroz, Y.S., Irwin, J.J.: ZINC-22─a free multi-billion-scale database of tangible compounds for ligand discovery. J. Chem. Inf. Model. **63**(4), 1166–1176 (2023). https://doi.org/10.1021/acs.jcim.2c01253
van den Daele, W.: Der Traum von der ‚alternativen' Wissenschaft. Zeitschrift für Soziologie **16**(6), 403–418 (1987). https://doi.org/10.1515/zfsoz-1987-0601
Wang, Z., Walker, G.W., Muir, D.C.G., Nagatani-Yoshida, K.: Toward a global understanding of chemical pollution: a first comprehensive analysis of national and regional chemical inventories. Environ. Sci. Technol. **54**(5), 2575–2584 (2020). https://doi.org/10.1021/acs.est.9b06379
Weber, J.M., Guo, Z., Zhang, C., Schweidtmann, A.M., Lapkin, A.A.: Chemical data intelligence for sustainable chemistry. Chem. Soc. Rev. **50**(21), 12013–12036 (2021). https://doi.org/10.1039/d1cs00477h
White, L.: The historical roots of our environmental crisis. Science **155**(3767), 1203–1207 (1967)
Wirtz, H.-G.: Natur und menschliches Handeln: Zum Naturverständnis in der gegenwärtigen Umweltdiskussion. Schulz-Kirchner, Idstein (1992)
Wynne, B.: Creating public alienation: expert cultures of risk and ethics on GMOs. Sci. Cult. **10**(4), 445–481 (2001). https://doi.org/10.1080/09505430120093586
Ye, J., Liu, C., Mei, D., Ge, Q.: Active oxygen vacancy site for methanol synthesis from CO_2 hydrogenation on Pd_4/In_2O_3 (110): a DFT study. ACS Catal. **3**(6), 1296–1306 (2013). https://doi.org/10.1021/cs400132a

Ye, J., Liu, C., Mei, D., Ge, Q.: Methanol synthesis from CO_2 hydrogenation over a Pd_4/In_2O_3 model catalyst: a combined DFT and kinetic study. J. Catal. **317**, 44–53 (2014). https://doi.org/10.1016/j.jcat.2014.06.002

ZuinZeidler, V.: Digitalization paving the ways for sustainable chemistry: switching on more green lights. Science **384**(6701), eadq3537 (2024). https://doi.org/10.1126/science.adq3537