Electronic Supplementary Material (ESI) for Chemical Science.

Supporting information for

AN ANTHROPOCENE-FRAMED TRANSDISCIPLINARY DIALOG AT THE CHEMISTRY-ENERGY NEXUS

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SI-1 Who we are

A brief overview here: this group of authors comes as the continuation of a reflection which started during an interdisciplinary winter school “Catalysis at the Energy-Chemistry Nexus” (CatEnerChem) Winter School that took place in March 2022 in Aussois (France),[1] and consists of scholars with different profiles (ages, careers, nationalities) and disciplinary backgrounds, from chemistry to economics and ethics. Among all the on-site participants that experienced at least two full days of lectures and activities, a subset decided to continue the reflection, motivated by the collective concern about the consistency of our research activities with the imperatives of the ecological transition and by the collective elation felt at experiencing an approach combining physical sciences (chemistry, chemical engineering, life cycle analysis, and Earth system sciences), social sciences (economics, psychology, history, and psychology), and humanities (ethics and epistemology) as tools to address this concern.

SI-1.1 Situating ourselves

While working together during the March 2022 Winter School we realized that our diversity of views, education, disciplines, age, and interest were an important part, not only in terms of the originality of the authorship, but in the perspective we built. The main purpose of this section is to acknowledge and share how our position in society influences our opinions and our way of interpreting scientific results. We recognize that our voices are marked by our individual and social situations and that the way we interpret the world, even the scientific world, is shaped by our sociocultural backgrounds. In this paper, we developed what we found relevant to our understanding of the current planetary crisis, which is the central focus of the main body of the article. **Figure SI-1** shows the distribution of ages, gender identification, and career positions of the group. We are a group of researchers aged between 25 and 60 years old, covering different research positions. The vast majority has a scientific education in chemistry and works on research themes relevant to catalysis and the energy-chemistry nexus; others are researchers in social sciences (economics, history, geography, anthropology) or philosophy. The majority has mainly European origins while only one group member is from Latin America.

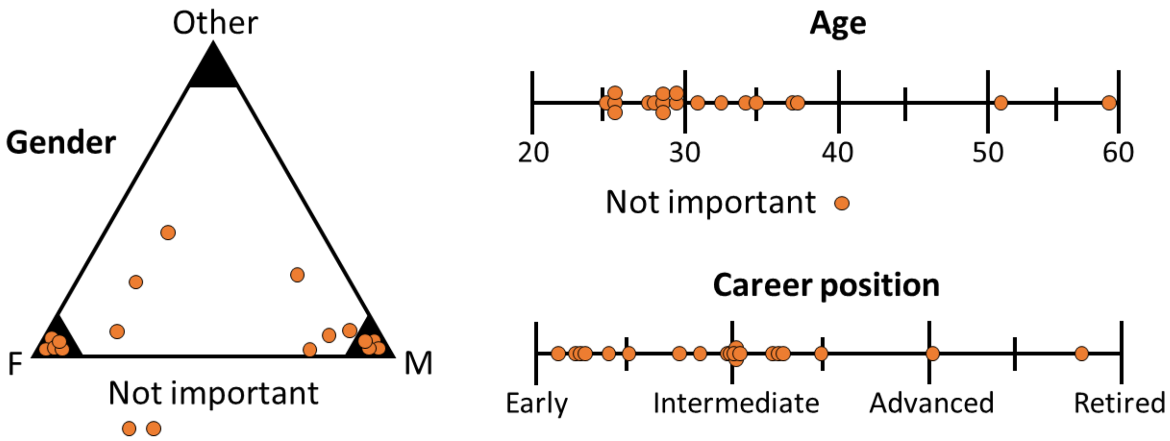


Figure SI-1. Gender, age and career position distributions by self-assessment. The groups "not important" include the number of people who did not consider a specific parameter relevant. The survey was answered anonymously by the authors present during the June 2022 plenary meeting.

Our shared experience. We first met at the 2022 "Catalysis at the Energy-Chemistry Nexus" (CatEnerChem) Winter School, that was originally conceived as a second edition to the international Winter School "Innovative Catalysis and Sustainability – Scientific and Socio-Economic Aspects" held in Bardonecchia, Italy in 2019. Much like this first installment, the CatEnerChem 2022 winter school aimed at training the upcoming generation of researchers and current staff in catalysis to operate the connection between the shifting techno-economic panorama of energy-related production systems and state-of-the-art development addressing catalysis challenges. The school organization was steered by a scientific committee (a list of its members can be found on http://catenerchem.cpe.fr [1]), who shaped the content and located the funds to support the event (see **Figure SI-2** for list of supports).

Figure SI-2. Logos of institutional bodies having financially supported the organization of the CatEnerChem Winter School.

This school was an opportunity to discuss the current role and challenges of research in catalysis at the energy nexus. This was organized around five chemicals central to the current model shifts undertaken by the global chemical industry under the impulse of its transition towards a low-carbon economy. To this end, particular care was given to the inclusion of oral interventions not only from influential academic researchers, but also prominent actors of the chemical industry, as well as social science experts working on themes relevant to the scope of the school. Importantly, during the planning of the 2022 event, fruitful discussions with scientists of the Lyon Urban School (LUS) corroborated and helped implement the scientific committee's decision to further explore the role and place of chemistry and chemists in the Anthropocene through the prism of practical workshops animated by philosophers and sociologists during the Winter School. The program was finally completed with practical chemistry training for students and serious games on cognitive biases animated by psychologists. Overall, this gave birth to an event adopting a decidedly transdisciplinary approach to the treatment of the energy-chemistry question. A definition of interdisciplinarity and transdisciplinarity and how we use these terms here is given in **section SI-1.3**.

During the school, to capitalize on the high quality of the presentations, large time slots were allocated to discussions between the audience and the speakers under the form of round tables. During these discussions, students took the floor and ask in-depth questions to the speakers, often going beyond the purely chemical aspect of their research and questioning their general role as scientists of the Anthropocene. This aspect stood out in a positively unusual way, since many young researchers recognized that, especially at the early stages of a chemist's academic career, little space is devoted to the investigation of the ethical implications of technical research and the wider context in which it is carried out. We perceive that the exiguity of this space contributes to narrowing the perspectives that the chemists among us have on an enormously complex issue that is the climate crisis. During the school, the involvement of students was further fostered by the recording of their thoughts, hopes and concerns about their future as researchers and actors in a world supposedly in transition. The emphasis on transdisciplinarity was also provided through various original expression workshops and serious games, ultimately allowing to tackle the questions and challenges raised by the talks from a different perspective. The transdisciplinary nature of the school allowed it to extend the questioning, reasoning and discussion beyond the traditional boundaries of chemistry conferences, and this approach was largely approved by the attendance of the school, according to a survey conducted on site.

Some of us were originally driven by social factors such as proposals from our PhD supervisors, because this was the first in-person event after the covid-19 pandemic, and because of the networking possibilities of the encounter. However, for most of the authors the initial participation in the winter school was motivated by its interdisciplinary approach to the topics combined with a thematic research interest. In fact, the general feeling most attendees were left with at the end of the event was that of an eye-opening experience, especially on the cross-sectional topics related to social sciences and humanities. An example is the theme of cognitive biases (see **section SI-1.4**).

The thoughts, reflections and analysis stemming from the interactions within this diverse pool of people and expertise were found to be relevant enough to be shared with the wider scientific community. To this end, us, a group of participants who recognized the original value generated by these interactions decided to gather and produce a first written contribution primarily destined to the academic community: the article at hand.

The collective production of this paper (see **section SI-1.2** for details), combined with common academic paper-writing practices (such as systematic reference to peer-reviewed literature) rooted in scientific values (such as intellectual honesty to the best of our capacities, and loyalty to reality to the best of our understanding, which included agreement with dominant current stabilized scientific knowledge and methods), is both the route we chose and its current output. The motivations behind the writing of this paper are to transform, continue and share the experiences, feelings, and shared point of views around the energy transition. Also, this experience allowed us to create a group of people concerned by the crisis and willing to work and to act upon the emergencies. As such, we recognized our desire to highlight and communicate about the current (chemical) inconsistencies/limitations we perceived in the proposed roadmaps and our desire to highlight the need for interdisciplinarity and help from other sciences to articulate such inconsistencies early on. We hope that this will allow us to not only work efficiently on current problems, but hopefully also find new solution pathways, in our research topics, for example, that are today obstructed by, *inter alia*, biases and a lack of system understanding.

As it becomes evident, we believe we should start acting on the crisis of the Anthropocene, as we do not believe to have infinite time, so we are concerned on how the scenarios and narratives to mitigate the crisis are built and accepted.

To fight the energy transition crisis we face, we see two paths as researchers. (i) We could incorporate teachings and conclusions from other disciplines to our practice, so as to improve the pertinence of the solutions we propose to the technological and societal challenges of our times. (ii) We could educate ourselves to the practice of other disciplines and work closely with a complementary range of experts to encompass as many as the technological, social, human, economic aspects as possible in the formulation of our proposed answer to the challenges of the Anthropocene. These two paths, while similar at first glance, are quite different in their methodology, philosophy and scope, and adepts of both could be found in our group. Some of us think that a purely disciplinary approach is likely to oversee dead-ends or inconsistencies early on, and that it will lead – by definition – to a narrower solution space, which appears to lead to ineffective resource allocation to overcome problems.

Furthermore, we believe these two paths are not two alternatives to choose from, but that we should transit both: we need to work solving the crisis with what we know, and we need to create new alternatives on how to think, model and practice science in the Anthropocene.

Overall, we agree that the current proposed dominant approaches to mitigate the climate crisis and contain the runaway consequences of the Anthropocene fall short in the face of the large amount of available technological, economic, sociological, historical, humanitarian, and philosophical data available to us. We therefore believe that better and more ambitious alternatives should and must be built to match the scope and urgency of the crisis we are facing.

SI-1.2 Our authorship policy

All authors should be considered as co-first authors in line with the methods and values that have guided the creation of this paper. In particular, the ideas building and the writing have been a collective process with horizontal interpersonal dynamics inspired by non-violent communication tools. We cherish the recognition of the collective, which implies in our case to value the collective creation of the current work, and the impossibility to rank the importance of the ideas shared, or even identify individual ownership of collective final ideas. In other words, we think that our dialogues and our work is not mirrored in current practices of authorship orders and we want to abstain from these usual academic capital distribution patterns. In the same spirit, we do not want to have one person or a subset of people among us be earmarked as “corresponding author(s)”, a distinction that carries a similar asymmetric academic capital distribution among the group of authors. In the printed version, the first author is the one whose birthday falls closest after June 26th, a close-to-random day in the year for us (June 26th 2023 is the day we obtained the first full draft of paper); the other names follow by being similarly ordered in terms of birthday (year of birth not considered). At the same time, since this order is just fortuitous and does not reflect any particular merit with respect to the manuscript, the authors retain the right to choose the order of their choice, in their CV for example, as an equal co-author among the others. The choice to publish open (diamond) access in a community-owned academic journal is also important to us. In order to comply with Author Guidelines which state that “if there are more than 10 co-authors on a manuscript, the authors should provide a statement to specify the contribution of each co-author”, we disclose hereafter more information on our process. Table SI-1 identifies, for each section, the authors who were in charge of the first draft and of coordinating the feedback to the section that all the group made by writing or during the plenary meetings. Table SI-2 gives an overview of individual author’s anonymized feedback to each possible item of conclusion that emerged during the April 24th 2023 plenary meeting. The results of this survey formed the basis for the manuscript conclusion section. We thank the five people that were present at part of our initial meetings for their initial contributions.

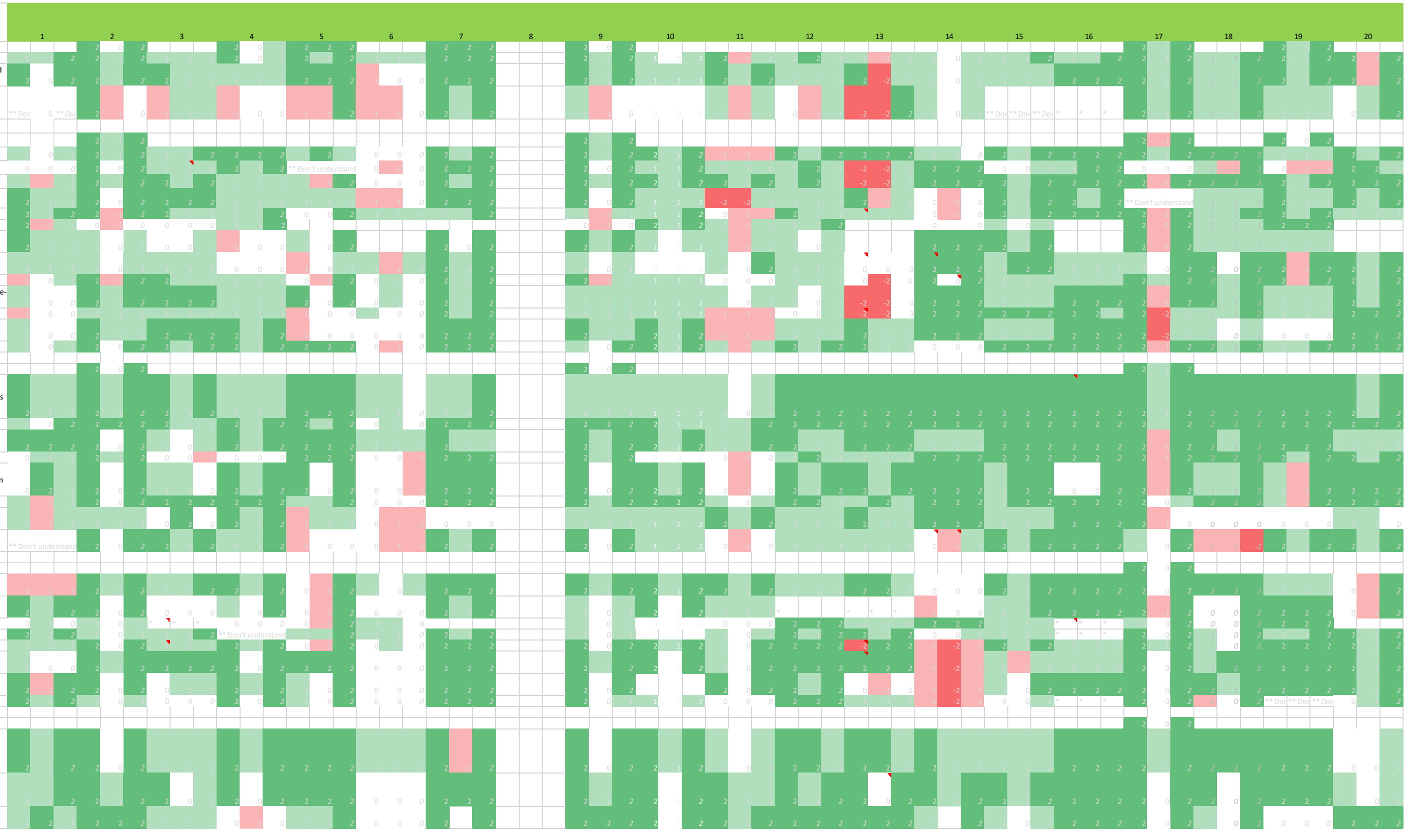
Table SI-1. Table showing which sections of the manuscript (columns) was curated by which author (see text).

	Outline*	Introduction			Earth system analysis and projected dominat future						Interdisciplinary considerations								Conclusion	Supp mat & other tasks
		1.1	1.2	1.3	Intro	CO_2	H_2	CH_4	NH_3	MM	Intro	CO_2	CH_4 & H_2	NH_3	Plastics	Scalability	Transitions	Discussion		
Mathieu Prevot	Plenary Meetings **			Plenary Meetings **	x				x		Plenary Meetings **			x		x		Plenary Meetings **	Plenary Meetings ** & anonymous survey (see Table SI-2)	As needed
Valeria Finelli								x												
Xavier Carrier							x						x							
Gabriele Deplano							x													
Margherita Cavallo						x														
Alessandra Quadrelli									x			x		x						
Juliette Michel		x																		
Marie-Hélène Pietraru						x														
Clément Camp			x					x												
Giulia Forghieri													x				x			
Anna Gagliardi										x					x					
Sebastian Seidel						x									x					
Antoine Missemer												x					x			
Bertrand Reuillard					x							x								
Barbara Centrella										x					x					
Silvia Bordiga									x											
Maria Grace Salamanca			x												x	x				
Vincent Artero					x		x									x				
Keanu Birkelbach		x			x				x					x		x				
Niklas von Wolff			x					x												

* Intended as: Collectively deciding the direction and content of the manuscript, leading to evolutive outline layouts
** Plenary meetings (on line or hybrid) took place 8th-10th June 2022, 3rd October 2022, 14th November 2022, 16th January 2023, 13th March 2023, 24th April 2023, 16th June 2023, 15th-17th November 2023.

Table SI-2. Table showing how each author (3 columns by author) evaluated each line's statement item which corresponds to one of the 44 concluding statements that emerged during the April 24th 2023 plenary. The first column collected how the author ranked the importance of the item in their own eyes, the second column asked whether the item should be in the manuscript in the author's opinion and the third if the author evaluates that the item has been sufficiently corroborated in the main manuscript. The color coding for the answers is: deep green ("Very much"); light green ("Yes, rather yes"); white ("Neutral/do not care"); pink ("No, rather not"); red ("Strongly disagrees"); yellow ("Don't understand"). The results were used for collective writing of the discussion and conclusion sections.

Statement
1. There is a Recurrent presence of strategies that are blind to N-S inequalities in the scenarios studied for the enrgy transisition
- Risk of Continuation (or even increase) of North-south inequalities is expected through the scenarios envisioned
- The scenarios are expected to Maintain inequalities of access to resources throughout the world to resources that are considered important for the European energy transsiiton
- [decolonial cannot be stated as conclusion (ex. we have not made distinction between colonialism and coloniality) but we can put in conclusion that the decolonial theory can suggest new roads to research [- Consider the decolonial and postcolonial interpretation of the north-south inequalities]
2. Domination of strategies that rely on corporate actors:
- We have identified some limits of industry-targeted research
- We need more efficiency
- We need less consumption
- Mechanisms of corporate profit to produce waste (along service and profit) and public money to handle waste is unfair and policies toward mitigation (CO2)seem recurrent an dare overall unjust
- We should be able to do research in other ways than targeting industry.
o what is research not targeted to industry ?
o research looking for different ways of thinking about energy transition without big industry? For example: decentralized, small scale, local, appropriate, not looking at scaling up at all prices, ...
- Remind Examples from economic literature showing the economy of scale is not necessary (taken from non- mainstream economics)
- There are invariants: scaling up is projected as the only (reasonable) alternative/value in modernity.
- New technologies are projected as the way out, with fast and massive scale up. However we do not know the impact of such scale-ups. "Could go very wrong? "
- Non zero chance that one or more of these new massive scale-up coud go very wrong
- But in some cases scaling up could be necessary. (not necessary anti large scale industril production, more againt necessarily profitable)
- Necessity to allow to think of alternatives to corporate industrialization
3. An established hierarchy
- Our juxtaposition of planetary boundaries analysis and scenarios analysis highlights that respecting the planetary boundaries is not explicitly stated as a goal of the scenarios. And the authors of the scenarios don't expect the respect of the planetary boundaries as an outcome of their own scenario. Going back inside planetary boundaries is not an expected result of analyzed the scenarios
- Planetary boundaries crossing could even be worsened , even in already dramatic situations (ex. ammonia)
- *sustainability* is barely clearly defined, and claims of said sustainability are supported by a few chosen criteria - in particular the carbon footprint - while others may be left under the rug - waste management, land or water management, ...
- extractivism, productivism are also two of recurrent mechanisms in projected scenarios
- The recurrent triple bottom line of sustainability (TBL) of the « three Ps » (People, planet and Profit, i.e. economically viable, socially just and ecologically sound) is mentioned throughout these scenarios. But these three values are established and projected in a hierarchical order (1st Profit, 2nd or 3rd People or Planet)
- Through the scenarios we see the alternatives tend to be thought of on the same terms, logics and hierarchies of values.
- Piling up of updating scenarios that propose more of the same; some scenarios support one another, i.e. one scenario may be justified by the choices made in another scenario (e.g. the IEA is often used as a reference)
- At least, it could be useful to "edge our bets" with respect to (economic) profit-requiring strategies. And look for scenarios that do not obey this hierarchy
4. Policies, politics, integrity, ethical
- The scenarios that we are exposed to are political – which trickle down to the research we perform (see differences in Germany and French energy scenarios)
- A legitimate question: Is it the researchers' job to implement politically-driven scenarios agendas thta we might consider deleterious or inefficient for example? (some of us are civil servant)
- How do we reconcile a hiatus with announced but less sought after values such as planetary boundaries respect
- How do we ensure that invokig planatry boundaries respect goes beyond pious (or green-washing)posture?
- Ethical implications: responsibility of our acts, which belong to a chain having an effect in the world.
- We are researchers specialized in a discipline, and at the same time we bear the ethical responsibility of our acts, that have consequences well beyond our discipline.
- Personally re-owning a form of at least understanding, and upon that understanding basing our choices to our actions seems necessary, timely
- There is a personal-individual-professional ethics involved, on our desire to have a word to say on our discipline and our job...
5. The necessity and usefulness of a method
- Integrity is also part of our method as scientist; however we tend to claim sustainability of our research or results, without defining the term, nor providing arguments to justify its use. What is actually sustainability? Transdisciplinarity allowed to assess the "shaky nature" of some of the grounds that the scenarios tend to build, or of the criteria chemists usually use to claim sustainability (e.g. carbon footprint).
- Circling back to ethics or values? What chemistry would we like to contribute to? => actually I would have stated that as questions, at the very end of the conclusion; a series of questions which would look like our personal interrogations, as future perspectives, but which would appeal to the readers themselves as well.
- Should we state that this paper is a first step towards more? Should we state that this paper intends to "share our understanding to the community"... to start a more general discussion?



SI-1.3 Clarification on how we use the concept of 'transdisciplinarity' in this paper.

Transdisciplinarity generally refers to approaches which actively incorporate information, goals and interests, values, knowledge, etc. of non-academic agents, often in a participatory way.[2] Transdisciplinarity studies is a field concerned with how to incorporate these values, interests, etc. into systematic scientific investigations. As scholars, who originate from academic fields (mostly chemistry, history, economics and ethics), we mobilize concepts from our own expertise and other disciplines, and are hence following an interdisciplinary approach rather than a transdisciplinary one. At the same time, as stated in our conclusion part of the main manuscript, we wish to highlight the transdisciplinary ambition of our work. To exemplify based on the latin etymology of the word "*trans*", as discussed by French-Romanian physicist Basarab Nicolescu:[3] we aim to work "between, across and beyond" academic disciplines – resonating with our desire to bridge across the great (perceived?) divide between natural & physical sciences on one side *vs.* social sciences & humanities on the other, and beyond. In particular we want to explicitly highlight the importance of non-academic sources to the construction of knowledge, which is too often limited to academic ones (see also **section SI-1.4**). Transdisciplinarity is what we aim for: our references to the ongoing epistemicide in the conclusion of the main text[4] point to reconsider knowledges that are not academic and hence not organized in disciplines.

SI-1.4 A part of our understanding of role of cognitive bias in scenarios projections: breaking cognitive barriers?

More than 125 years ago, and about 50 years after the early (separate) works by Eunice N. Foote[5] and John Tyndall,[6] Svante Arrhenius published his famous treaty on the green-house gas effect of CO_2.[7] More than a century ago newspaper articles alerted on the climate-changing risk of CO_2 emissions from burning fossil fuels (**Figure SI-3**).

The furnaces of the world are now burning about 2,000,000,000 tons of coal a year. When this is burned, uniting with oxygen, it adds about 7,000,000,000 tons of carbon dioxide to the atmosphere yearly. This tends to make the air a more effective blanket for the earth and to raise its temperature. The effect may be considerable in a few centuries.

Figure SI-3. Text excerpt from the "Waitemata and Kaipara Gazette" of August 14th 1912 (p. 7)[8]

Given the unprecedented challenges ahead (see main manuscript), especially as a community of mostly chemists who are aware of those early reports, we can also try to understand and question the decision-making processes at hand. Decisions can be modeled and understood in their individual or collective and political dimensions and we will try to share our understanding of some literature-mobilized governing factors mostly focusing on individual ones.

Neurological, psychological, and behavioral sciences tend to put forward the existence of different mostly individual-level factors said to be hampering efficient, rational, just, and adapted decision making. The framework of heuristics and bias was developed in the early 1970s by psychologists Amos Tversky and Daniel Kahneman,[9] who sought to justify irrational decision-making in the economic field. To simplify hereafter, we will not make the distinction between heuristics and biases, and will only refer using the "bias" term. A cognitive bias, for example, is described as an individual-level thinking mechanism that causes an alteration in judgment and often a misleading and false logical thought pattern that influences our choices.[10] This can become especially important when dealing with large amounts of information and/or limited time, influencing our decision-making and the way we address certain issues, both individually and in systems.

Among more of the 250 referenced cognitive biases, some can be contemplated to better understand the biases affecting the energetic transition. These concepts have been mobilized to provide insights on the difficulty we have to adapt and/or adopt new behavior, here concerning transition. If technological solutions existed (e.g., replacing carbon-based energies with renewables), what individual, structural, systemic or political factors and biases prevent us from acting accordingly? In order to understand differences between technological impossibilities and other types of hurdles, to what extent are our decisions affected by our thinking patterns?

Cognitive biases are, of course, not presented as the magical response to questions similar to the ones above. At the same time, many biases exist and some are said to directly influence both the rate and fate of the energy transition. For example, *status quo* (or *inertia*) *bias*[11] is a term used in behavioral finance to refer to an exaggerated preference for the status quo in decision making. Novelty is seen as bringing more risks than possible benefits and leads to resistance to change. The *ambiguity effect*[12] is a cognitive bias that occurs when decision making is affected by a lack of information, or "ambiguity". The effect implies that people tend to select options for which the probability of a favorable outcome is known rather than unknown. The *hypothesis confirmation* bias concerns to preferring evidence that confirms rather than refutes a hypothesis, while the *matching* bias is referred as focusing on the elements contained in a problem statement. *Reification of knowledge* is defined as considering knowledge as immutable and external to objects. *Myopia* is as focus on short-term objectives as opposed to long term ones, and *herding* is the tendency to base choice on actions of others.[13] The *over-confidence* bias, by which individuals overestimate their capacities can also lead to errors in decision making linked to the energy-transition. Finally, *cognitive dissonance*, a kind of cognitive bias, applies when we avoid having conflicting beliefs and attitudes because it makes us feel uncomfortable. The conflict is usually solved by rejection, mystification or avoidance of new information.

Some scientific literature tends to suggest that, based on the "universality of human cognitive capabilities" and survival, this type of biases are currently at hand and threaten human development, especially when applied to planning and collective decision-making processes.[14] We notice that, in some cases, explanations offered by other sciences (such as history, sociology, economy, ethnology, etc.) can reduce some of the universality claim contained in this type of reasoning. For example, a posture informed by neuroscientific evidence, consists in believing that it is at least in part because we are human, and therefore because we individually suffer from *myopia* and related biases, that we are collectively prevented from long-term planning.[15] History and anthropology (to name academic disciplines) as well as the practices of the very peoples, for example, informing them (to acknowledge the non-academic source[4] of this academic knowledge) can attest of other dynamics: for example, the deemed capacity of Iroquis to think in term of seven generations for taking short term decisions,[16,17,18] in apparent contrast with the *myopia* and related cognitive bias said to be consubstantial with "human nature". A second example can be offered through the case of people deciding to build their home in floodable areas notwithstanding the risk: while cognitive science-based explanations would put forward the role of biases such as *inertia* or *cognitive dissonance,* some social scientists have highlighted the central role that social vulnerability plays.[19] Rather than being cognitively-biased individually, which would lead them to underestimate the risks, the people making the decision to live in such area can also be oriented by social vulnerability (an aspect correlated to collective social factors). We therefore put forward the hypothesis that these discourses on cognitive biases may also in themselves carry the bias of *ethnocentrism*, that is the bias to project as universal the characteristics that are typical of its group,[20] extending to a general "human natural state" some thinking processes that remain culturally and historically situated.

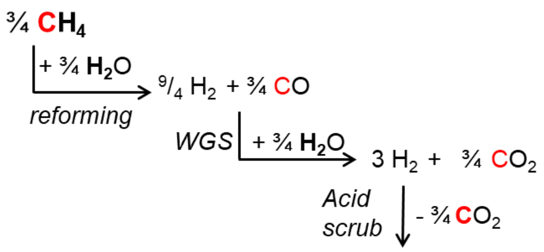
SI-2 Details on links between chemical entities and Planetary Boundaries (PB)

Table SI-3 Links between the five selected chemical entities and the nine Planetary Boundaries (PB): scale (data in 2022), uses, and systemic consequences of their presence.

Entity	Anthropogenic amounts	Current production	Current main use	PB affected by its presence	Issues identified
CO_2	37 Gt/y [21]	Byproduct of oxidation of organic compounds Fossil fuel combustion	Urea synthesis, beverage industry, enhanced oil recovery	Climate change Ocean Acidification	Atmospheric accumulation (GHG)
H_2	95 Mt/y [22]	Steam Methane Reforming (SMR)	Refining, & chemical industry, processing	Climate Change Freshwater Use Land-system change	Synthesis mainly from fossil resources causes CO_2 emissions Converted to H_2O (GHG)
CH_4	347 Mt/y [23,24]	Extraction from fossil resources	Fuel, H_2 production	Climate Change	Atmospheric accumulation (GHG) Combustion or oxidation to CO_2 (GHG)
NH_3	185 Mt/y [25,26]	Haber-Bosch process, involving N_2 from air and fossil-based H_2	Fertilizers	Biogeochemical flows Climate change Biodiversity	Accumulation in water systems as ammonium salts and nitrates, leading to eutrophication and anoxia, with contributions to loss of biodiversity Atmospheric accumulation as N_2O (GHG), produced by biological denitrification
Plastics	400 Mt/y [27]	Polymerization of petrochemicals obtained from oil cracking	Materials	Novel Entities Climate Change	Synthesis from fossil resources causes CO_2 emissions Chemical inertness leads to accumulation in the environment or partial degradation to microplastics

SI-3 Precisions on Haber Bosch -related CO_2 emissions

Simplified Steam reforming reactions:



Simplified Haber- Bosch **Reaction** Stoichiometry: $3\,H_2 + N_2 \longrightarrow 2\,NH_3$ (ideal C-free hydrogen)

Haber-Bosch **Reaction** Stoichiometry with explicit simplified steam reforming :

$$^3/_4\,CH_4 + {}^6/_4\,H_2O + N_2 \longrightarrow 2\,NH_3 + {}^3/_4\,CO_2 \qquad 0.92\ t_{CO2}/t_{NH3}$$

Haber-Bosch Stoichiometry Explicitly including concomitant exothermic oxycumbustion ($CH_4 + 2\,O_2 \rightarrow 2\,H_2O + CO_2$), present in the process for heat generation to reach reported 1.12 t_{CO2}/t_{NH3} (i.e. per 2 NH_3 : $0.17\,CH_4 + 0.34\,O_2 \rightarrow 0.34\,H_2O + 0.17\,CO_2$)

$$0.92\,CH_4 + 0.34\,O_2 + 1.16\,H_2O + N_2 \longrightarrow 2\,NH_3 + 0.92\,CO_2 \qquad 1.12\ t_{CO2}/t_{NH3}$$

Overall Haber-Bosch **Process** Stoichiometry from above and Modeling further process-related CO_2 emissions (due to steam-to-turbine, steam-to-reformer, heat losses, methane extraction and other, see Fig 4 main text) with oxycumbustion to reach final 1.67 t_{CO2}/t_{NH3} (i.e. per 2 NH_3 : $0.46\,CH_4 + 0.92\,O_2 \rightarrow 0.92\,H_2O + 0.46\,CO_2$)

$$1.38\,CH_4 + 1.26\,O_2 + 0.24\,H_2O + N_2 \longrightarrow 2\,NH_3 + 1.38\,CO_2 \qquad 1.67\ t_{CO2}/t_{NH3}$$

Overall (reaction + process) Haber-Bosch stoichiometry

Scheme SI-1. Representative chemical equations for the Haber Bosch process with connected ton of CO_2-emitted per ton of ammonia produced (from gray hydrogen, in optimized HB plants, see main text).

SI-4 Details on green H_2 production infrastructure technologies

Alkaline electrolyzer is the most mature technology and the most largely deployed to date,[28] such as HyDeal Espana for example with a projected electrolyzer capacity of 7.4 GW by 2030.[29] Proton exchange membrane (PEM) electrolyzers, a more efficient but historically more costly technology, has recently experienced important cost reduction and should gain increasing market shares in the coming years. Both technologies are considered to have reached a technology readiness level (TRL) of 9.[28] Other maturing technologies include high-temperature solid-oxide electrolyzer cell (SOEC) at TRL 7 and anion exchange membrane (AEM) electrolyzers at TRL 6.[28] Another longer-term generation of infrastructure for H_2 production is proposed in the 2020 SUNRISE technological roadmap. It concentrates on the European energy landscape with different scenarios, namely P2X (Power to X with 80% reduction of GHG and large development of e-fuels) and H_2 (with a massive hydrogen deployment in addition to 80% reduction of GHG). The first one (P2X) is leading to a hydrogen consumption of around 10 Mt (about 350 TWh), while the second one (H_2) would require around 52 Mt (about 1700 TWh) in 2050. Such scenarios rely on three technological processes that are currently more or less mature. First, the maturing photovoltaic- or wind-driven electrolysis that should allow for a centralized and efficient large-scale production of hydrogen with a vision for 2050 to provide cost-effective (100 €/kW) and efficient electrolyzers (electricity to molecules yield 80–90%). Second, a less mature technology with direct solar to hydrogen conversion through photoelectrochemical devices, which would permit a decentralized, local production of hydrogen, even down to the scale of single households. The 2030 vision is to design a fully integrated system with 10% solar-to-hydrogen efficiency and 1-year stability. A 30% efficiency should be reached in 2050. Third, an extremely low-cost technology based on autonomous systems made of transparent plastic bags with microorganisms and photocatalytic systems to drive (bio)chemical reactions for a decentralized, local production of hydrogen for single households and niche applications. Such systems are currently at a low TRL (3–4). If solar-to-fuel yield is significantly improved, they could reach TRL 6–8 by 2030.[30]

SI-5 Overview on critical materials

Achieving net zero emission in the proposed time frame (typically before 2050) is said to require the rapid development of new technologies relying on large-scale infrastructures that often need to be built from scratch. Indeed, the implementation of *Carbon capture, utilization, and storage* (CCUS) technologies and the shift towards a global hydrogen economy for example – while maintaining current production levels – will require a large amount of raw materials, some of them already considered critical. In broad strokes, material requirement in connection to "transition to clean energy" [31] can be divided in two categories: (i) resources necessary for the electrification of the industry and transportation sectors, namely copper, aluminum, iron for the construction of electrical grids and cobalt, graphite and lithium for the production of storage units (in particular within electric vehicles, EVs, which require six times more mineral input than conventional models), and (ii) active materials such as, for example, metallic silicon and indium required in photovoltaic panels, rare-earth elements used in the magnets of electrical motors or iridium and platinum acting as catalysts for water electrolysis and hydrogen fuel cells. Some materials are already produced on a large scale (copper, steel) and are already extracted at near-peak capabilities and suffering from declining ore quality, which impacts price and production volumes, and leads to increased volumes of waste. Other materials require a rapid increase in production in the coming years (lithium, cobalt, rare earths) to achieve the foreseen development. For instance, it is expected that the lithium demand will be multiplied by fifteen by 2040, due to the popularization of EVs. At the same time, with the current EV battery technology, replacing the totality of traditional vehicles with EVs would cause the depletion of known cobalt reserves by 2050. Furthermore, because the extraction of energy from renewable sources is generally less trivial than from fossil resources, the amount of minerals required per unit of power generation capacity is expected to mechanically increase as the energy transition takes place. Indeed, the IEA forecasts that the "clean energy" sector will see the fastest growing demand in critical minerals in coming years.[31]

SI-5.1 Can hydrogen technologies help buffer critical mineral demand related to electricity networks?

In the IEA net zero by 2050 scenario, the demand for critical minerals will increase by a factor 6 by 2040,[32] with the construction of the electricity network and the EVs and battery storage accounting for two thirds of this increase. Electrification is currently prioritized based on better energy yield over the complete cycle (both for direct use but also through storage in batteries), when compared to hydrogen yield for production, storage and reuse (40–50%) and to carbon-based synthetic fuels one (20–30%). It was suggested that coupling hydrogen production with renewable-generated electricity can bring several benefits, such as lowering costs and maximizing the decarbonization potential of renewables.[33] Furthermore, amongst different pathways, the use of pipelines for hydrogen transportation is positioned to be the less energy intensive solution. Therefore, as most of the demand in critical materials is related to electricity networks, EVs and battery storage, revising the ranking of solutions to net zero by including renewable fuels (i.e. as alternative storage strategies) is said to help buffering – at least partially – the expected rise of critical materials demand. At the same time, H_2 as an energy carrier underpins major growth in demand for nickel and zirconium for electrolyzers, and for platinum-group metals for fuel cells EVs.

SI-5.2 Metal supply limitations.

Pure metal content in natural ores is typically very low (e.g. around 0.1% for lithium, between 0.5 and 1% for copper, around 1% for cobalt), making the mining industry the biggest producer of gas, liquid and solid waste,[34] through the processing of these ores. Indeed, the "responsible mining" claims of some current large-scale mining operation are disputed for example on the fact that every gram of processed mineral ends up as waste.[35] In fact, the environmental impact and the toxic waste generated result in land erosion, loss of biodiversity, and contamination of soil and water, sometimes causing health, social and political issues in local populations, further strengthening existing inequalities.[36]

The necessity of intensifying the mining industry to achieve the proposed energy transition has sometimes been labeled as "green extractivism", a notion referring to a hierarchy of values that places mining interests above human rights and ecosystem sustainability in the name of the energy transition.[37,38] In practice, new mining projects are often met with strong pushback from local populations, as the mining industry is the industry sector causing the highest number of socio-environmental conflicts.[39] In fact, several of the metals critical to the energy transition are extracted from extremely localized deposits: the majority of cobalt production originates from the Democratic Republic of Congo, while almost half of the global copper originates from Chile and Peru, 75% of lithium is produced in Australia, Chile and China, and the majority of rare earths are produced by China. This lack of national diversity increases the risk of supply chain failure and can contribute to, or worsen, existing geopolitical tensions and power dynamics,[40] with colonial-informed richness-extraction from the global South to supply demands in the global North.

Deep-sea mining has also been proposed as a possible solution to meet the foreseen demand in critical metals for the energy transition. However, this idea has been met with several pushbacks ranging from history-informed call for very cautious way forward[41] to stark criticism by scientists from more than 40 countries, claiming that it will surely lead to extensive environmental destruction and contamination.[42]

SI-5.3 Overview of some accompanying strategies

If the availability of critical minerals is recognized by all as another piece of the puzzle for the development of a net zero emission economy and for so-called clean energy technologies in general, opinions diverge on the severity of this aspect depending on the scenario envisaged.

It is in general agreed that the manufacturing of so-called clean technologies, including electric vehicles, solar panels, and wind and geothermal energy systems, will require considerable resource expansion. Some resources such as copper for electrical transmission or steel for wind turbines are already produced at large scales whereas production of metals such as lithium, cobalt, and indium, among others[43] will need to expand rapidly to meet global needs,[40,44] Their criticity emerges as a major bottleneck in most global “clean energy” scenarios due to physical scarcity of geological supply. In some cases, increased recovery, recycling, substitution, and careful design of new high-tech devices are put forward to help circumvent the physical scarcity of the mined ore to the growing demand.[45,46] In these cases, metal recovery is challenging and energy intensive because “clean energy” technologies often involve complex metallic alloys (e.g., in battery electrodes). The supply complexity is compounded by the challenge to develop recycling channels without setting off negative rebound effects.

Some analysts anticipate that the current metal reserves are sufficient in most cases to enable renewable production, but do not fail to identify physical scarcity for some specific metals (such as lithium, and possibly cobalt) [43] or concede the presence of substantial environmental, social, and political barriers to extraction of the necessary materials.[44] As it takes an average of 16 years for a mine to go from discovery to production, suppliers may struggle to match sudden surges in demand,[31] especially if the mining activities are fueling socio-environmental concerns. A governance at the planetary level that would ensure continuity of global mineral supply, is projected by some as necessary to overcome some of these challenges.[49] A necessity that invites to further necessities: to make more explicit the governance’s values with respect to the multi-level, complex, and sometimes divergent challenges raised by the topic

SI-6 Limits to growth scenarios updated by Herrrington

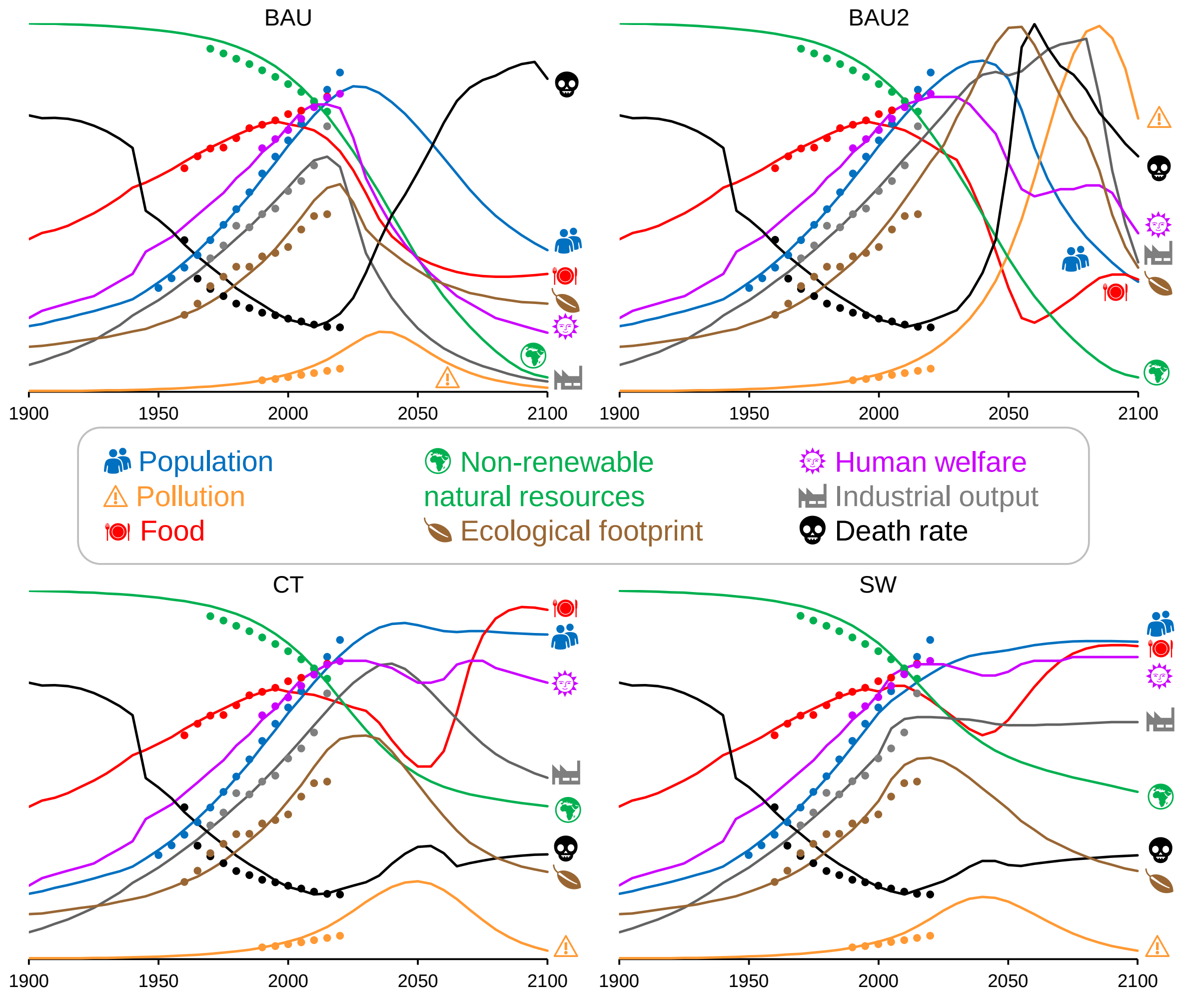


Figure SI-4. Four scenarios for the projected evolution of population (blue lines), pollution (orange lines), food per capita (red lines), non-renewable resources (green lines), ecological footprint (brown lines), human welfare (pink lines), industrial output (gray lines), and death rate (black lines), and comparison with corresponding empirical data (dots), adapted from Herrington[50] and Meadows.[51] BAU (*Business As Usual*) depicts continuation of the current economic, political, and social model, and shows collapse around 2030s due to lack of resources. BAU2 is similar to BAU with double the amount of resources available; the collapse is then not avoided, but delayed, due to massive pollution. CT (*Comprehensive Technology*) includes projections of significant and optimistic technological progresses, which would help curb the consequences of anthropogenic pollution and ecological footprint, and thus prevent total collapse. SW (*Stabilize the World*) is referred as the sustainable model: indicators are stabilized on the long-term thanks to meaningful policy changes (see also Table SI-4). Regarding the fits with the empirical data, Herrington concluded that BAU2 and CT are the closest fit, while SW is the farthest.

Table SI-4. Explanations of the scenarios considered in “the Limits to growth scenarios” analysis performed by Herrrington [reproduced form ref].[50]

Scenario	Description	Cause
BAU	No assumptions added to historic averages	Collapse due to natural resource depletion.
BAU2	Double the natural resources of BAU	Collapse due to pollution (climate change equivalent).
CT	BAU2 + exceptionally high technological development and adoption rates	Rising costs for technology eventually cause declines, but no collapse.
SW	CT + changes in societal values and priorities	Population stabilizes in the twenty-first century, as does human welfare on a high level.

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