Showcasing the IUPAC "Top Ten Emerging Technologies in Chemistry", in an article published in Chemical Science and co-authored by Dr Fernando Gomollón-Bel, a science communicator based in Cambridge, UK, and Prof. Javier García-Martínez, from the Department of Inorganic Chemistry, University of Alicante, Spain.

Connecting chemical worlds for a sustainable future

Inspired by Raphael's 'School of Athens' fresco, this artwork depicts a symbolic personification of various sciences: mathematics, engineering, physics, biology, astronomy, and, of course, chemistry. Each discipline is shown in dialogue with the others, emphasizing their interconnections. This work communicates the central concepts of the paper, highlighting the role of chemistry as the "connecting science" that fosters the creation of new bonds, interdisciplinarity, and diversity. It underlines the importance of chemistry as a catalyst for a more sustainable future for all.

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Connecting chemical worlds for a sustainable future

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Chemistry plays a central role in science and is the basis of one of the major, more impactful, and diverse industries. However, to address the most pressing global challenges, we must learn to create connections in an effective and meaningful way, with other disciplines, industries, and society at large. Here, we present the IUPAC Top Ten Emerging Technologies in Chemistry as an example of an initiative that highlights the value of the most promising advances in chemistry and contributes to creating connections to accelerate sustainable solutions for our society and our planet.

Introduction

Chemistry is often called the central science, because of the connections that arise from bibliographical analyses (Fig. 1) as well as historical, educational, and conceptual links.[1] However, we prefer to refer to chemistry as the "connecting science," to emphasise its key role in intertwining diverse disciplines,[2] such as energy, materials science, and biomedicine. Additionally, chemistry is closely connected to several societal issues, such as climate change, supply chains, and the energy crisis; an intricate and interdependent network of problems often called "polycrisis".[3] We believe that chemistry holds the key to a brighter, more sustainable future. In 2019, IUPAC introduced the "Top Ten Emerging Technologies in Chemistry" initiative to highlight fascinating and promising discoveries, hovering between the early stages of laboratory work and commercial reality.[4] Since then, the "Top Ten" has become an established initiative, which impacts areas as diverse and important as sustainability, technology transfer, and education (Fig. 2).[5] Herein, we explore the possibilities that the "Top Ten" technologies offer to create connections in chemistry and beyond, in line with the motto of the last IUPAC World Chemistry Congress, which took place in The Hague, Netherlands, in the summer of 2023 – "Connecting chemical worlds".

Creating new bonds

From strong static bonds to dynamic adaptive networks

Sometimes, discoveries in chemistry uncover completely new fields, creating untapped opportunities. For example, just last year, the concept of "dynamic covalent bonds" reshaped our understanding of key chemical concepts such as chirality and aromaticity.[7] These results challenged the previous belief that carbon–carbon covalent bonds are immutable, opening doors to dynamic systems with interesting possibilities in the design of sustainable solutions, such as systems that actively adapt to the environment around them. Additionally, some of these molecules and materials could exhibit different behaviours based on external stimuli, "smart systems" with great potential in applications such as medicinal chemistry.[8] Other opportunities include the design of molecules with features like sustainability already built-in – chemists could create connections and design efficient "disconnections" that ensure efficient degradation to the original building blocks for recycling and upcycling.[9] Similarly, organocatalysis (selected within the first IUPAC Top Ten list in 2019) is realising the potential of non-metallic compounds to catalyse enantioselective transformations efficiently and sustainably,[10] supported by the award of the 2021 Nobel Prize in Chemistry to David MacMillan and Benjamin List. Currently, our chemical technologies transform only one-third of all raw materials into useful products – therefore, the vast majority is wasted.[11] New discoveries, such as dynamic bonds, could expand the toolbox of adaptive chemistry, a strategy that explores the potential of responsive materials to yield fascinating features such as self-

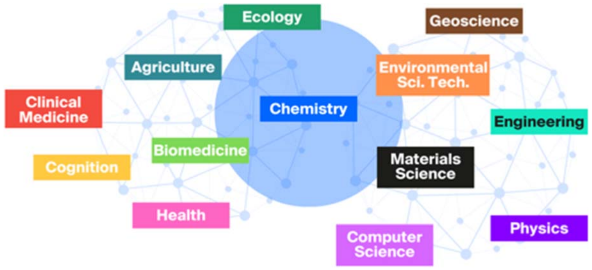

Fig. 1 Chemistry is usually depicted as "the central science". This simplified scheme depicts how chemistry is connected to many other fields based on the connectivity maps generated from bibliographical analyses (adapted from Rafols, Porter, and Leydesdorff, 2010).[6]

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healing and responsive properties.[12] Accordingly, the IUPAC "Top Ten" have highlighted the importance of dynamic systems in several instances, particularly to address the problem of plastic pollution. With dynamic bonds and adaptive chemistry, combined with comprehensive studies, including computational simulations and life-cycle analyses (LCA), chemists could make molecules safe and sustainable by design.[13] The reimagination of chemical bonds is one of the cornerstones to circularity. It's time to transcend the chemistry of transformation, and establish the foundations for the chemistry of re-use, which will enable the circular economy.[14] Similarly, the design of new two- and three-dimensional chemical networks, such as covalent- and metal–organic frameworks (MOFs), has opened a new world of possibilities in recent decades. MOFs, selected in the first "Top Ten" list in 2019, have catapulted applications that range from water harvesting and carbon capture to gas storage and more efficient, directed drug delivery.[15] Thinking of new networks beyond the classic connectivity rules created the field of reticular chemistry[16] – but perhaps more interestingly, it could serve as an example on the importance of collaboration and connections in chemistry. Although nobody could guarantee the "Top Ten" technologies will transform the world, so far, the initiative has been extremely successful at raising awareness across different disciplines. Such a step is significant on its own, since visibility is the first step towards establishing new collaborations between areas, including the social sciences, in line with the principles of Responsible Research and Innovation (RRI).[17]

Connections across disciplines

The division of knowledge in siloes is counterproductive, as these artificial compartments don't exist in the natural world. Recent studies clearly demonstrate that multidisciplinary research is key to tackling the most pressing global challenges.[18] This includes the interactions with experts in social sciences – building bridges with a broad range of disciplines is a cornerstone of RRI and, most importantly, a catalyst for quicker change. Comprehensive collaborations in the RRI framework could help integrate aspects such as cultural competence and social justice, both indispensable aspects for a sustainable future.[19] The recent IUPAC World Chemistry Congress in The Hague gathered thousands of delegates who presented and discussed chemical solutions to accelerate innovation and bridge the gap between academic and industrial discoveries. As part of this major chemistry conference, the World Chemistry Leadership Meeting (WCLM) connected chemistry researchers, industry leaders, policy- and decision-makers, and other key players in the chemical community, all working together towards identifying the most important challenges ahead, including access to resources, regulation, and generally, the transition to a more sustainable future.[20] The theme of the WCLM 2023 has its roots in the Top Ten Emerging Technologies in Chemistry, selected by a panel of experts appointed by IUPAC. One of the goals of the "Top Ten" is bringing the former into the attention of, early adopters, industry leaders, and entrepreneurs.[21] Nowadays, public funders have also identified the importance of shattering silos and establishing stronger collaborations between academia and industry – examples include different programmes within the European Innovation Council (EU) and the National Science Foundation (US), among others. Collaboration requires communication and trust, to bridge the differences across fields and sectors, but they're key to the advancement of science.[22] The different "Top Ten" lists include several successful cases, such as mRNA vaccines, which have jumped from the laboratory to the market in record time and helped overcome one of the largest pandemics in recent history. Venturing outside our comfort zone to explore new opportunities, such as industrial collaboration, private funding, and relationships with researchers in other fields, is almost a guarantee of

Fig. 2 A picture showcasing the latest "Top Ten" Emerging Technologies in Chemistry, an initiative pioneered by IUPAC.

success, and usually impacts all sides in a symbiotic way – it benefits all.[23]

Re-thinking chemistry and education

Planetary boundaries

Earth Overshoot Day marks the point when humanity has exhausted the "budget" of natural resources available for a single year. Since 1971, the Earth Overshoot Day has come earlier each year, coming down to August 2 in 2023.[24] Similarly, the concept of Planetary Boundaries, proposed by an international team of researchers in 2009, identifies and assesses the critical risks of crossing certain biological and natural thresholds. The identification and quantification of boundaries could further help halt the progress of climate change and other ecological threats.[25] More recently, a study unveiled that 99% of the industrial processes in chemistry breach the boundaries – therefore they contribute to the climate crisis, to polluting our planet, and overall, they could be considered unsustainable.[26] Most of the "Top Ten" picks are strongly related to renewable principles, including the sustainable production of ammonia, efficient sodium-ion and solid-state batteries, solvent-free reactive extrusion, and different technologies to improve the recyclability of plastics. This IUPAC initiative should inspire others to "rethink" chemistry and envision strategies to make molecules in a more efficient manner, ensuring sustainability and safety by design, and creating processes that avoid the depletion of critical raw materials. Chemistry could catapult the transition to a circular economy, by designing both molecules and processes that reduce waste, recycle products better, and save economic and environmental resources.[6]

"Systems thinking" in chemistry education for sustainability

In 2020, IUPAC launched an international project on system thinking in chemistry to promote sustainability for the 2030 Agenda and beyond.[27] This effort involves reimagining chemistry research, education, and implementation.[28] "Systems thinking" achieves the understanding of complex topics by looking at broader relationships, connections, and circularity, as opposed to the more traditional analytical approach, which tends to dissect and separate problems into smaller pieces. Instead of considering chemistry the central science – an idea that only reinforces the separations between different fields and implies the existence of hierarchies among them –, we should concentrate the efforts of researchers and educators into the establishment of connections across sectors. Chemistry is only central in the sense that it will provide many of the tools that we need to achieve a much larger goal – the transition to a sustainable future. Intertwining chemistry with other fields, particularly with societal systems and social studies, is a fundamental step towards reimagining our world for the better.[29] In the field of chemical education, systems thinking provides an opportunity to support students. To address today's global challenges – pandemics, the climate crisis, access to energy and water – we must recognise the importance of interactions across different disciplines.[30] Small changes, *per se*, sometimes seem easy to dismiss and futile; however, social studies have proven that communities could catalyse a transition towards a more sustainable future.[31] "No one is too small to make a difference," the title of Greta Thunberg's book, perfectly summarises this idea. Similarly, connections and community building with other disciplines and the broader society help integrate aspects such as cultural competence and social justice into the discussion, which helps challenge the establishment and accelerate change. Both in chemistry and chemical education, connections must take place between researchers, industry experts, policymakers, activists, and global citizens – every piece of the puzzle matters to put together the complete picture.[32] Some of the 2023 IUPAC Top Ten Emerging Technologies in Chemistry, such as chloride-mediated removal of ocean carbon dioxide, depolymerisation technologies, and artificial muscles, as well as technologies selected in previous years, require the tools and mental frameworks provided by system thinking to connect the dots and go beyond the obvious solutions. For example, to understand where the raw materials and energy required come from, the processes involved in producing and using them, and what happens at the end of their life span. In early December 2023, the American Chemical Society organised a summit to reimagine chemistry education in response to the emerging technologies that are transforming chemistry jobs. The summit included discussions on the incorporation of "systems thinking" into chemistry curricula to promote green and sustainable development while expanding educational opportunities for both students and professionals.[33]

AI and the future of chemistry

Artificial Intelligence (AI) has made the "Top Ten" list twice, both in 2020 and 2023. However, this year's edition highlights the importance of large language models (LLMs), such as OpenAI's ChatGPT, for chemistry research, education, and industry. Although these technologies present interesting challenges to chemistry education, some threats to scientific integrity, and may contribute to fuel the current "publish or perish" model,[34] the advantages seem to outweigh the problems.[35] For many experts, LLMs represent the future of chemistry,[36] offering endless possibilities for a wide variety of applications – and better results than previous AI alternatives such as deep learning models. LLMs also offer outstanding opportunities in the advancement of sustainability research and, provided the methodologies follow the principles of "green AI",[37] its contributions to climate research surpass its concerns.[38] Additionally, some of these tools could convey great advantages to chemical education, complementing the abovementioned efforts of renewed strategies such as systems thinking. Chatbots and other generative models could streamline the search for information, as well as the discovery of interconnections across fields, often overlooked in an always-growing pile of published papers. Overall, LLMs – and AI tools in general – could rescue chemists from "the morass of the mundane, from meetings and memos," thus clearing time for creativity.[39] Beyond the "Top Ten", IUPAC is leading efforts towards the implementation of AI in chemistry, as well as the standardisation of tools, including InChI, to ensure that data follows the FAIR (findable, accessible, interoperable, reusable) principles. The IUPAC Top Ten Emerging Technologies in Chemistry exemplifies the need to connect the different fields of chemistry and chemistry with other disciplines. The development of some selected technologies, such as GPT models in chemistry, biological recycling of PET, and wearable sensors will need of collaboration between experts in linguistics, mathematics, medicine, and electronics, to cite just a few examples. Likewise, for the industrial application of the "Top Ten" technologies we will need entrepreneurs who will run with these laboratory discoveries and take them to the market. Even if we believe that chemistry has a role as the central science, we must embrace the fact that other sciences are also central to solving the problems that lie ahead. To be more effective in this endeavour, we must connect the different fields of chemistry and break down the silos that artificially separate fields whose boundaries are increasingly blurred.[40] Connecting the chemical worlds also involves embracing diversity in chemistry, meaning including the experiences and knowledge of people from different backgrounds, origins, and career paths.[41]

Conclusions

Now, as world leaders gather in Dubai for the 28th meeting of the Conference of the Parties (COP28), to join efforts in the fight against climate change, the world's plan to make humanity sustainable is failing. Science must do more to save our planet, as stated in a recent editorial in Nature.[42] To achieve this complex goal, and to do so quickly, we could connect the knowledge, technologies, and disciplines that are currently siloed, fragmented, and isolated. IUPAC's successive "Top Ten" lists of emerging chemical technologies represent a concrete contribution towards achieving this goal, raising awareness of the opportunities that chemistry could provide to build a sustainable future for all. But science and technology alone will not suffice. We need a new generation of scientists with the passion and knowledge to tackle these complex global challenges. To do so, they must be equipped with the skills and tools to understand, analyse, and connect the complex interdependencies and delicate balances involved in meeting people's needs without compromising the ability of future generations to enjoy a healthy and prosperous life. Tools like systems thinking will help create connections between the molecular world and our societal and environmental challenges. But, more generally, we need a new paradigm shift in the way we teach, research, and apply chemistry. Every molecule, material, and process should be designed with recovery, reuse, and recyclability in mind – the basis of circular chemistry. It won't be easy, but we are not alone, other scientists across disciplines will help too. We just need to make the connections. Luckily, bonding is something chemists are very good at.

Author contributions

F. G.-B. and J. G.-M. equally contributed to the conceptualisation, writing, review and editing of this paper.

Conflicts of interest

F. G.-B. is paid by IUPAC to write the feature articles on the Top Ten Emerging Technologies in Chemistry, published in Chemistry International (DeGruyter). J. G.-M. was the president of IUPAC until the end of 2023.

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