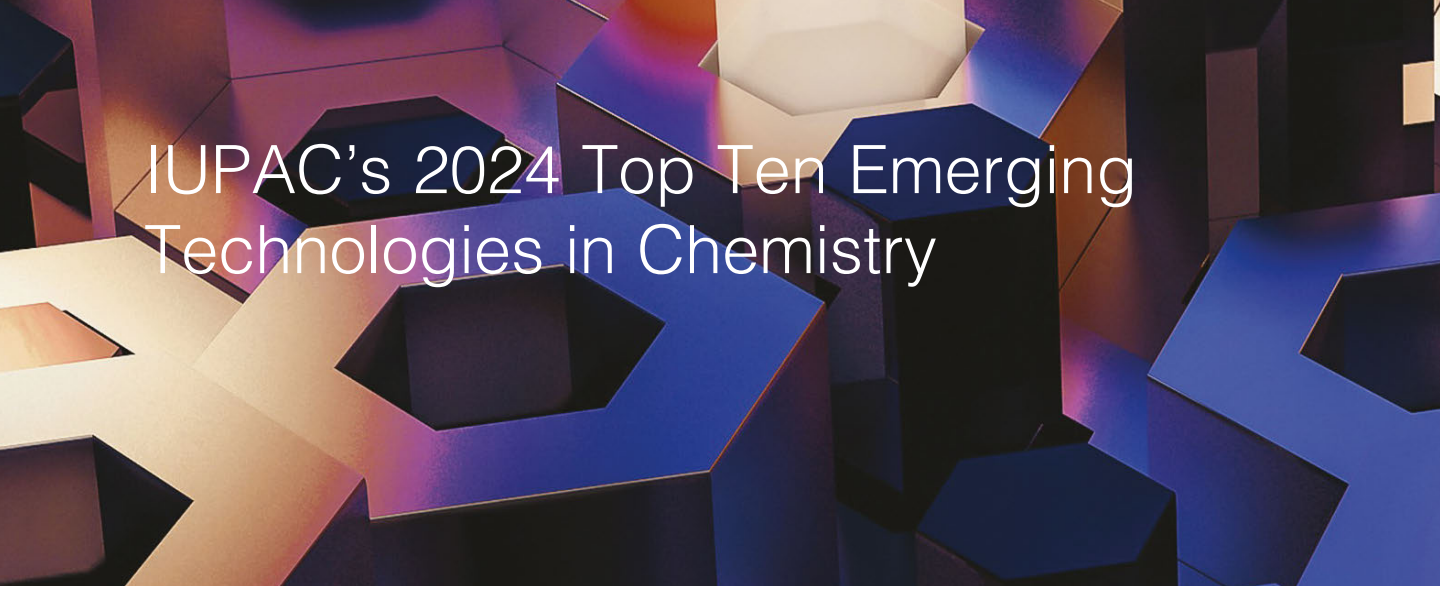


IUPAC's 2024 Top Ten Emerging Technologies in Chemistry

by Fernando Gomollón-Bel

In 2019, the IUPAC started a quest to select the most interesting emerging technologies in the chemical sciences [1]. Now, this established initiative continues year after year—adding ideas to a list of innovations with an enormous potential to transform fields as diverse as materials science, energy, healthcare, agriculture and computing, among others [2]. Overall, the IUPAC "Top Ten Emerging Technologies in Chemistry" align with the United Nations' Sustainable Development Goals, in a quest to secure a sustainable future and pave the way to a circular economy [3]. This new list delves into new materials, unexplored physical phenomena, and creative solutions to global challenges, including prevalent diseases and the still ongoing energy and fuel crisis. As in the first "Top Ten" paper, the technologies hover over a broad range of readiness—from laboratory discoveries to commercial realities, hence "emerging." But all of them, carefully curated by a panel of experts nominated by IUPAC, are equally exciting. Read on.

Frustrated Lewis pairs

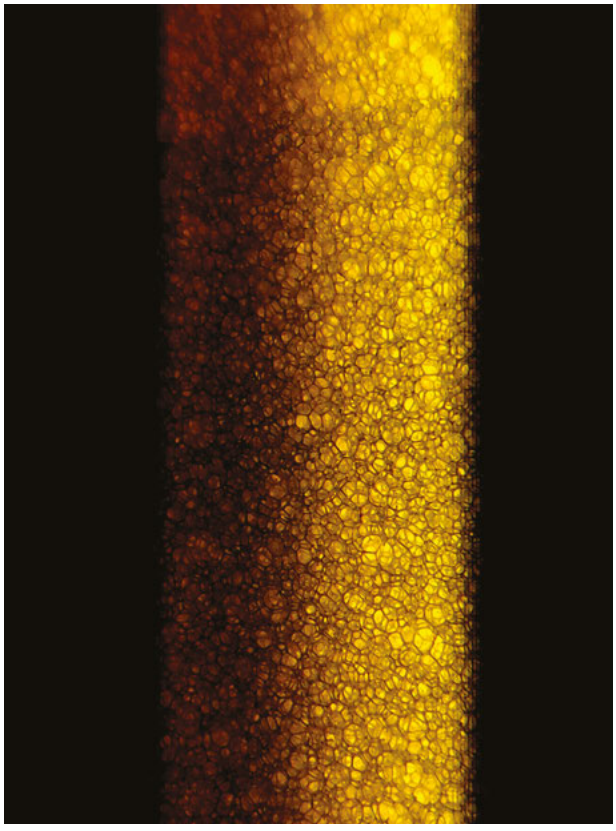
In 2006, frustrated Lewis pairs (FLP) compounds debunked a chemical "dogma" over one hundred years old—transition metals weren't alone in activating and splitting hydrogen. Armed with lighter elements, such as phosphorus and boron, FLP structures started the reaction even at mild conditions [4]. The concept is compelling—a combination of Lewis acid and base that cannot form a classical adduct because of steric or electronic hindrance, leaving their most reactive fragments exposed and ready for other molecules to enjoy. [5] This unique reactivity opened new possibilities for metal-free catalysis, and kickstarted a whole field that soon expanded to several substrates and possibilities, including enantioselective reactions [6]. Such versatility has enabled a wide variety of applications, including the activation of carbon–hydrogen and carbon–fluorine bonds, key in synthetic organic chemistry and, most particularly, in the functionalisation of pharmaceuticals and fluorine-18 imaging agents [7]. Other applications include the synthesis of biodegradable polymers, self-healing materials and sensors—widening the possibilities of FLP beyond organic chemistry and into the realms of materials science [8]. Additionally, on top of successfully activating hydrogen, FLP also activate the carbon dioxide molecule, which could create new capabilities in carbon capture and conversion into value-added products, including methane, methanol and acetic acid [9]. Although still far from commercial applications—probably because most FLP compounds are sensitive to air and moisture—some studies have shown great potential for the implementation of FLP compounds and catalysts on industrial scales. For example, FLP can decorate metal-organic frameworks (MOF) and still catalyse chemical transformations, such as hydrogenations and imine reductions. Once used, the MOF-FLP combination is easily filtered and recycled up to seven times without a decrease in catalytic activity [10]. Similar successes could catapult the industrial implementation of this technology in the near future.

Triboelectric nanogenerators

Triboelectricity is a tantalising property—it causes static stickiness between a balloon and hair, or Styrofoam and a furry cat. More technically, triboelectricity transforms mechanical energy into electricity. And triboelectric nanogenerators make the most of its capabilities and generate power from small movements and vibrations. This finds applications in sensors, energy harvesting, wearables, and healthcare. In the past decade, triboelectric nanogenerators have evolved from an early idea and proof-of-concept to a variety of commercial ventures and technologies in a market that is expected to double by 2030, according to some preliminary studies [11]. Until now, chemists have created triboelectric nanogenerators from a myriad of materials, including polymers (polydimethylsiloxane, polytetrafluoroethylene, polyvinylidene fluoride), graphene oxide, metals (gold, silver, copper), and textiles—as well as from a combination of compounds to craft composites with synergetic effects [12]. More recent efforts have focused on greener devices designed with natural materials, which offer a low-cost, biodegradable, and biocompatible alternative to synthetic solutions—while still showcasing increased instability, short service lives and lower power densities than the traditional alternatives [13]. Although triboelectric nanogenerators have demonstrated interesting uses in energy harvesting and storage, the most exciting applications arise in sensing—which ramifies into robotics, [14] actuators, wearables and, perhaps more importantly, medical devices [15]. The triboelectric properties permit self-charging from the subtlest vibrations, creating capabilities such as self-charging and enabling the detection of vital signs and pathogens with unprecedented accuracy and sensitivity [16]. Early studies also suggest applications in sustainability, including both water and air purification. Several companies in the US, UK, and China are currently studying the possibilities of scale-up and commercialisation of the technology, which could disrupt several sectors in sensing—and beyond.

Aptamers

Discovered in the 1980s, aptamers have evolved from an early-stage technology to a solution with several success stories in clinical trials. “Aptamer” literally means “the fitting part,” and refers to short, single-stranded series of nucleic acids, DNA or RNA, that bind other molecules with high affinity and specificity. The single stranded nucleic acids provide a unique versatility in terms of shapes and adaptability, which enables aptamers to adopt many different shapes and bind targets that include proteins, peptides, sugars, toxins—basically anything from small molecules to entire cells [17]. The applications range



from analytical systems and molecular imaging to drug delivery and targeted treatments. The aptamers are extremely specific to the different targets thanks to a process that evolves and enriches different strands, commonly called SELEX [18]. In a first step, a library of single-strand oligonucleotides is eluted through an affinity column previously packed with the target molecule. From the selection of best-performers, the DNA and RNA strands are amplified with a PCR [19] and then the process is repeated over and over—until the best candidate is isolated, purified, and characterised [20]. The selectivity and sensitivity of aptamers is comparable to antibodies, detecting substances in the nanomolar and picomolar range. But the activity of aptamers is much more uniform—plus production is cheaper and more reproducible. Aptamers also present other advantages in the field of drug delivery and advanced treatments, showcasing better penetration into tissues while generating a lower, less aggressive immune response [21]. In analytical chemistry, aptamers have successfully detected drugs such as cocaine, antibiotics like tetracyclines, [22] and even enabled the live and continuous monitoring of many molecules in the bloodstream of awake animals, thanks to the combination with a microfluidic array [23]. Moreover, aptamers have showcased great promise as specific therapeutics. The US Food and Drug Administration has already approved two aptamers for medicinal use: pegaptanib (commercialised as Macugen) for macular degeneration [24] and avacincaptad (commercialised as Izervay) for geographic atrophy—another degenerative disease that leads to loss of vision. Other aptamers are currently undergoing clinical trials to treat cancer, cardiovascular diseases, neurodegenerative diseases, and viral infections, among others [25]. New studies also suggest that aptamers could contribute to better drug delivery systems for chemotherapy, including the treatment and monitoring of aggressive cancers such as glioblastoma [26]. Overall, they offer a great step towards safer health solutions.

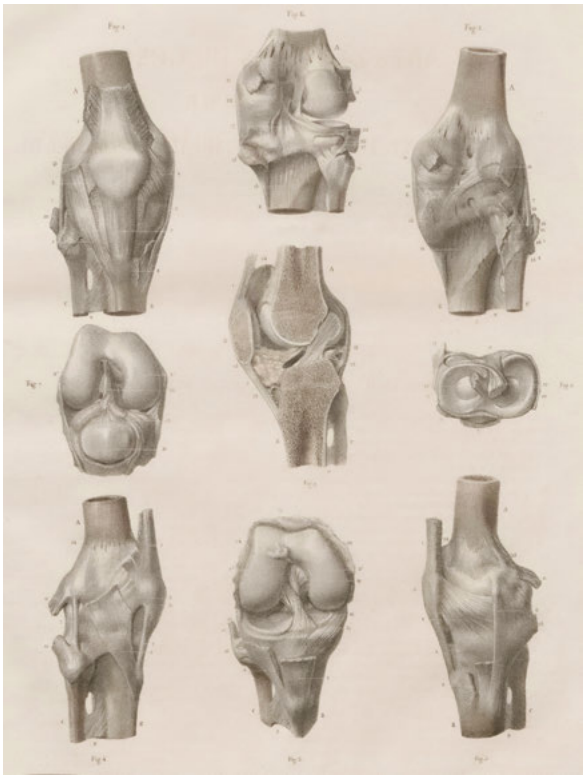
MXenes

The isolation of graphene in 2004 triggered the exploration of two-dimensional materials, also called layered materials, since not all of them are technically flat [27]. Among these many marvellous materials emerged MXenes, layered inorganic compounds such as carbides, nitrides, and carbonitrides, first reported in 2011 [28]. Within ten years, researchers reported applications in energy storage, environmental remediation, electronics, telecommunications, gas adsorption, water filtration, and more [29]. With over one hundred

possible combinations in terms of composition and fabrication strategies ready for scale-up, MXenes have been dubbed "the influencers" among two-dimensional materials—and catapulted the publication of patents, licensed by major players in the semiconductor and electronics industries such as Intel and Samsung [30]. Part of the promise of MXenes relies on a remarkable versatility—(semi)conductors a la carte according to composition—durability and elasticity. Like graphene, MXenes dispersions and inks enable the fabrication of different devices with production-ready processes, such as printing and spray-coating. But unlike graphene, films and flexible MXene-devices maintain the superior properties of the isolated flakes—a "killer point" in comparison, according to experts [31]. Among the most promising applications of MXenes is electrochemistry and energy storage, including key technologies such as batteries and supercapacitors. In both liquid and solid electrolytes, MXenes seem to boost redox reactivity, catalytic activity and other performance indicators that are usually studied in electrochemical reactions, including hydrogen evolution and the carbon dioxide reduction reaction. MXene-doped electrolytes have also showcased an increased performance in solid state batteries and supercapacitors—two key technologies that could untangle the energy crisis and solve the intermittency problem of renewable energies [32]. The energy-storage capabilities of MXenes could convey applications in functional memories and artificial neurons—the future could be full of surprises [33].

Hydration lubrication

This idea is a particular paradox. In certain materials and conditions, layers stay stuck together thanks to electrostatic interactions, but rapidly relax in response to shear, which provides an impressive fluidity and an



extremely efficient lubrication. It's hydration lubrication, a phenomenon observed in hydrated ions trapped between surfaces, as well as surfactants, liposomes, and other molecules, often observed in biological systems such as the synovial liquid that lubricates joints [34]. The remarkable properties of water reduce the frictional energy. Although the exact mechanism is still under investigation, some studies suggest that viscosity somehow increases under pressure without inducing solidification—probably because solid water is less dense than its liquid form, contrary to other solvents [35]. This sparked the study of applications in biomedicine, mostly in mobility issues, related to the lubrication of cartilage around our joints. Joints, especially hips and knees, experience massive stress, which in turn creates degradation and diseases such as osteoarthritis, suffered by over five hundred million people and experimenting a worrying increase in prevalence, according to the World Health Organisation (WHO) [36]. Some start-up companies work in related technologies, mostly in liposome lubrication, which seem to provide an effect comparable to healthy cartilage. Specifically, Israeli company Liposphere Ltd has successfully completed a clinical trial that confirmed both a reduction of pain in patients with osteoarthritis and no reported adverse effects. The same company has also started a multi-centre, double-blind, randomised trial with 150 subjects. Others research the application of hydration lubrication in the production of low-friction gels, with uses in soft contact lenses, catheter coatings, and other systems such as scaffolds for tissue engineering and recuperation. Additionally, such synthetic hydrogels for hydration lubrication could shed light on how biological lubricants really work [37]. Even if still in its starting stages, the understanding and study of hydration lubrication could convey extraordinary results in the near future.

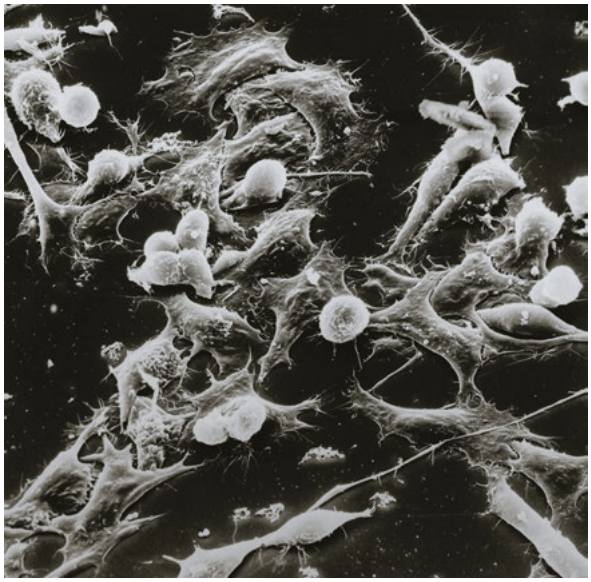
Bioinspired nanofluidic iontronics

Imitating the behaviour of the brain is the bedrock towards developing more efficient computers—and, in this quest, chemistry is key. In 2021, researchers described bioinspired nanofluidic iontronics, a technology that could catalyse the creation of chemistry-based computing systems and, in turn, brain-computer interfaces, artificial neurons, sensory protheses and much more. Mimicking the mechanism of neural synapses, in which ions carry signals and information, researchers envisioned a nanofluidic system filled with electrolytes that could behave like a memory-effect transistor, or memristor. Simulated monolayers of electrolytes showcased

a similar behaviour to synapses—with spontaneous voltage spikes. Although the first proof-of-concept was purely computational, [38] it sparked a series of studies in the field. For example, just a couple of years after the first study, nanofluidic iontronics successfully showed signal processing and transmission, demonstrated by regulating the cardiac activity of bullfrog hearts. This suggests that nanofluidic devices could become biocompatible—and effectively transmit and translate stimuli and signals between biological and artificial systems. [39] Soon, researchers also uncovered practical applications, with a working experimental example of a nanofluidic device that worked as a memristor—a promising step towards neuromorphic computing, [40] which would involve systems that replicate the way a biological brain processes information, in parallel processes and learning, communicating, and adapting. Such systems would reduce the energy demands of classic computers, which is an increasingly worrying environmental problem with the rise of artificial intelligence—especially large language models—and cloud-based internet-of-things solutions. Moreover, nanofluidic iontronics could convey key functionalities to biomedical devices, particularly in analytical systems that require high sensitivity and accuracy, as well as energy harvesting and energy storage [41]. The possibilities seem promising—and endless. Surely, it is possible that nanofluidic iontronics could soon circumvent the limitations of Moore's law [42].

KRAS inhibitors

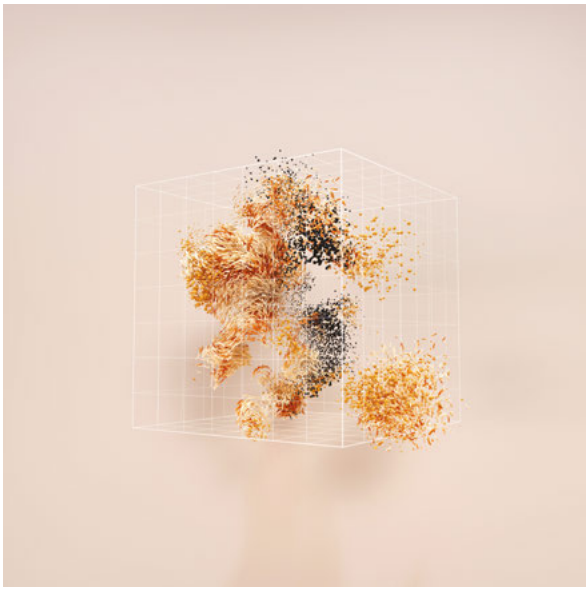
Cancer is the second leading cause of death worldwide, according to WHO [43]. And KRAS (the abbreviation of Kirsten rat sarcoma virus) is the most common oncogene—a mutated gene with the potential to cause cancer. Therefore, the understanding of KRAS and the development and design of drugs to block its effect has become a huge challenge in the fields of medicinal and pharmaceutical chemistry. But until recently, the efforts to repress KRAS' action had deemed unsuccessful—to the point that many had dubbed the oncogene "undruggable." [44] Luckily, in 2013, researchers discovered the first molecules that would bind covalently and selectively to the mutated cysteine residues in KRAS-related proteins [45]. Then in 2016, a small series of successful inhibitors entered the scene [46]. Soon, patient studies started, surprisingly obtaining positive and encouraging results with drugs such as sotorasib (Lumakras®) and adagrasib (Krazati®)—of which the former became the first KRAS inhibitor approved for clinical use in 2021. As it turns out, the action mechanisms of the molecules were previously unknown, nevertheless uncovered thanks



to the multidisciplinary efforts of chemists, biologists, and medical professionals—a major milestone in drug discovery. According to experts, many patients suffering from KRAS-mutated cancers will likely live longer, and better, thanks to these simple small molecules [47]. Clearly, the first KRAS inhibitors sparked innovation in the field. Many molecules have now joined sotorasib and adagrasib in the library of KRAS inhibitors, and companies continue to carry out clinical trials with these new drugs—as well as combinations with existing chemotherapy and immunotherapy agents. The advancements in KRAS inhibitors have paved the way towards tackling one of the major and most common challenges in oncology [48].

Neural network potentials

In the past few years, Machine Learning (ML) and Artificial Intelligence (AI) have revolutionised chemistry and materials science, as highlighted in previous editions of the "Top Ten" in 2020 and 2023 [49]. Once again, algorithms accompany us with neural network potentials (NNPs)—a ground-breaking tool to simulate systems at molecular scales with speed and accuracy. The dream of NNP experts is realising Paul Dirac's vision—using quantum mechanics to unify physics and chemistry, potentially providing powerful tools to better understand materials science, biology, earth sciences, and much more [50]. NNPs, trained with data sets such as solutions to the Schrödinger equation, have successfully showcased several applications in computational chemistry, simplifying and accelerating otherwise complicated and time-consuming tasks, with improved results as well [51]. Among the advantages



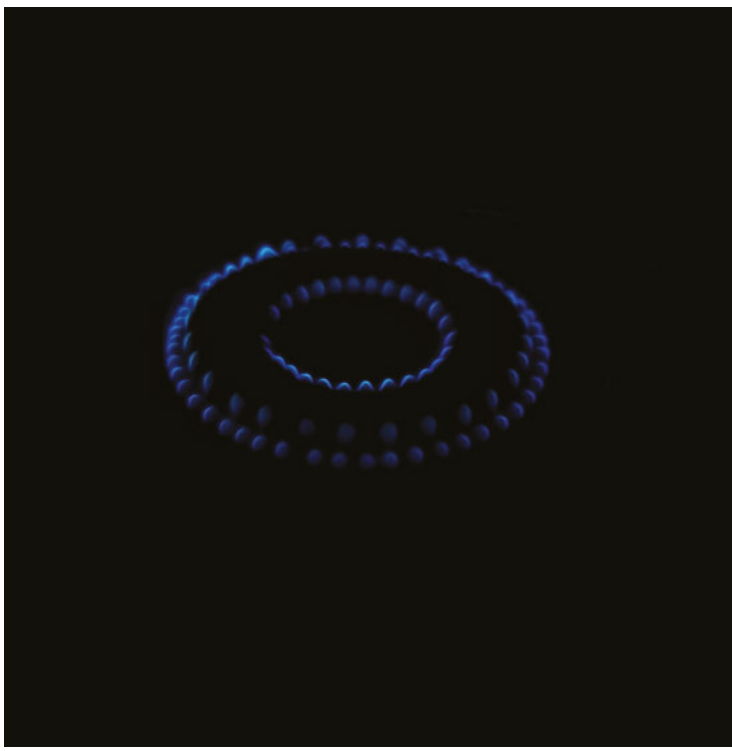
of NNPs are making the most of ML, large-language models and other technologies to speed up molecular simulations, learning to predict properties such as energy levels and forces from basic inputs, giving access to previously unreachable results. Traditionally, such calculations required monstrous amounts of resources and power. Since AI and access to computational capabilities—particularly high-performance computers—is increasingly limited and associated with environment, energy and climate concerns, [52] NNPs could circumvent several issues, particularly related to the size of simulations. Big technological companies have already started researching in NNPs, including Google's Deepmind and others [53]. This innovative ML methodology could catalyse faster simulations and, therefore, more creative chemistry ideas.

Active adsorption

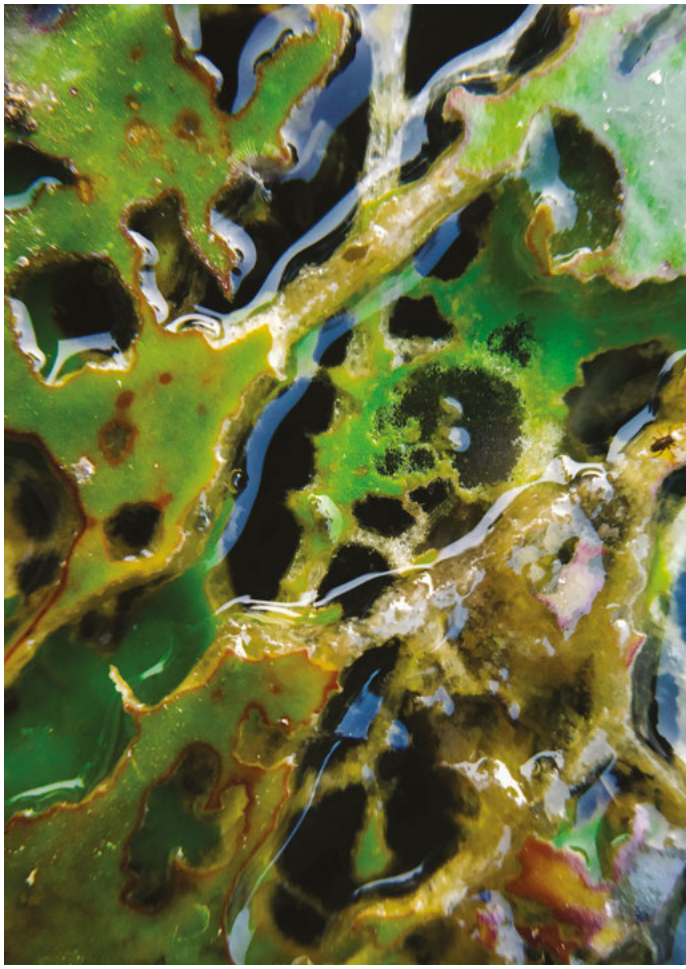
During the big boom of physical chemistry in the 1930s, Irving Langmuir and John Lennard-Jones laid out the rules and laws of adsorption. They established that adsorbates stuck to surfaces in two different ways—physisorption, the product of van der Waals interactions, and chemisorption, a consequence of electronic interactions. Additionally, adsorption was analysed as a "passive" process, in which the adsorbate tends to transfer from high concentration to low concentration areas to maintain an overall equilibrium. In 2021, however, a discovery defied this dogma [54]. Could chemists make adsorption an active process? Apparently, active adsorption happens—thanks to Nobel-prize winning molecular machines. If secured on surfaces, synthetic molecular machines may "grab" and move molecules opposing the equilibrium with just a small push of external energy. The first example of active adsorption (also dubbed "mechanisorption," because of its mechanical mechanism) used redox reactions to both adsorb and desorb a paraquat-phenylene polyaromatic ring onto the surface of a metal-organic framework—decorated with molecular machines or "pumps." [55] Although still a basic proof-of-concept, some studies have used the mechanisorption concepts to develop self-assembling materials and other supramolecular structures [56]. Additionally, because active absorption acts against equilibrium, some researchers speculate it could create new technologies for energy generation and storage, as well as enable chemical computing, because of the resemblance of these synthetic systems to components such as capacitors. Other applications could emerge in solutions with lots of surface and interface action—such as catalysis, gas capture, water purification and drug delivery. Mechanisorption could create new methodologies for manipulating molecules in a controlled manner—potentially a true game-changer.

Electrochemical nitrogen cycle

The sustainable synthesis of ammonia—as an alternative to the energy-hungry Haber-Bosch process, which is directly responsible for 1.5% of all global carbon dioxide emissions [57]—made the "Top Ten" list back in 2021 [58]. Then, electrocatalysis emerged



as a powerful tool to decarbonise Haber-Bosch, and provided power production proceeds from renewable sources, such as solar and wind. However, making ammonia is just a small part of a larger problem—the nitrogen cycle. Other reactions, such as the oxidation of ammonia to nitrates (the Ostwald process) or the reduction of said nitrates to nitrogen, still pose several electrochemical challenges. Therefore, the overall electrification of the nitrogen cycle is far from reality [59]. But such electrification could bring abundant advantages in terms of sustainability. For example, the overuse of synthetic nitrogen fertilisers has provoked pollution problems such as eutrophication, the increased growth of unwanted microorganisms in nutrient-rich areas, which compete with crops for nutrients and oxygen. The reduction of nitrates back to ammonia could contribute to cutting the contamination in crop fields, as well as provide an alternative source of nitrogen with higher reactivity than atmospheric dinitrogen. Like in electrochemical nitrogen reduction, studies suggest that metallic copper could catalyse the transformation of nitrates into ammonia [60]. This approach follows the principles of green chemistry and the circular economy, and could literally "transform trash into treasure." [61] On top of copper, other catalysts with abundant metals such as zinc, nickel, and iron have successfully shown activity in the reduction of nitrates to ammonia, as well as other species including urea, nitrous oxide, and dinitrogen gas. Although ammonia is a good fertiliser, electrochemists still study the direct transformation of atmospheric nitrogen into nitrates—mostly because salts are easier to transport and distribute. Moreover, oxidation of dinitrogen also gives access to nitric acid, a valuable feedstock in the chemical industry. Electrocatalysts based in ruthenium, titanium, zinc, iron, and cobalt have demonstrated promising results [62]. Finally, another interesting reaction is the conversion of ammonia back to nitrogen, which on top of applications in environmental remediation could provide new possibilities in power generation and green fuels. Ammonia is a common hydrogen "carrier" and a valuable vector for environmentally friendly energy, [63] since it has high volumetric and gravimetric energy density, plus is cheaper and safer to store and transport. Then, ammonia is either transformed back into hydrogen and innocuous nitrogen or used directly as a power source in fuel cells. Here, precious metals such as platinum, palladium and iridium outperform more abundant alternatives. However further research will surely yield better results with cleaner catalysts [64]. Lots of different hurdles ahead—electrifying the nitrogen cycle means remodelling and rethinking the heart of the current chemical industry [65]. An interesting idea, nevertheless.



Conclusions

It is fascinating that, year after year, the "Top Ten" uncover chemical technologies with a true potential to transform our world. It reflects the real diversity of chemistry as the connecting science, a catalyst across disciplines that can and will accelerate sustainable solutions for our society [66]. This IUPAC initiative is growing and becoming a beacon of innovation—an inspiration, too, creating new opportunities for collaborations to eventually "bridge the gap" between academic laboratories and impactful industrial applications. The "Top Ten" family has grown to sixty technologies now. If you recognise any meaningful developments in the chemical sciences, please take the time to send us your ideas! IUPAC collects contributions through a publicly available link, so stay tuned and submit your nominations for 2025

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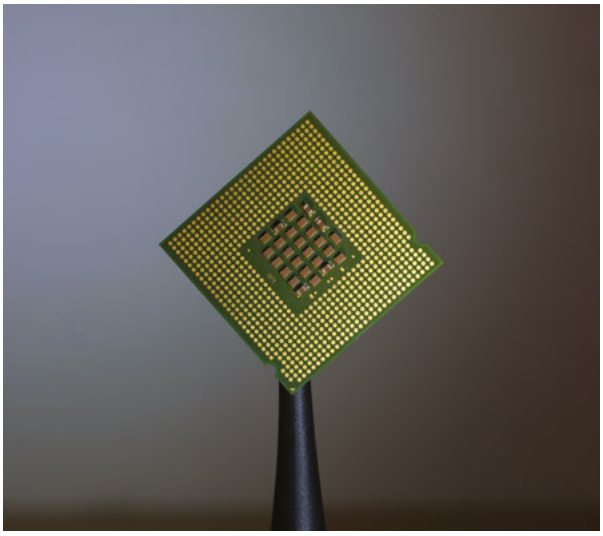

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