

# Ten Chemical Innovations That Will Change Our World

## The developing science that will fight the pandemic and reshape the chemical landscape

by *Fernando Gomollón-Bel*

In 2019, IUPAC introduced the “Top Ten Emerging Technologies in Chemistry” [1]. This initiative commemorated both IUPAC’s 100 anniversary and the International Year of the Periodic Table, a worldwide event that celebrated 150 years since the first publication of Mendeleev’s most famous chemistry icon. Now, IUPAC wants to transform this project into yet another landmark. Every year, the “Top Ten Emerging Technologies in Chemistry” will identify innovations with tremendous potential to change the current chemical and industrial landscape [2].

Throughout the past year, chemists around the globe have suggested remarkable technologies and innovations in their respective fields. A team of experts recruited by IUPAC curated the proposals and selected the most disruptive and forward-thinking—promising ideas with excellent chances for achievement. Some of them have already started weaving a network of spin-offs and attracting the interest of the chemical enterprise.

The “Top Ten Emerging Technologies in Chemistry” are also aligned with the United Nations’ Sustainable Development Goals (SDG). The selected technologies will change our world for the better, making a more thoughtful use of our resources, favouring more efficient transformations, and providing more sustainable solutions in applications ranging from new materials and more efficient batteries to extremely precise sensors and personalised medicine.

Furthermore, this year the world is facing an unprecedented challenge—fighting one of the worst pandemics since the Hong Kong flu in 1968. COVID-19 has affected our society across many levels, and will most likely transform our lives in ways we are yet unable to anticipate. In this global fight against coronavirus, chemists will play a key role. From soap and clean water to tests and new drugs, chemistry will be paramount to defeat this new threat. Thus, two of the technologies focus on solutions that will be crucial—rapid tests and RNA vaccines.



### Dual-ion batteries

Electricity as we know it has a major flaw—it is surprisingly hard to store. To date, one of our best solutions are lithium-ion batteries, an advancement that was recently recognised with the 2019 Nobel Prize in Chemistry. During the past few decades, these devices have enabled the miniaturisation of energy-storage devices, currently used in laptop computers, mobile phones, and electric vehicles. Despite their high energy density, lithium-ion batteries still present some downsides. In fact, if you were to use state-of-the-art batteries to power your house, you would need a device of over one ton to store enough energy for one week. Moreover, the scarcity of lithium and cobalt limit future developments, and their links to conflict minerals clashes with SDG 12 on sustainable production patterns. Hence, newer devices such as dual-ion batteries (DIBs) have attracted the attention of the scientific community [3]. Whereas in classic lithium-ion batteries, only cations move along the electrolyte, in DIBs both anions and cations participate in the energy storage mechanism. They also exhibit some fundamental differences in the cell setup—in DIBs the ions in the electrolyte are also active, which directly influences characteristics such as capacity and voltage [4].

DIBs could be an interesting alternative for grid storage applications. Their electrodes can be manufactured out of cheap and abundant materials using greener routes. Traditionally, the fabrication of lithium-ion batteries involves the use of toxic organic solvents. On the other hand, researchers envisioned fabricating DIBs using water processing, enhancing sustainability and reducing the cost. Although the first DIB prototypes also relied on lithium, now chemists have found new solutions that use sodium, potassium, or aluminium—all of which are copious and widely available worldwide. Discovered only a few years back

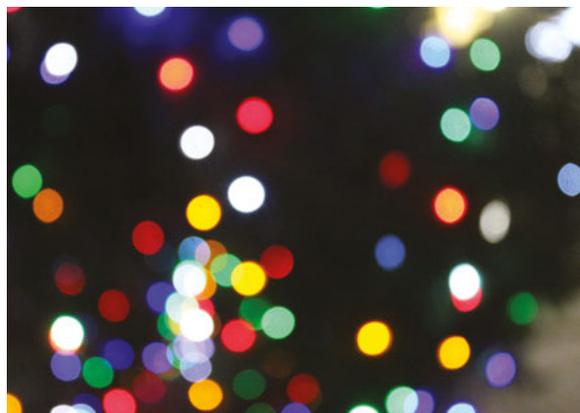
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[5], DIBs are still facing some challenges – researchers need to better understand their mechanism in order to improve their capacity, reversibility, and lifetime. Yet, industrial innovations are starting to blossom. Recently, a team in China reported the first prototypes for viable pouch cells based on the dual-ion approach [6], and companies such as Ricoh and Power Japan Plus are already investing in this attractive technology. The latter has even tempted electric car maker Tesla with “a fully recyclable battery that charges faster than lithium while still allowing a range of 300 miles.” In brief, DIBs present a series of advantages in terms of cost, lifetime, and sustainability that align with SDG 7. Besides, they provide a safer choice, according to experts. Since there is no intrinsic oxygen available in the cell, the ‘fire tetrahedron’ is incomplete, preventing accidental combustion.

### Aggregation-induced emission

Nowadays, luminescent materials are ubiquitous: from LEDs to bio-imaging techniques. Since most of these substances usually feature a plethora of aromatic moieties, molecules tend to stack at high concentrations, which eventually kills luminescence. This effect is known as aggregation-caused quenching. In contrast, back in 2001 researchers observed the opposite phenomenon [7] – certain luminogens showed very weak emission in diluted solutions and an intense emission when the molecules piled up. At first, the concept received very little attention, but now it has become a vast field of study [8]. Aggregation-induced emission (AIE) has transformed the way people think about luminescence.

Molecular shapes are the key to understanding this effect. Unlike classic luminogens, the molecules that are AIE-active are non-planar. They are like miniature propellers, continuously moving. However, when they aggregate, rotation stops, and all of their energy is released in the form of light. Since the discovery of AIE, chemists have identified several families of compounds



that exhibit this effect, including classic luminogens such as polyaromatic compounds and organometallic complexes, and more exotic products such as polymers, oligosaccharides, and nanoparticles [9]. AIE has opened new avenues in the development of luminescent materials—it has already found applications in OLED devices, sensors, and novel bio-imaging tools. *The New York Times* highlighted AIE’s potential to reach the real-world very soon. In fact, start-ups that market AIE technology are blossoming—two good examples are AIEGEN Biotech, in Hong Kong, and Luminicell, in the US. The latter also sells their fluorescent nanoparticles for live cell tracking through leading chemical supplier Merck.

### Microbiome and bioactive compounds

We contain multitudes. Over 10 trillion microbes live in our guts, respiratory track, and skin. Our microbiome may be modifying our behaviour, and research suggests it could also trigger diseases such as cancer, as well as determine our response to treatment. All of these bacteria constantly release metabolites in response to different stimuli in their environment. Chemistry could play a key role in screening and identifying all these different molecules, which could eventually be isolated and used as novel therapeutic candidates.

Very recently, a team in Princeton took this approach to the next level [10]. Using different computational tools, they analysed bacterial genomes and identified gene clusters that codified the biosynthesis of small molecules. Then, they expressed these instructions in genetically-modified bacteria and obtained a series of molecules with strong antibacterial activity. Although this field—functional metagenomics—has progressed slowly in the past few decades, this new development has been characterised as “a game-changing approach, [with] the potential to revolutionise discovery.” [11] The microscopic life within us is immensely diverse. Chemists and biochemists may find a myriad of new bioactive compounds encoded in the genomes of bacteria, contributing directly to SDG 3. Understanding and unravelling the secrets of our microbiome could revolutionise the future of healthcare.



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## Liquid gating technology

The idea of using liquids as a structural material to build responsive gates sounds counterintuitive—even verges on science fiction. However, this idea, originally proposed in 2015 [12], has already become a reality, and could soon bring many novel applications. Usually, liquid membranes work thanks to differences in concentration and potential astride the border. However, liquid gating membranes respond to pressure changes that rely on capillarity. At the microscale, phenomenon allows certain liquids to selectively open and close pores on-demand.

Liquid gates can selectively process mixtures of fluids without clogging. Thus, researchers predict that they could become extremely useful for large-scale filtration and separation processes. Among other things, liquid gates could accelerate the progress towards SDG 6, which looks to ensure access to clean water and sanitation for all. Moreover, since liquid gates require no electricity at all, they ensure huge energy savings.

Besides separation, liquid gates could find uses in many other fields, such as chemical sensors, microfluidic arrays, high efficiency catalysis [13], biological tissue printing [14], and lab-on-chip applications. Despite its novelty, liquid gating technology has already been recognised as a key innovation by prospecting company TechConnect, in the U.S. “It is sufficiently mature and attractive for licensing and investment,” they said. Hopefully, liquid gates will soon be scaled-up and adopted by key players in the chemical enterprise.

## High-pressure inorganic chemistry

We all perform differently under pressure. Chemicals are no exception, and the most exceptional phenomena take place at extreme conditions. For instance, researchers have squeezed benzene into super-strong, ultra-thin diamond nanothreads and recently provided spectroscopic evidence of having prepared metallic hydrogen. High-pressure science is no longer a niche field. The newest technological advances allow to closely monitor

samples under high-pressure environments, enhancing our understanding of materials [15].

These experiments involve pressures of up to 500 GPa—equivalent to five million times the average atmospheric pressure. To reach these immense strengths, scientists need to trap their samples between two diamond tips, which is commonly known as a diamond anvil cell. Further enhancements, such as combining diamond anvils with high energy X-rays, allow even higher pressures, reaching limits around 640 GPa.

Under ultra-high pressure, the rules of chemical bonding reshape. Stoichiometry laws blur—researchers have isolated ‘cousins’ of common salt from  $\text{Na}_3\text{Cl}$  to  $\text{NaCl}_7$ . In addition, some compounds that are undoubtedly inert at ambient conditions suddenly become reactive. Traditionally inactive species, such as dinitrogen, carbon monoxide, and carbon dioxide polymerise under extreme pressure and temperature, yielding products that, in some cases, survive depressurization and can be isolated at atmospheric pressure [16]. High pressure also enhances well-known effects such as luminescence and superconductivity.

Chemistry gets very complex in these conditions, but at the same time it gets really interesting. Discerning the transformations that take place under ultra-high pressures could lead to new molecular species and novel materials with unprecedented properties, such as room temperature superconductivity or superhardness. Moreover, some of the knowledge acquired could be translated to room pressure processes—researchers hope to open new frontiers in chemistry.

## Macromonomers for better plastic recycling

2020 marks the 100 anniversary of Hermann Staudinger’s prestigious manifesto on polymerisation. Chemistry played a key role in the development of artificial polymers—durable and versatile materials that transformed our civilisation. However, said durability has turned against us: the building blocks of the twentieth century are now everywhere, accumulating in our landfills and polluting our oceans. Some experts predict that by 2050, the total amount of plastic in the oceans will weigh more than the total amount of fish [17]. Now, chemists must find a solution.

Many research groups are looking into more efficient ways to recycle the polymers we know, as reflected by last year’s IUPAC Top Ten Emerging Technologies in Chemistry [1]. Additionally, other groups are investigating new types of polymers that can be easily recycled. Solutions include plastics that break down upon exposure under UV light, and macromolecules bearing responsive “end caps” that trigger depolymerisation on-demand.





Redesigned monomers and macromonomers are an up-and-coming strategy to craft more sustainable plastics. Chemists rely on radical ring-opening reactions, which allow them to incorporate heteroatoms and functional group—such as ester—in structures that, traditionally, have an all-carbon backbone. The resulting polymers are easier to hydrolyse and recycle. Recently, several groups have optimised this technology, delivering a broad-range of biodegradable plastics that keep the attractive characteristics of conventional polymers [18]. Starting from a widely-available lactone, researchers developed a strong and stable polymer that can be recycled again and again under mild conditions [19].

These methods are far from being widely adopted. Nevertheless, chemists are moving in the right direction—re-thinking polymers and designing structures that ensure recyclability. Undoubtedly, chemistry is our best chance to find a solution to the plastic problem, contributing to at least five different SDGs at the same time.

### Artificial intelligence

Artificial intelligence is transforming our society. Its market value is growing exponentially as it finds uses in finance, justice, transportation, and even healthcare. Chemistry is no exception. Researchers train algorithms to speed-up structure elucidation, enhance retrosynthetic analyses, design optimised reaction sequences, discover new drugs, and even run futuristic robotic laboratories. The possibilities are endless. “In the future, we will forget chemists used to be humans,” believes chemist and inventor Lee Cronin.

The applications of artificial intelligence in chemistry are only just beginning—the biggest leaps in progress are yet to come [20]. Researchers predict that these technologies have a tremendous potential. Among other things, they expect chemical reactions will become more reproducible, more easily scalable and eventually, greener and more efficient. Thanks to the combination of high-throughput methodologies and automated analyses, chemists could control and accelerate serendipity—turning accidental discoveries into a thorough and carefully-planned search [21]. All these strategies could expedite scientific breakthroughs and solve increasingly-sophisticated problems.

Algorithms could also tackle broader issues. For

instance, machines can systematically analyse the scientific literature and learn from virtually every piece of data ever published. This could not only help us recognise trends, but also identify possible solutions to bigger challenges related to energy, climate change, environment, and health. In fact, recent studies suggest that artificial intelligence has a positive impact towards achieving the SDG—enabling the accomplishment of 134 targets across the goals.

Technology will upgrade our role as chemists. Rather than replacing us, artificial intelligence will enhance chemical discoveries while freeing us from mundane and repetitive tasks. Thus, we will focus on creativity, enabling leaps only limited by our imagination [20].

### Nanosensors

Sensors detect changes in the environment. In chemistry, the process of sensing involves two steps—recognition, when analyte molecules meet their receptor; and transduction, the ‘translation’ of that event into an output signal [22]. Nanosensors work in a similar way, only they use nanomaterials as the active element. Chemical nanosensors are used in a myriad of applications, from monitoring pollution and food quality control to security and healthcare.

The field of sensors has progressed to the point of detecting single molecules. This has been dubbed “the



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ultimate sensitivity,” and is paramount in healthcare applications [23], where detecting a single entity can be a matter of life or death. Single-molecule sensing provides additional benefits, such as easily measuring heterogeneity in a sample or enabling calibration-free measurements. Experts believe that these technologies could be “paradigm changing” [23].

Advances in chemistry and materials science have allowed significant improvements. Researchers have explored a tremendous variety of nanostructured materials—metal, oxides, carbon nanotubes, graphene, polymers—that, thanks to their high surface to volume ratio, provide significant benefits for sensing. Nanosensors are used across a number of fields in analytical chemistry. Recently, antibodies have attracted a great deal of attention due to the pandemic caused by coronavirus SARS-CoV-2. Luckily, chemists have used the unique properties of nanomaterials to create antibody nanosensors that are extremely sensitive and specific [24]. Gold nanoparticles, for instance, enable the detection of SARS-CoV-2 in under 15 minutes.

We are surrounded by sensors—they are inside our phones, fitness bands, smartwatches, and computers. Nanosensors will become increasingly popular, helping us distinguish fresh food from products about to expire, or upgrading our ability to detect previously unknown brainwaves, unlocking potential treatments for diseases such as epilepsy. Sensors will help us better understand the world in which we live.

### RNA vaccines

Vaccines prepare our immune system to fight diseases. Through different agents, vaccines induce the production of antibodies, molecules that recognise and trigger the destruction of pathogens. In particular, RNA vaccines have a very clever approach to this goal—the patient is administered an RNA sequence encoding the production of antigens, which eventually stimulate an immune response and the synthesis of antibodies. Although RNA vaccines have not been approved as yet for human use, they have shown promising results in clinical trials [25]. Their potential to supply a speedy solution to prevent the infection caused by the novel SARS-CoV-2 coronavirus has again put them under the spotlight.

One of the advantages of RNA vaccines is that their synthesis can be easily scaled-up. To develop classic vaccines, researchers need to grow the infectious agent in a cell culture, which requires using high volume reactors and a significant amount of time. On the other hand, RNA strands can be synthesised using methodologies that have been optimised—and even

automated—for decades. Moreover, RNA vaccines can be designed very quickly. Robin Shattock’s team at Imperial College London developed a candidate vaccine against COVID-19 within two weeks of getting the virus’ genomic sequence. The team is confident they could have preliminary results by next year. This is a true advantage when compared to classical vaccines, which usually need up to ten years of development—and an average investment of half a billion dollars—before they reach the market.

In addition to COVID-19, scientists are exploring the potential of RNA vaccines to prevent other infectious diseases such as Zika, rabies, HIV, the flu, and even cancer. Studies show that RNA vaccines could stimulate an immune response against cancer cells, making them an attractive alternative for novel immunotherapy treatments [26]. The Bill & Melinda Gates Foundation have invested an initial amount of \$52 million for the further development of this technology.

Moreover, several companies are investigating RNA vaccines. Among them stand out CureVac and BioNTech, both in Germany, and Moderna in the U.S. All of them have adjusted their pipelines to investigate RNA vaccines against SARS-CoV-2, and are confident that they could upscale production if needed. RNA vaccines advance quickly—in fact, Moderna’s candidate (mRNA-1273) was ready to start Phase III clinical trials on thirty thousand volunteers in mid-June.

While still young, the field of RNA vaccines will probably grow tremendously in the coming years—especially given how rapid and adaptable production is. Plus, if RNA vaccines against COVID-19 are successful and get fast-tracked into the market, this could further foster the advancement of the technology [27].





### Rapid diagnostics for testing

Rapid diagnostic tests are chemical assays suitable for swift medical screening. They normally involve a series of easy-to-follow steps and provide results within a few minutes. Moreover, these tests seldom require additional equipment, facilitating their use in resource-poor settings. Probably the best-known example is the home pregnancy test, of which more than thirty-five million units are sold annually in the U.S. alone. There are also rapid tests to diagnose diseases such as malaria, aids, and the flu.

Rapid tests work thanks to chemical reactions. Often, they use antibodies to detect the presence of antigens. Antibodies are linked to different types of probes that undergo a certain chemical reaction if the test is positive—this usually involves a colour change, making the interpretation of the results very straightforward.

The current COVID-19 pandemic has led to shortages of laboratory equipment to perform more thorough PCR tests. Thus, scientists around the globe have prioritised the development of rapid tests to detect SARS-CoV-2 and diagnose people suffering the disease this virus causes, COVID-19. Some of them rely on the detection of RNA strands rather than antigens, and deliver results in under half an hour. Pharmaceutical company Abbott, developed a COVID-19 test that

allegedly [28] uses loop-mediated isothermal amplification, which gives results in only five minutes. However, the latter requires some laboratory equipment.

At the moment, the World Health Organization (WHO) does not recommend the use of rapid diagnostic tests that detect antigens for COVID-19 patient care. So far, only three companies have received both an emergency use authorisation from the U.S. Food and Drugs Administration and the CE Mark from the European Commission—Autobio Diagnostics, CTK Biotech, and Hangzhou Biotech. Hence, chemists need to race against the clock to develop a suitable alternative that can yield significant results in a timely manner.

### Chemistry for a sustainable future

Chemistry provides us with an unlimited set of tools to reshape our world into one that is safer and promises a more sustainable future. From designing more efficient tests to developing a successful treatment, chemistry will be central to tackle the current COVID-19 pandemic, one of the most difficult challenges our society has faced in the last few decades. Furthermore, while we flatten the curve to stop the spread of the coronavirus and grant access to healthcare for those in need, we must remember other threats on the horizon, such as pollution, climate change, and circular

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economy. Innovation in the chemical sciences is essential to attain most of the SDG, the aspirational goals set by the United Nations to promote prosperity while protecting the planet. This aligns flawlessly with the main mission of IUPAC -to apply and communicate chemical knowledge for the greatest benefit of humankind and the world. This new edition of the “Top Ten Emerging Technologies in Chemistry” keeps the same spirit—promoting the fundamental role of chemistry to protect society and our planet. 🌍

## Acknowledgements

This initiative would not have been possible without the outstanding group of experts who identified and curated the list of technologies; they are: Michael Droscher, Javier García Martínez, Rai Kookana, Ken Sakai, and Bernard West. Many thanks to Bonnie Lawlor, for all the help all along the crafting of this article.

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More than 100 references are embedded in the online version of this article.

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The next search for the Top Ten Emerging Technologies in Chemistry is on.

The deadline for nomination is 31 March 2021.

<https://iupac.org/what-we-do/top-ten/>