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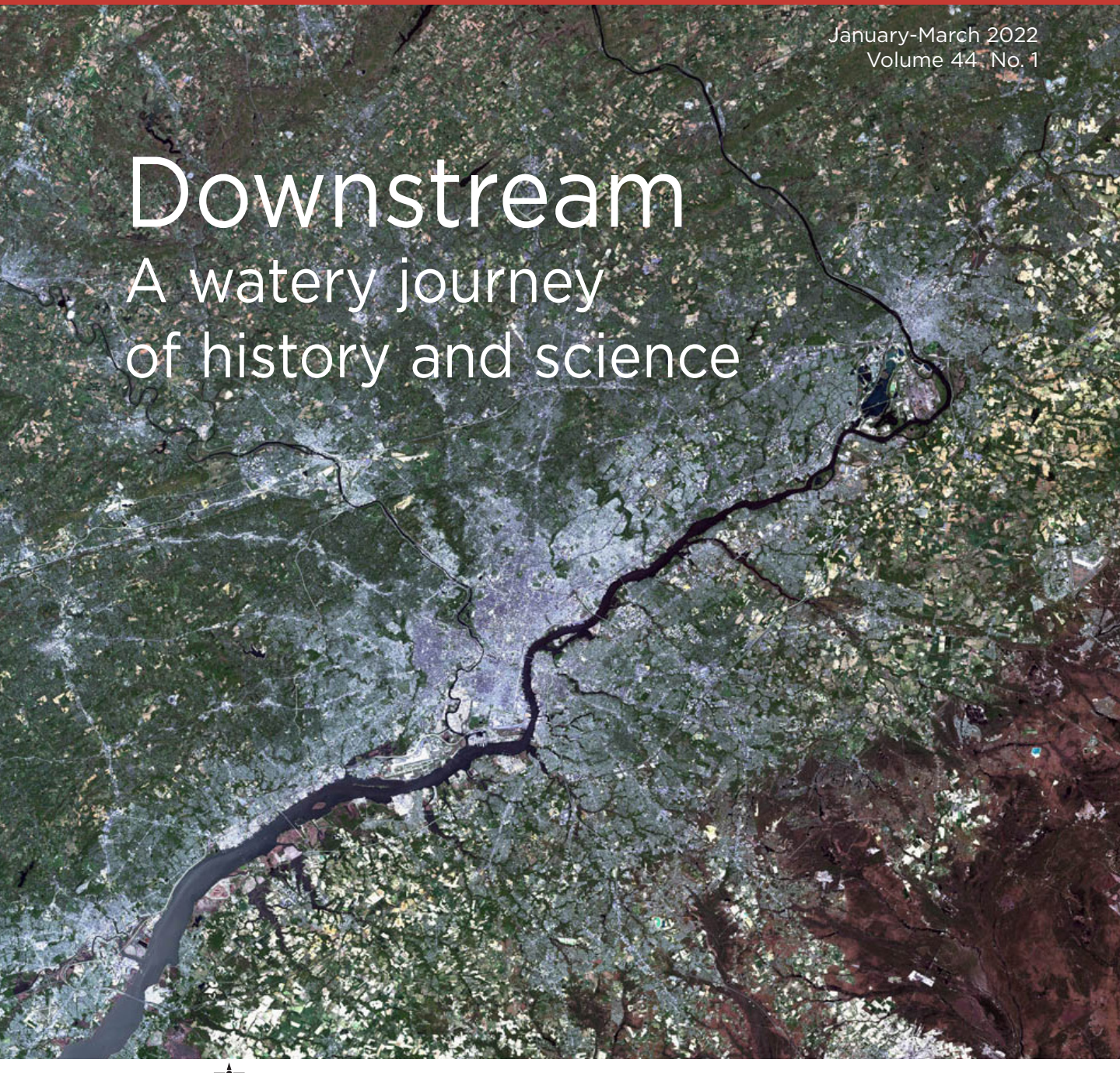

Downstream

A watery journey of history and science

Young chemists voice in support of the SDGs ▶

AI and Drug Discovery and Development ▶

INTERNATIONAL UNION OF
PURE AND APPLIED CHEMISTRY

Chemistry International

CHEMISTRY International

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Managing Editor:
Fabienne Meyers
IUPAC, c/o Department of Chemistry
Boston University
Metcalf Center for Science and Engineering
590 Commonwealth Ave.
Boston, MA 02215, USA
E-mail: edit.ci@iupac.org
Phone: +1 617 358 0410

Design/Production: Stuart Wilson

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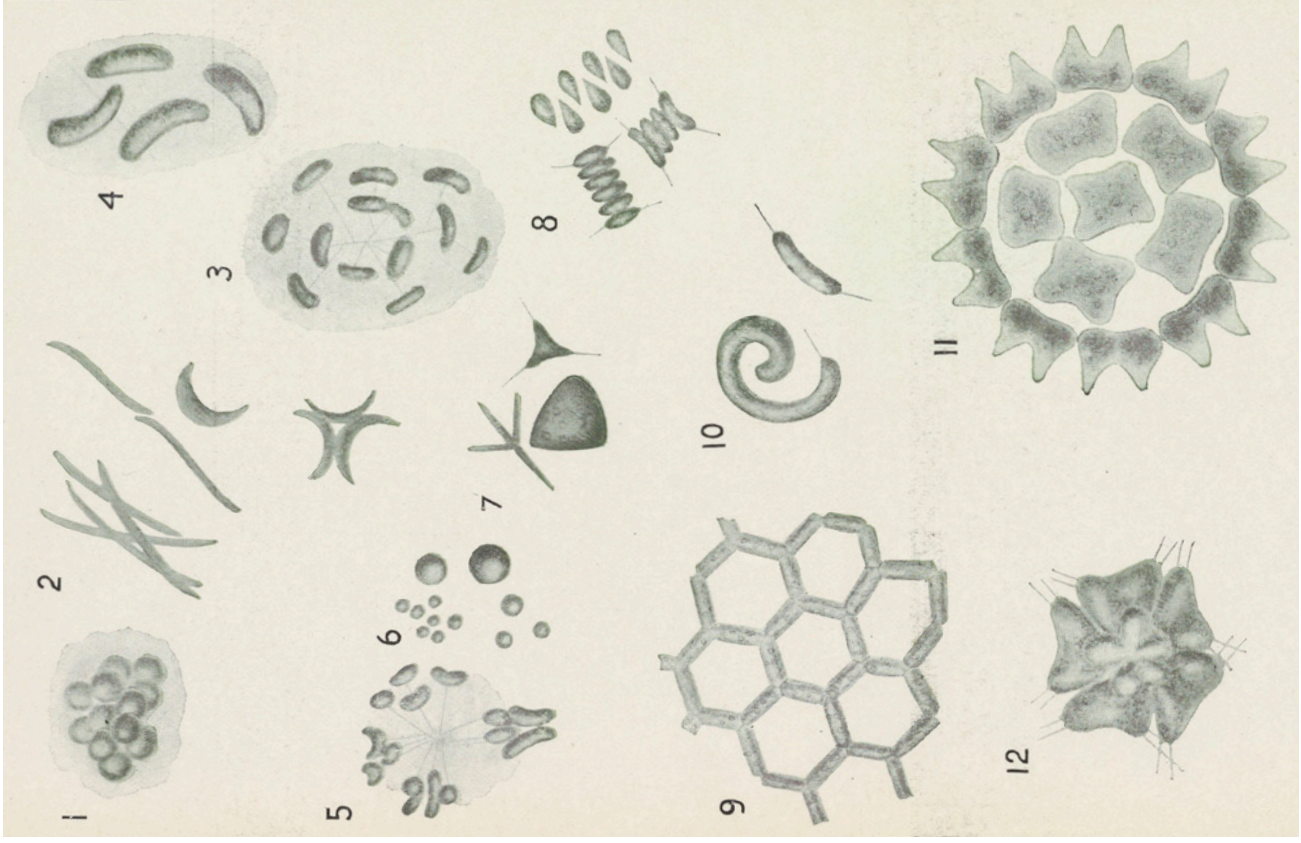
Cover: Downstream is the Science History Institute latest exhibit that explores more than 200 years of water analysis and protection in the United States; read more p. 11, by Jess Smith. The cover image originally appeared in the NASA Earth Observatory story Philadelphia, Pennsylvania. Image courtesy Ron Beck, USGS Land Processes Data Center, Satellite Systems Branch, published May 19, 2003.

While staying with the theme of Downstream, let us #colorourcollections. From February 7-11, 2022, libraries, archives, and other cultural institutions around the world are sharing free coloring sheets and books based on materials in their collections. Learn more at https://library.nyam.org/colorourcollections/

Here below is a collection of various forms of microscopic plant organisms living in water: Whipple, George Chandler, "Plate VI: Chlorophyceæ." The Microscopy of Drinking Water, 1914. https://digital.sciencehistory.org/works/zs25x934s.



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Bonding the Chemistry Community

by Javier García-Martínez

None could have imagined what history had in store for all of us when, just a couple of years ago, we were celebrating our Centenary and planning for the future of IUPAC. These past months, marked by a pandemic, have shown how fragile and interdependent we are. We have also learned the key role of science in understanding, tackling, and solving our most pressing challenges. Chemistry, in particular, is playing a central role in the fight against the coronavirus, from the production of disinfectants to the nanoparticles that carry the mRNA in the COVID-19 vaccines. However, this is not the last global challenge we will have to face and chemistry will continue to be essential in our fight against illness, hunger, and poverty.

Like so many other organizations, IUPAC too has had to adapt to a difficult time, when self-care and care for the people around us have been the top priority. A time in which we have had to learn on the fly how to work from home, adapt to new technologies, and be in countless virtual meetings while trying to balance our personal and professional life. Because of this, I would like to start this Column by acknowledging and thanking the excellent job that our staff has done to quickly adapt and to facilitate the work of all our volunteers. Our Secretariat has been above and beyond the call of duty, working tirelessly and with great efficiency to ensure that our organization not only carried on with its normal scientific activity but also held its first-ever virtual General Assembly, conducted a major review of its organizational structure, and significantly grew its online activities including the Global Women Breakfast, the Periodic Table Challenge, The Top Ten Emerging Technologies in Chemistry, and ChemVoices. I have no words that can thank our team enough for making all this possible. I would also like to take this opportunity to thank our past President, Chris Brett for leading during these difficult two years, our former Treasurer Colin Humphris, our Division Presidents, Committee Chairs, Titular and Associate Members, Affiliates, Task Force Members, partners, and all our volunteers for carrying on such a tremendous amount of work in a critical time under less than ideal conditions. Their availability and positive attitude speak volumes about their commitment to this Union and its mission.

However, we cannot continue operating in this way and, therefore, we must evaluate which activities and ways of working that we have implemented in the past months we should keep and which we should replace. To answer this question, we will be conducting a survey that is being designed to understand what our stakeholders liked about the way we operated during the last months, what they would like to change, and what they expect from us moving forward. With this initiative, we aim at capturing the lessons learned and at getting new ideas about the most efficient ways to communicate and engage with our stakeholders and among ourselves. This effort, which will be conducted by the Evaluation Committee led by Ehud Keinan, will greatly help us decide and define how to better use the new technologies while maintaining the clear benefits of in-person interaction. We are making every effort to facilitate the work of our volunteers and increase the impact and outreach of our scientific work. We are currently simplifying the project proposal format and submission process and from January 2022, Chemistry International will be freely available to all, which will help us to promote and give visility to our projects, activities, and recommendations.

I am delighted that some of the recommendations of the Review Group are already being implemented. Some are already a reality. For example, the new Committee on Ethics, Diversity, Equity, and Inclusion (CEDEI) has been established and its founding members have already been appointed. I would like to use this opportunity to thank Mary Garson for agreeing to chair this new Committee, which, I am sure, will be critically important to set up the guidelines that will help us to operate following our values and the highest standards. CEDEI will also produce recommendations on topics related to its mandate, which will be useful not only to IUPAC but to the entire chemistry community. Similarly, the IUPAC Centenary Endowment Fund was established last August during our General Assembly.* This represents a great opportunity and constitutes a new tool that will allow Fund Donors to support our work and to engage with the activities and initiatives of the Union.

Since our General Assembly, and in just a few months, we have done tremendous progress regarding the changes in our Statutes and Bylaws. This is not, by any means, an easy task but it is vital for the future of IUPAC. We have done our best to hear, debate, and

include as many views as possible through multiple meetings and conversarions. I want to thank the members of the Executive Committee and the Bureau, and other stakeholders for their comments, suggestions, and feedback and to ask Council Delegates for their support during the special Council meeting that will be held in June , 2022. The simplification of our decision making process to create a more agile and lean organization will allow us to react faster and more effectively. At the same time that we are strengthening and streamlining our governance structure, we are making a significant effort to improve our communication and engagement with our NAOs and other stakeholders. In addition to the frequent meetings we are having with them thanks to the use of online tools, we are creating new opportunities to discuss and answer any questions in an informal format. This is the NAOs Forum, an online meeting that will be held in the off-years of our General Assembly to have a conversation and address any concerns that anyone may have. The experience of the last months has taught us that these informal and frequent dialogues are essential to have a fluid and engaging communication with our constituents. Similarly, during our General Assemblies, the IUPAC President will invite the representatives of all chemical societies and federations to a meeting, that we have called the Presidents Forum, to discuss topics of common interests, potential synergies, and opportunities for collaboration. One example of of these kinds of opportunities, which will involve many sister organizations, is the International Year of Basic Sciences for Sustainable Development. It provides us with a unique and far-reaching opportunity to raise awareness on how chemistry research and innovation are key in building a more resilient and circular economy. From reusable plastics to green ammonia, chemistry contributes to achieving the Sustainable Development Goals. These two innovations are, in fact, some of the top ten emerging technologies in chemistry that we have been highlighting since 2019 and that are having a major impact. This is an initiative that is promoting both IUPAC and the public image of chemistry helping us to reach wider audiences and other stakeholders. During our Centenary, we launched this and many other activities that have become so successful that we decided to continue them beyond 2019. This turned out to be an excellent decision because, during the pandemic, our online activities, including the Global Women Breakfast, the Periodic Table Challenge, and ChemVoices have grown beyond anyone´s expectations and have opened many doors to IUPAC. We have now a much stronger and frequent collaboration with our sister organizations, especially

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Interdivisional Committee on Terminology, Nomenclature and Symbols

(Executive Committee members are denoted in bold).

with the International Younger Chemists Network, which is doing a terrific job and constitutes not only an opportunity but a priority for IUPAC.

But among all my priorities for this biennium, I want to highlight IUPAC Digital. Under this label, we include a series of actions that we are conducting at IUPAC to lead the digital chemistry space. This ranges from the creation of a chemical nomenclature for machines, namely the International Chemical Identifier (InChI), to the adoption of the FAIR principles to ensure that all chemical data is Findable, Accessible, Interoperable, and Reusable. It became very clear during our last General Assembly, which had a session entirely devoted to IUPAC Digital that this is the way to go so IUPAC will keep leading the global chemistry community during the next decades, as most of the chemical information and data is now contained, stored, and shared in bits, not in paper. On this note, the digitalization of our Gold Book represents a unique opportunity to make all our content not only more accessible, but also more relevant, impactful, and useful. Finally, I want to bring here some of the conclusions of our recent World Chemistry Leadership Meeting that under the title "The Future of Chemistry in the World of AI" provided us with a clear and compelling vision for the future of IUPAC. This two-day online meeting, masterfully coordinated by Chris Ober was a clear call to lead in this emerging field, which is already having a profound impact on chemistry discovery.

We are living in a time of uncertainty and profound changes, but also of great opportunities. Chemistry in general and IUPAC, in particular, are especially well-positioned to contribute to proving the solutions we need so urgently. I know I count on all of you to create an agile, effective, and inspiring organization, and to continue being the international community of chemists, widely recognized by its reputation, independence, and high standards. It will not be an easy task, that is for sure, but it is a challenge worth pursuing.

Javier García-Martínez <j.garcia@ua.es> is a Professor of Inorganic Chemistry and Director of the Molecular Nanotechnology Laboratory of the University of Alicante where he leads an international team working on the synthesis and application of nanostructured materials for the production of chemicals and energy. Javier is IUPAC President since January 2022. Previously, he served as Vice President and member of the Executive Committee, and as Titular Member and Vice-President of the Inorganic Chemistry Division.

*For a list of the actions taken at the IUPAC Council, held Virtual last August during the General Assembly, see https://iupac.org/actions-taken-at-iupac-council-virtual-2021/

Ethics, Diversity, Equity and Inclusion

Some National Adhering Organizations or other organizations affiliated with IUPAC have in place committees or reference groups that address issues of ethics or diversity and inclusion. There are numerous womens' chemistry groups worldwide, many linked to the IUPAC Global Womens Breakfast series, and emerging chemists' groups, including the International Younger Chemists Network (IYCN). Specialist groupings include those for chemists of color, for less-able bodied chemists, or from LGBTQ communities. Each of these groupings requires our recognition, respect, and support. IUPAC is in the unique and privileged position to deliver global leadership on their behalf. There are still chemistry communities globally where the principles of equity are less well recognized, and IUPAC can provide support through networking and informal education or advice.

In August 2021, the 51st Council of IUPAC approved the formation of a Standing Committee on Ethics, Diversity, Equity and Inclusion (CEDEI). Plans for this newly established Standing Committee include providing guidelines for diversity and inclusiveness at IUPAC conferences, for editorial board memberships, task group memberships, and on selection panels (e.g. IUPAC awards). The role of CEDEI is outlined in the committee's terms of reference (see below).

IUPAC has a global base of members who are guided by the set of core values and behaviours identified in its strategic plan. Where an incident or behaviour inconsistent with these values is alleged, initial investigation should occur at the same level and with the people implicated involved, and only those incidents/behaviours unable to be resolved should be forarded, and in complete confidence, to CEDEI.

The current terms of reference for CEDEI are:

1. To provide independent advice to the President, Executive Committee, Executive Director, other Standing Committees, Divisions, and Commissions on matters relating to ethics, diversity, equity, and inclusion within the policies, business, and

activities of the Union, or when undertaken by volunteers on behalf of the Union.

2. To make recommendations to the President and the Executive Committee, where appropriate, on matters relating to ethics, diversity, equity, and inclusion within the policies, business, and activities of the Union, or when undertaken by volunteers when engaged in business or activity on behalf of the Union.
3. To develop in-house policies on ethics, diversity, equity, and inclusiveness that are in accord with the IUPAC strategic plan, which are widely publicized on the IUPAC website(s), and which act as a reference point for the behaviour of IUPAC members, volunteers, and staff when engaged in activities or business on behalf of the Union.
4. To provide confidential advice or act as a confidential point of contact for IUPAC members, staff, and volunteers when engaged in business or activity on behalf of the Union, where an incident inconsistent with the Mission and Core Values of IUPAC may have occurred.
5. To establish, subject to approval by the President and Executive Committee, Advisory Boards, Subcommittees, and Working Groups as needed to carry out specific functions of the committee.

Mary Garson (Australia) is the inaugural Chair of CEDEI; additional members include Supawan Tantayanon (Thailand) Secretary, Mark Cesa (USA), Peter Mahaffy (Canada), and Marvadeen Singh-Wilmot (Jamaica).

<https://iupac.org/body/060>

Young chemists voice in support of the SDGs

by Janine Richter and Emiel Dobbelaar

In 2015, the United Nations General Assembly agreed upon 17 Sustainable Development Goals (SDGs) that are to be achieved by the year 2030. These goals were adopted to ensure an economical, socially just and ecologically sustainable development on a global scale and to protect natural resources and the environment [1].

A leading role in the achievement of the SDGs falls to the chemical sector as developments in the chemical industry as a primary industry may shape the whole supply chain [2,3]. The implementation of sustainable chemistry not only affects chemical production, but also has an impact on industrial and consumer products, including (positive) effects on health and working conditions as well as economic growth [3-5].

A fundamental approach for the chemical sector to become active is couched in SDG 12 "Ensure sustainable consumption and production patterns" [6]. By implementing this SDG, the chemical sector moves to the center of various demanding challenges of our time, from plastic waste to solar energy conversion to air pollution, and can promote a development towards more sustainable solutions [7].

In this important discussion, the voice of the young generation (ages up to 35), representing over 56 % of humanity (4.4 billion individuals in 2020) [8], must not be ignored. As today's decisions will tremendously affect their future, a huge desire for meaningful contribution can be deduced from the increasing global environmental and climate activism. Young chemists especially possess the willingness as well as the chemical knowledge to improve processes in the whole chemical sector by the implementation of sustainable chemistry principles and are looking for ways to be part of the transformation. Their opinions and expectations are key for the sustainable development of industry and society alike.

In order to make young chemists' voices heard, we recently analyzed an overview over their opinions and expectations on the role and responsibility of the chemical sector for a sustainable societal and industrial transformation [9]. While the collected statements are summarized and presented in our previous publication, we now aim to put them into a broader context by comparing young chemists' views to other works and expert opinions on the topic in order to examine their expectations according to their feasibility with respect to the current circumstances.

Role and Responsibilities of the chemical sector

Regarding the role of the chemical sector, young chemists have clear demands for future development, calling for more responsible, indicatory and cooperative actions. First of all, the chemical industry is expected to pledge itself to the SDGs and sustainability in general. Thereby, young people see its role as a forerunner and demand the chemical sector to recognize this. The development towards a pollution-free, high-tech industry, serving as a role model for other (industrial) sectors, must be pursued. The chemical sector should avoid linear business models, be wary of product lifecycles, and recognize its responsibility towards building a circular economy. In order to reduce carbon emissions as well as the dependence on limited resources, the chemical sector must cooperate closely with other sectors and invest in renewable, green, and sustainable technologies. In these processes, transparency is significant to gain the trust of the civil society and especially the young generation, who represent the future work force [9].

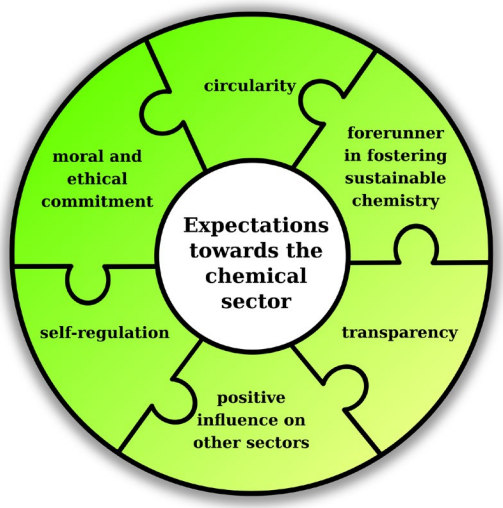
The overall sentiment of the statements is in line with Cole-Hamilton's recent opinion piece in *Science Voices*, who sees chemistry and chemical engineering processes at the forefront of the transformation, encourages repair and reuse, demands better recyclability and highlights the importance of ethics in education as well as governmental incentives [2]. Moreover, complementing the idea of a moral and ethical science as well as the thought of cooperation for the benefit of society, Matlin *et al*. have introduced the concept of "one-world chemistry" [10]. Close partnerships of industry to academia and the public (media) are pointed out to enhance the flow of ideas and benefit all, supporting young chemists' propositions to increase multi-lateral cooperation. When considering the actual transformation of the sector, Anastas' vision of the chemical sector taking the step from conventional reductionist methods to systems thinking appears to be compatible with their views [11]. Although the simplification of complex chemical matters brought numerous benefits since the beginning of the industrial era, it also led to many unintended, negative consequences, affecting both people and ecosystems. Thus, chemists can only address today's sustainability challenges (and young chemists expectations) by considering the whole

complexity of our world, being attentive to full product life-cycles and investing in sustainable strategies rather than in old technologies that cannot meet todays' requirements.

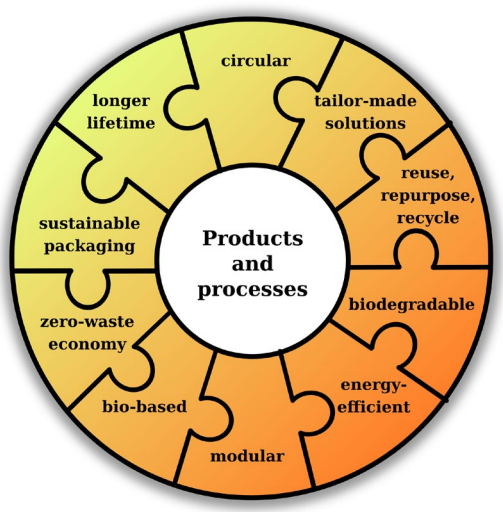
Products and Processes

Two main developments in industrial products and processes are considered crucial by young chemists: First, the product composition regarding the consumption of limited resources and the accrual of waste need to be optimized for a zero-waste approach. Second, a shift towards a circular economy and advanced recycling processes should occur. On the one hand, a modular product design with less composite or layered materials is proposed to facilitate the exchange and repair of individual components and separation processes for recycling. On the other hand, products of the future, according to young chemists, need to be produced from bio-based, and, therefore, renewable resources. In addition, special attention should be directed towards the application of safer, less toxic, and less pollutant chemicals and energy-efficient, carbon-neutral production. The chemical industry is also demanded to drive the development of power storage facilities, technologies for the use of sustainable energy sources and electronics with low energy consumption [9].

Many concepts named by young chemists have long been known, though their relevance has only increased. In a model circular, zero-waste economy, when the end of life of a product is reached, it should be recycled [12,13]. However, not all products can be recycled. For open-environmental applications such as cosmetics or pesticides, materials have to be developed that undergo degradation fast and completely [12]. In this case, careful attention should be directed towards the environmental impact and toxicity of the degradation products when released into the biosphere [14]. According to Kümmerer *et al*., products that cannot be degraded safely or recycled should be stored in an appropriate way to allow for future recycling through advanced processes. Thus, there seems to be a need to assess the properties of an end-of-life product during product design already, especially when it comes to reducing the complexity of material compositions for better recycling properties, as well as a need for the advancement of recycling processes, in line with the propositions of young chemists (*vide infra*) [12,15,16]. This need is exemplified by Matlin *et al*. and their analysis of the whole life cycle of aluminium, plastics, and textiles, representing three very different industrial fields [3]. In each field, improvements by chemists could have a significant impact on material circularity. To achieve betterment, Mohan and Katakojwala name ten specific drivers for circular chemistry, such as systems thinking (*vide supra*), renewable raw materials and the *Five R* (reduce, reuse, repurpose, recycle, and recover), that should be implemented by industry [17]. Another issue observed in the case study of Matlin *et al*. is the prevalent use of energy from fossil fuels which is also perceived by young chemists [3]. Beyond a transition towards the use of more renewable energy sources for chemical production (including concepts such as Power to X) [18,19],



Expectations towards the chemical sector. *A summary of key aspects in the answers of young chemists when asked about expectations towards the role and responsibility of the chemical sector. [reproduced from ref. 9]*



Products and processes. *A summary of key aspects in the answers of young chemists when asked about the kind of products and processes that are needed to shape a sustainable future. [reproduced from ref. 9]*

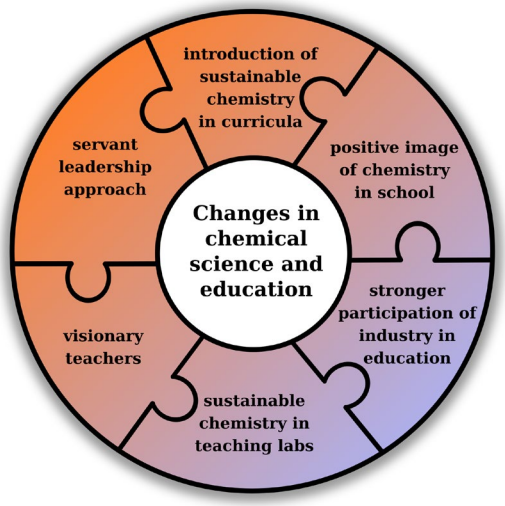
to achieve a sustainable and carbon neutral future, Cole-Hamilton points out that currently privileged parts of the global population have to reduce their consumption while the development of currently deprived parts of the population has to proceed without a huge consumption of fossil fuels. This also applies to general consumption behavior. Besides a rethinking at the consumers' side on repair versus replacement, more and better take-back schemes, reparability and recyclability should be crucial considerations in product design and should be supported by a governmental framework and a good infrastructure [2].

While young chemists demand a lot of the chemical sector itself, they also specifically demand the ban of single-use plastic packaging and the development of sustainable alternatives. This action can be (and is being) taken and incentivized by governments and policy-makers [20]. New bio-degradable materials from natural sources are named to replace conventional plastics. However, linear product use even of more sustainable alternatives can again represent a massive waste problem if not executed responsibly, as is evident *e.g.* by the ill-informed use of fertilizers and statements made by Kümmerer *et al*. regarding open-environmental applications (*vide supra*) [2,12]. Additionally, potentially more costly sustainable solutions may harm poorer populations disproportionately. Thus, careful considerations of consumer behavior are necessary when such supposedly more sustainable alternatives are proposed [21].

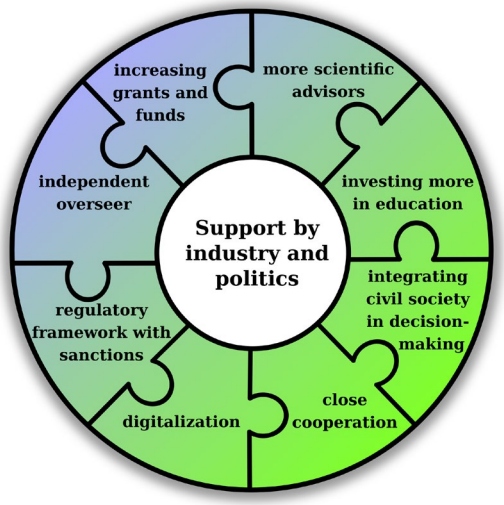
Science and Education

To face the challenges of developing sustainable products and processes, fundamental and applied research as well as a well-educated workforce with innovative ideas is required. Young chemists, currently, feel a lack of education in the field of sustainability and express a strong desire for the implementation of environmental and sustainable chemistry in chemical education. More practical classes and interdisciplinary teaching should thoroughly prepare them for future tasks. Young chemists also ask the chemical industry to participate in science education, *e.g*. by sponsored scholarships, training programs or the provision of well-equipped laboratories in developing countries. Moreover, young chemists highlight the need for chemistry education in schools to start much earlier. Modern teaching techniques, the use of modeling software or artificial reality, and everyday examples where chemistry improves our lives could increase children's interest in chemistry and its impact on individuals as well as on other disciplines [9].

Already 10 years ago, Wiek *et al*. presented an extensive review about the necessary key competencies individuals should have for promoting a sustainable development. Systems thinking, strategic, normative, anticipatory and interpersonal competences were identified as crucial, however, not sufficiently imparted in adult education [22]. When reflecting on young chemists' statements, this has not changed to date and adult education still seems to be devoid of teaching these proposed sustainability competencies. This is also



Changes in chemical science and education. *A summary of key aspects in the answers of young chemists when asked what needs to change in chemical science and education. [reproduced from ref. 9]*



Support by industry and politics. *A summary of key aspects in the answers of young chemists when asked how politics and industry can support the realization of the expectations of the younger generation. [reproduced from ref. 9]*

evident by a recent piece by Garcia-Martinez, where it is stated that chemistry education (still) needs to be rethought and updated to the needs of the 21st century. This is, according to him, the most effective way to also adapt chemistry research and industry to these needs [23]. Thus, the urges of young chemists echo a call for change that has been proposed for a long time but not properly addressed. To foster change, Zuin and Kümmerer propose that sustainability practices should be taught *e.g.* by case examples in existing lectures and lab courses rather than adding more subjects to the already crowded university curricula [24]. Here, young chemists also seem to be very much in line with their proposition that green and sustainable chemistry should "become the norm rather than the novelty" [9].

Beyond this, Zuin *et al.* point out the importance of green and sustainable chemistry education not only for schools and universities, but also as a lifelong education and learning process for professionals [4]. This includes regular exchange and a cooperative discourse among stakeholders from all dsciplines. Thereby, considering only the field of chemistry will not be sufficient, but the concept of sustainability (and sustainable chemical practices) has to be implemented into other curricula, such as economics and social science, as well. Regarding interdisciplinarity, Cole-Hamilton considers especially the topic ethics underrepresented in scientific education. He regards a course like "Good chemistry—methodological, ethical, and social dimensions" [25], designed by the European Chemical Society (EuChemS), as an essential precondition for any scientist [2].

Support by Politics

To ensure a sustainable and wealthy future, politics must give science a higher priority, according to young chemists. This involves more financial funding for research and education, especially in sustainable science, as well as more scientific advisors on a worldwide scale. Politics also should not miss the chance to make people part of the solution. Furthermore, it has a heavy responsibility to guide the industry's development towards more sustainability and its rising demands of (sustainable) energy. This requires a regulatory framework with strict sanctions for non-sustainable actions by companies. Likewise, companies conducting a sustainable transformation could benefit from incentives such as tax reductions or rewards that give sustainable products competitive advantages. Thus, policy guidelines and regulations could give a framework for close cooperation between the industry and environmental authorities as well as the civil society. This should go along with strict self-supervision by the chemical industry as well as independent observers to avoid 'green-washing' [9].

Beyond our work on expectations of young chemists towards the chemical sector, representatives of the European Young Chemists' Network (EYCN) have also highlighted the importance of early-career chemists contributing to policy making in a recent article [26]. The authors strongly suggest the further development of the "science for policy" approach, where scientific evidence is the main foundation for political decisions. This agrees with the results of our overview and complements the named article's call for (early-career) scientists to make their opinions and knowledge heard, namely among policy-makers.

An analysis of 37 national-level strategy documents published by Weiser *et al.* in 2020 revealed that there is indeed a lot of room for this, as concrete measures to foster sustainability are regularly missing. Therefore, they phrase recommendations for future resource strategies. However, it is emphasized that such strategy papers by themselves can merely have small effects if not closely linked with regional, national and international action [24]. For future development, Weiser *et al.* already demanded more flexibility and anticipatory action from politics and industry alike in 2017 [15]. Since rarely all risks and hazards of new processes can be foreknown, it is even more important to constantly evaluate products and processes and be prepared to adapt them as necessary and chemists play a significant role in this.

Conclusion

The comparison of young chemists' expectations towards the chemical sector with recent literature and experts' opinions on the topic shows that young chemists have a differentiated and realistic image of what should and could be done. Their demands are in good agreement with measures considered necessary by experts to promote a transformation towards sustainability. The similar claims of both relevant groups mutually complement each other and demand proper attention and action. Chemical industry and politics alike appear to be reacting too slowly to recent developments and impede themselves in necessary transformations. To meet current and future challenges, the different stakeholders (chemical industry, politics, academia, organizations, civil society) should work together; transparency and trust are needed. The challenging transformation of the chemical sector should be met with strict self-supervision, external stimuli and quality contemporary education.

Multi-lateral dialogues that include more scientists and a young generation that will be most impacted by today's decisions can be a chance for a strategic, sustainable development of the chemical sector for the benefit of society.

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Emiel Dobbelaar <e.dobbelaar@jcf.io> is on the Faculty of Chemistry at Technische Universität Kaiserslautern, Kaiserslautern, Germany. https://orcid.org/0000-0002-5650-9231. Janine Richter is on the Faculty of Chemistry and Food Chemistry at Technische Universität Dresden, Germany. https://orcid.org/0000-0002-0271-5873.

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Downstream

by Jesse Smith

In the 1940s, the Delaware River at Philadelphia was so dirty that pilots could smell it from the air. The water was so harsh it corroded metal and discolored paint. Fish killed by pollution washed up on the Delaware's banks. The lack of oxygen in parts of the river blocked the critical migration of others.

The Delaware River was strained along much of its length by the middle of the 1900s. States fought over its water in times of drought, and they struggled to contain its water in times of flood. Salt water from the tidal Delaware Bay threatened to infiltrate drinking water supplies. Exploding populations also contributed to the mess, with sewage output growing faster than sewage treatment. During World War II, shipyards, oil refineries, and manufacturers that supported the United State's military efforts further burdened the river.

By the mid-1900s the problems of the Delaware were too big for any one state to handle alone. So in 1961, the four states through which the river flows—New York, New Jersey, Pennsylvania, and Delaware—entered into a partnership with the federal government to oversee the water resources of the Delaware River basin. Named the Delaware River Basin Commission, the partnership established pollution standards. It established water quality monitoring procedures. It promoted the creation of small watershed alliances across the basin to stimulate community involvement in environmental concerns. And water quality across the basin improved. Today, the Delaware River Basin Commission continues to manage those resources, which stretch across 13,000 square miles and serve more than 13 million people.

This history is part of *Downstream*, a new temporary exhibition at the Science History Institute in Philadelphia. The exhibition explores more than 200 years of scientific analysis and political interventions into the waters that surround the organization's home. Drawing on the Institutes's deep collection of scientific instruments, books, and ephemera—as well as loans from partner organizations—*Downstream* invites visitors to explore the changing relationship between knowledge and action behind efforts to keep water clean from the late 1700s through the present. The exhibition also represents the Institute's ongoing efforts to use the public history of science to educate, entertain, and engage as broad an audience as possible.

IMG 1.

Exhibiting Water

Downstream is organized according to five historical episodes. The first begins in the late 1700s in the Institute's Old City Philadelphia neighborhood. The city was a wet and stinky mess at the time. Pits used as household toilets overflowed into basements and backyards. Businesses making candles, soap, and leather dumped foul waste into small streams that flowed toward the Delaware River. The city's bustling port reeked of rotting garbage at low tide. Stagnant water fouled the city's famous public squares. Horses, cows, dogs, and pigs filled the streets, making the messes that live animals do. Dead animals were often left to rot.

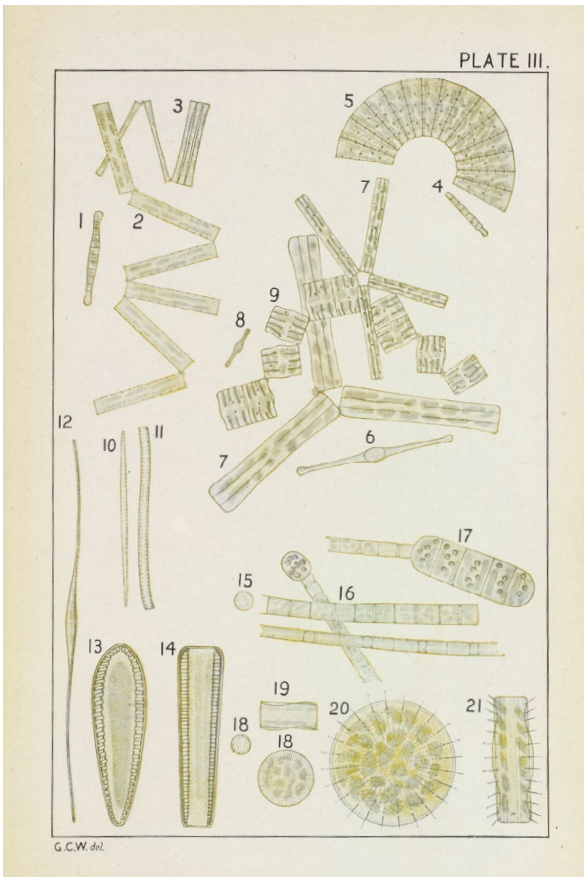
All this activity dirtied the natural springs and public wells that supplied water to residents and businesses of the growing city. And when yellow fever killed thousands in 1793, many blamed miasmas, or "bad airs" that emerged from rotting and decaying organic matter. Philadelphia identified the Schuylkill River, three miles to the west, as a safe and clean replacement for the foul water people pulled from polluted streams and wells around their homes and businesses. Though it was just three miles from the heart of Philadelphia, the Schuylkill was then surrounded by fields and forests, with few homes and little industry on its banks. In 1801, steam engines began pumping clean Schuylkill water east to the residents and businesses of Philadelphia.

The purity of the Schuylkill was short-lived. Across the 1800s, upstream manufacturers were putting more waste into the river. And the growing city was sending greater amounts of often deadly sewage into the Schuylkill. Between 1860 and 1890, waterborne typhoid fever killed 16,000 residents, or anywhere from three to 12 percent of the city's population in a given year. It made many more seriously ill. The bacteria that causes typhoid travels in sewage, and it sickens and kills when people consume food or water that's been touched by infected sewage.

But by the end of the century, the city (and much of the world) was armed with a better understanding of disease. The germ theory of disease gradually eclipsed earlier miasmatic ideas. Specific germs, and not broader environments, were the new enemy in the fight to keep people safe. Armed with this knowledge, Philadelphia adopted slow sand filtration to physically treat its water supply in the early 1900s; in 1914, it adopted chlorination and the chemical treatment of water. These interventions eliminated nearly all waterborne illness and disease in the city.

This story is told in *Downstream* with evocative objects from the Institute's collections, including a brass microscope, a copy of George Chandler Whipple's 1914 text *The Microscopy of Drinking Water*, and images from the 1915 book *Water Purification Plants and their Operation*. In addition, the Philadelphia Water Department loaned the Institute a sample of a wooden pipe from the 1800s. Part of an early underground infrastructure of water delivery, such technologies were also physically tapped to fight deadly fires in Philadelphia.

Around the same time that the city of Philadelphia was cleaning its water supply, the commonwealth of Pennsylvania was identifying water pollution as a statewide problem. One hundred miles upstream of Philadelphia, a booming mine industry poured coal dust and acidic byproducts into the river's headwaters. Sewage from growing towns and cities along the river flowed into the Schuylkill. Downstream, slaughterhouses and factories used the river as a cheap and easy way to dispose of their waste.



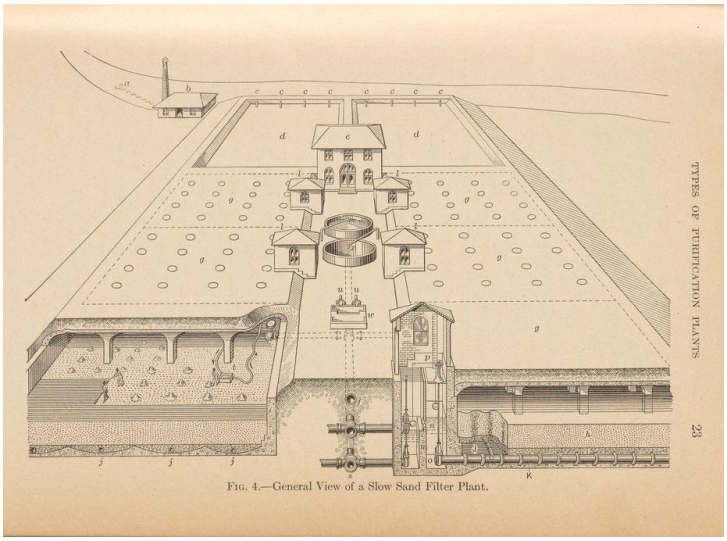
IMG 2.

Pollution from mines, factories, humans, and animals disrupted natural river processes, killed plants and animals, and posed threats to human health. Across Pennsylvania, similar patterns of urbanization, industrialization, deforestation, and mining damaged the state's rivers and streams. Scientists increasingly recognized that pollution in one place threatened the health and safety of another.

This is the second episode of *Downstream*. In this section of the exhibition, Institute objects including thermometers and and pH meters ground stories of scientists, doctors, and engineers working in new fields such as bacteriology, public health, and sanitary engineering in the early 1900s to learn more about water and the broader environment. They knew that sewage carried harmful organisms. But bustling factories and mines also added new toxic chemicals to water. Water researchers in Pennsylvania and other states found inorganic heavy metals such as lead and arsenic, as well as organic hazards such as phenol chemicals, in water. Oil from wells in western Pennsylvania leaked into streams. And mine acid runoff corroded metal and degraded concrete.

Downstream shares several critical interventions from this period. In 1905, the American Public Health Association and the American Water Works Association published *Standard Methods for the Examination of Water and Sewage*—a set of comprehensive and standardized water analysis techniques that are still updated today. And in Pennsylvania, with one water user unable to control what another did at a distance, the state took administrative and legislative action. In 1905, Pennsylvania became one of the nation's first states to pass a water protection law. The Purity of Waters Act gave the state's Commissioner of Health the power to regulate sewage. The Act, however, was limited to sewage pollution and didn't address the waste generated by the economically valuable coal industry. It took several more decades of pollution, science, and advocacy for Pennsylvania to address the problem of coal mine pollution. In the exhibition, a watercolor painting of a coal dredge (loaned to the Institute by Philadelphia's Independence Seaport Museum) depicts the massive cleanup of the Schuylkill

IMG 3.



IMG 4.

River between 1945 and 1955, which removed between 30 and 40 tons of coal waste from the river.

The exhibition then moves to the historical moment described above, when the water quality (and water quantity) challenges facing the Delaware River basin could not be solved by any single state alone. As the U.S. Senate wrote in 1961 of the proposed Delaware River Basin Commission, "there is one river, one basin, all water resources are functionally interrelated, and each use is dependent upon the other. Therefore, one comprehensive plan and one coordinating and integrating agency is essential for efficient development and operation." [1] This third episode of *Downstream* reveals the exhibition to proceed not only through time, but across increasing scales of action as well. As our knowledge of water (and of the environment more broadly) increased in this period, the scope of water oversight increased as well.

That knowledge included better understanding of the decreasing quality of water across the basin. Instruments in this section of the exhibition include a Jackson candle, nephelometer adapter for a pH meter, and a Secchi disk—all used to quantify the turbidity (or cloudiness) of water; a photoelectric colorimeter that could screen water for chlorine, fluoride, cyanide, iron, molybdenum, and zinc; and a portable oxygen analyzer that could determine the quantity of dissolved oxygen in a sample. It also includes a 1964, 16-foot-tall model of the Delaware River basin, donated to the Institute by the Delaware River Basin Commission. The Institute believes this model was used in the 1960s to identify the Commissions' activities to a broad public.

Just as the Commission was seeing improvements to water quality in the basin, a national environmental movement was emerging. Boosted by popular works and images such as Rachel Carson's *Silent Spring* and images of Ohio's Cuyahoga River on fire, public support for greater interventions into environmental challenges increased. Behind this movement was an increasingly sophisticated understanding of the environment. Methods for analyzing chemicals changed dramatically in the mid-1900s. These new techniques revealed many kinds of chemical pollution in waterways, including dangerous chemicals that could not be seen or smelled. Electronic instruments such as spectrophotometers and mass spectrometers measure physical characteristics of a sample to identify its composition. By combining new analytical instruments with older separation techniques such as chromatography, chemists could more rapidly and precisely determine the types and concentrations of chemicals in a complicated sample. An ion chromatographs on display, for example, could monitor drinking water for contaminants such as cyanide and arsenic. It could also detect charged molecules characteristic of fertilizer runoff or untreated sewage, such as nitrates and phosphates.

Intense public concern about pollution drove the federal government to act in the 1970s. President Richard Nixon created the Environmental Protection Agency in 1970. In 1972, the Clean Water Act set a sweeping national goal that all surface waters in the U.S. be "fishable and swimmable" by 1983. Every major discharger of wastewater had to obtain a permit from the EPA and reduce the contamination in their discharge. The Act also created the largest federal public works program in U.S. history. Cities and towns constructed sewage treatment plants using federal subsidies that covered up to 75% of the construction costs. And in

1974, the Safe Drinking Water Act directed the EPA to set health-based standards for contaminant levels in public water supplies. Local water utilities had to monitor for specific contaminants using EPA-approved technology.

Visitors to this fourth section of *Downstream* also learn how, in 1976, a citizen lawsuit forced the EPA to finally set allowable levels for 126 different chemicals being discharged into waterways by permit holders. Companies and water utilities would have to routinely measure many water samples to show they complied with EPA standards. The EPA also specified an analytical method, combined gas chromatography-mass spectrometry (GC-MS), and a recently developed instrument, the Finnegan Model 1015, that should be used to demonstrate that discharged water met EPA standards.

The exhibition concludes by examining the emerging concern of microplastics in water. Scientists aren't exactly sure what dangers microplastics pose to human, animal, and environmental health. But concern over microplastic beads in products such as toothpastes and face scrubs led the U.S. to ban microplastics from cosmetics in 2015. And scientists continue to use techniques such as Fourier transform infrared spectroscopy to study the types, amounts, and possible threats of microplastics that are increasingly found in waters around the world. This is work happening across all the scales of action explored in *Downstream*. The city of Philadelphia, the commonwealth of Pennsylvania, the Delaware River Basin Commission, and multiple federal agencies are all studying microplastics in water.

This is not a sweeping indictment of plastics. As the exhibition explains, In 2019, the World Health Organization cautioned that efforts to reduce plastics should not ignore the benefits of some plastics for health and safety. The WHO cited plastic packaging that extends the shelf life of food; of plastic medical equipment such as single-use gloves, syringes, and IV tubes; and of critical health devices made of plastic like

IMG 5.

IMG 6.

heart valves and prosthetics. The WHO also warned that concern over microplastics should not draw attention from the ongoing fight to provide clean water around the world. Today, drinking water contaminated with human and animal waste continues to sicken two billion annually. And it kills more than one million people every year.

Doing the Public History of Science

The development of *Downstream* included some longstanding challenges in the interpretation of the history of science for public audiences. Scientific instruments like an ion chromatograph, for example, can be unfamiliar and inscrutable for non-practitioners. The exhibition team also must consider how much is necessary for visitors to engage with the relationships between science and society more broadly. In *Downstream*, this was achieved through "How Did We Know?" exhibition content that introduces visitors to an analytical technique or knowledge practice; "How Does It Work?" content that explains that technique or practice; and "What Did We Do?" stories that reveal how knowledge informed political and social decisions about water.

At the same time, *Downstream* presented the Institute with novel opportunities for the public history of science. As an exhibition based in both the history of science and environmental history, the curatorial team was able to ground the stories of water analysis and protection in both time *and* place. Text and visual assets—including maps, posters, fine art, illustrations,

advertisements, and films from the 1950s and '60s—tell stories of the water around the Science History Institute and encourage visitors to think about the changing relationships between knowledge, action, and the specificity of place. Timelines in each of the exhibition's historical episodes, however, offer glimpses of contemporaneous efforts to know and protect water beyond the Delaware River basin. These include, for example, the first use of chlorination to chemically treat water in the United States in Jersey City, New Jersey, in 1908; the Massachusetts State Board of Health's discovery of the link between sewage and typhoid fever outbreaks; and the establishment of national water pollution laws in France, Japan, and India, among other countries.

Over the next year, the exhibition (which runs through January 2023) will be supplemented with digital lesson plans, supported by the Society for Analytical Chemists of Pittsburgh & Spectroscopy Society of Pittsburgh, and a digital exhibition, supported by Villanova University's Lepage Center for History in the Public Interest and Drexel University's Lenfest Center for Cultural Partnerships [2]. And the Institute's museum will continue to interpret the public history of science through upcoming exhibitions on the histories of synthetic colors and food science.

IMG 7.

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Jesse Smith <JSmith@sciencehistory.org> is Research Curator at the Science History Institute in Philadelphia.

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https://www.sciencehistory.org/downstream

The Role of Artificial Intelligence in Drug Discovery and Development

by Michael Liebman

Artificial Intelligence (AI) is an exciting, growing field. Due to the high and growing number of data, the comprehensive evaluation of information behind data makes AI tools indispensable. In Drug Discovery and Development the application of AI has become important to accelerate progress and enhance decision making in many fields and disciplines of medicinal chemistry, upscaling, molecular and cell biology, pharmacology, pharmacokinetics, formulation development and toxicology. In clinical testing AI has high importance in increasing success rates by enhancing trial design (biomarkers, efficacy parameters, dose selection, trial duration), selection of the target patient population, patient stratification and evaluation of patient samples. The increasing relevance of AI in drug discovery and development is reflected by the growing number of start-up companies specialized in this field, the growing number of collaborations from Pharma with AI platforms, and the high number of articles and reviews reporting current applications, their success and limitations.

In the first part of this article, Michael Liebman focuses on a general overview on AI in drug discovery and development; the second part provided by Yann Gasthon-Mathé and his colleagues from IKTOS (France)—an AI company specialized in drug discovery and development-related AI applications—highlights key points to succeed in AI drug discovery projects.

This feature is an integral part of the first D3SC Newsletter — See https://iupac.org/d3sc-newsletter-sep2021/>

1929: *Japanese biologist and professor Makoto Nishimura created Gakutensoku, the first robot to be built in Japan. Gakutensoku translates to "learning from the laws of nature," implying the robot's artificially intelligent mind could derive knowledge from people and nature. Some of its features included moving its head and hands as well as changing its facial expressions. (reproduced from [1])*

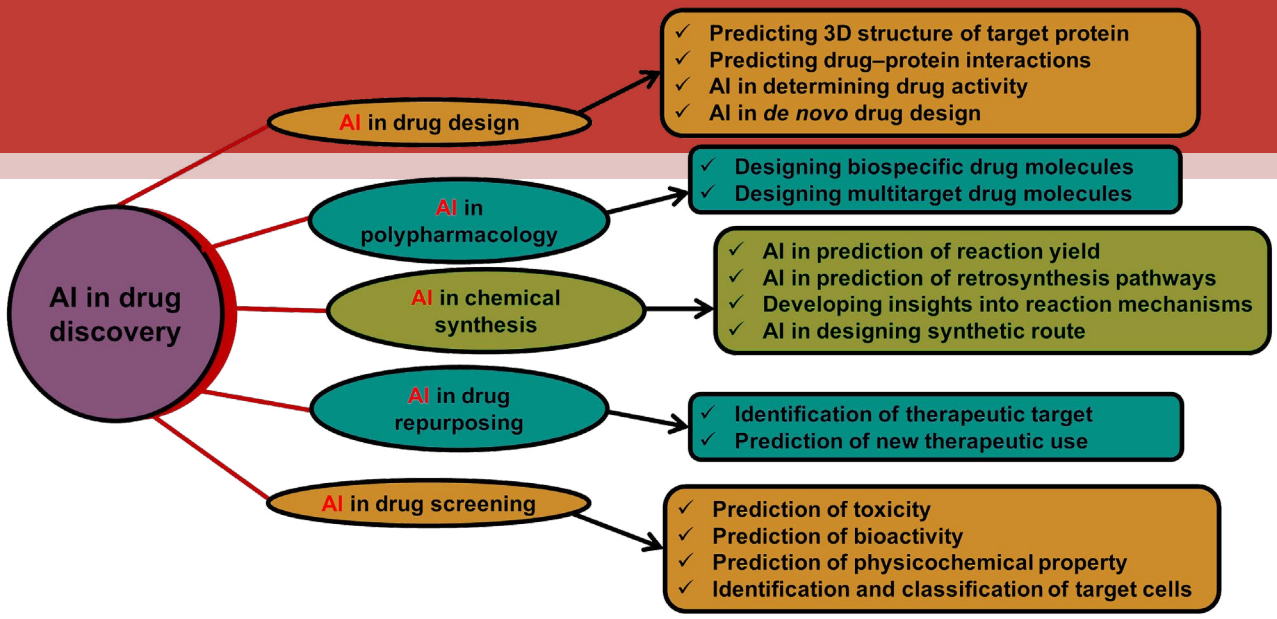
General Overview

Brief highlight of AI key advantages, current status of maturity and its impact on Drug Discovery & Development. A few review references, including a recent article on this very topic of AI in drug discovery and development brings us up to speed on the literature and are cited [1-4].

Two fields, artificial intelligence and drug discovery/development, have long histories that pre-date their current names and definitions. Although they have evolved separately and not necessarily linearly, their paths have more recently begun to converge as significant advances in computational and experimental/technological capabilities provide access to enormous amounts of data and computing power. This commentary provides an introduction to the state of this convergence and what critical gaps remain as challenges still to be addressed.

The term "artificial intelligence" (AI) was promulgated by John McCarthy in 1956, although the concepts stem from Greek mythology (Talus and Pygmalion), from Hebrew folklore (Golem) and later the alchemists, Paracelsus (Homunculus) and Roger Bacon. Although mathematical logic, critical to AI as we know it today, was developed in the 20th century by Russell and Whitehead and Hilbert, it originated with formal reasoning among the Chinese, Indian and, Greek philosophers. Today we recognize Babbage, Lovelace, Shannon, Turing and von Neumann, Minsky, McCarthy, Newell, and Simon in the recent family tree of AI.

We can also separate "drug development" into two main components: drug discovery/design/preclinical optimization and clinical drug development. The former's history extends to ancient times when natural products, *e.g.* herbals, minerals, animal substances, were used and continues to the highly refined



Role of artificial intelligence (AI) in drug discovery. AI can be used effectively in different parts of drug discovery, including drug design, chemical synthesis, drug screening, polypharmacology, and drug repurposing. (reproduced from [3])

experimental and computational approaches applied today. The latter largely reflects the introduction of regulatory processes and procedures that help to insure safety and efficacy and then leads to commercialization. Drug discovery initially involved trial and error and practitioners who could remember what worked and what did not. For many centuries it existed in conflict with religious views until being reborn in the Renaissance period, with pharmacology being born in the late 19th century. Drug design has evolved from the early experimental efforts to modify and improve natural products through medicinal chemistry to incorporate computational approaches in the 1970's. Clinical development may have started with Avicenna (1025), progressed to Lind's scurvy trial and Flint's first placebo trial in 1863, but it was not until 1943 that the first double blind controlled trial (Patulin for common cold) and until 1946 that the first randomized curative trial (Streptomycin for TB) were carried out. Today, regulatory agencies, epidemiologists and biostatisticians are involved in trial design for clinical development, and the marketing groups greatly impact the commercialization planning and effort.

AI in Drug Discovery/Design/Preclinical Optimization

Drug discovery/design/preclinical optimization focuses on 1) the identification of targetable processes or molecules that bear responsibility for a specific clinical condition, and sometimes in a specific patient population, and 2) the identification/design/preclinical optimization of an agent to modulate this modified physiology. AI methods are being applied to both these steps.

Target/Process identification typically stems from the collection and analysis of large data sets, *e.g.* population-based studies of clinical observations sometimes linked with genomic data. The application of ontologies and knowledge graphs to link disparate data provides an ongoing opportunity to continually update existing data sets and/or integrate new data sources into the analysis process which focuses on stratification of the disease and of the patient. Machine learning and deep learning methods are being applied as clinical observations are being enhanced with data from digital health applications, *e.g.* Fitbits, *etc*, that can provide almost continuous data feeds that require complex feature extraction. Diagnostic image processing, *e.g.* x-ray, MRI, pathology, *etc,* are being enhanced with AI methods to sharpen feature extraction and provide secondary confirmation of manual interpretations.

***1949**: Computer scientist Edmund Berkeley's book "Giant Brains: Or Machines That Think" noted that machines have increasingly been capable of handling large amounts of information with speed and skill. He went on to compare machines to a human brain if it were made of "hardware and wire instead of flesh and nerves," describing machine ability to that of the human mind, stating that "a machine, therefore, can think." (reproduced from [1])*

Natural language processing (NLP) is being used to "read and interpret" clinical notes. Knowledge graph methods are being used to integrate and represent the combined data/information and support potential analysis to suggest potential molecular or process/pathway targets.

Drug selection can involve *de novo* design, screening of the deck molecules for a Hit or modification of existing molecules, Hit to Lead optimization of pre clinical parameters such as PK/PD including both small molecules and peptides/proteins, *etc* as well as re-purposing of existing molecules for new indications and also potential combination therapies. As it focuses on both efficacy and safety, drug selection needs to consider potential drug-drug interactions, risk for adverse events and potential for differential response among diverse patient populations. The application of AI methods enables greater opportunity for computational screening of potential drug candidates as it can significantly increase the feature space used to define specific properties for inclusion or exclusion. Machine learning approaches have the potential to learn from existing data from existing compound libraries, including high throughput screening results, to help identify critical features in both categories and to enable ongoing, rapid computational screening of large compound databases using these features. Such analyses can also "infer" potential features for further molecular modification through medicinal chemistry approaches. Ongoing screening of existing libraries provides opportunities for re-purposing of compounds for new indications and/or development of combination therapies that can compensate for potential side-effects or establish multi-target treatments. It is notable that one of the first applications of AI methods in drug discovery focused on reverse engineering of existing patents and generation of novel synthesis pathways. Interestingly, one of the AI companies, Exscientia, announced the first AI-designed Immuno-Oncology drug to enter clinical trials (https://www.exscientia.ai/news-insights/exscientia-first-ai-designed-immuno-oncology-drug-trial).

AI in Drug Development

Drug development includes two major phases: the first, pre-clinical testing through clinical trials and the second, submission for regulatory approval. AI has been introduced more recently into the developmental phases, primarily to enable the aggregation, organization and analysis of "big data" with the goal of improving trial performance and regulatory approval.

Clinical trials involve the identification and evaluation of clinical test sites and personnel that meet specific criteria including: access to adequate trial participants, clinical competency, administrative and technical support that can meet performance requirements and identification of potential trial participants from clinical records. AI methods are being applied to screen potential sites for their history for meeting critical enrollment criteria and compliance, analyzing electronic health records to identify potential candidates who meet trial inclusion/exclusion criteria and integration of real world data that may support trial performance. More recently the addition of digital health monitoring into clinical trial protocols and the need for advanced data processing have also required the addition of machine learning technologies. AI is also providing dynamic indications of participant status as well as identifying early indications of potential adverse events.

Regulatory submission closely follows strict protocols and procedures that are evolving to include both the data digital monitoring systems and real world evidence. The use of real world data may additionally require integration of multiple data sources with ontologies or knowledge graphs as noted earlier in this commentary.

Challenges and opportunities

The complexities of drug design and development provide a natural target for the application of the methods and technologies of artificial intelligence to achieve greater success and at potentially lower cost and shorter time to market. To date, however, the results have been more incremental than disruptive but hold much promise for the future. The technology alone, however, does not directly address some critical challenges which, in turn, present potential opportunities that could enhance clinical and commercial success.

Target selection: How well is the disease/condition diagnosed and stratified, *i.e.* is the phenotype adequately defined? How comprehensive is patient stratification, *i.e.* clinical history, co-morbidities, lifestyle, environment, genomics, *etc.?* Is the target generalizable across the real world patient population, *i.e.* observed diversity?

Drug design/selection: Can we "decode" deep learning to interpret results? All patients reflect co-morbidities and poly-pharmacy, how are these being addressed? How well are pathway modulators being modeled as to individual targets and response?

Clinical trials: How do inclusion/exclusion criteria approximate real world patients? How does this impact commercialization post-approval? Could disease and/or population stratification lead to shorter, more directed clinical trials?

Conclusions

Drug design and development will continue to be an early adopter of new and evolving technologies, both experimental and computational. Among the challenges is whether to apply these technologies to enhance the existing pipeline and processes or is the real opportunity to re-engineer the processes in light of these technologies? Big data, digital healthcare, remote monitoring, and genomics will drive the need to explore how computational and reasoning approaches can be applied to enhance the process both in terms of clinical significance and cost reduction. Artificial intelligence methods hold great promise towards these goals but their success will depend on aligning the right question with the right technology.

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Key points to succeed in Artificial Intelligence drug discovery projects

by Quentin Perron, Vinicius Barros Ribeiro da Silva, Brian Atwood, and Yann Gaston-Mathé

Drug discovery and development is an expensive, complex, and time-consuming task [5]. Recently, the development of artificial intelligence (AI) approaches to drug discovery, specifically *de novo* drug design through the use of deep generative models, has triggered a lot of interest in the drug hunter community, especially as an important tool to speed up the process [6].

Since 2017, we at Iktos have worked in collaboration with industry and academia in many different projects, from hit discovery to lead optimization, using AI with ligand and structure-based techniques. In a recently published preprint work, we described the results of a successful collaboration between Iktos and Servier in a late-stage lead optimization project [7]. At this occasion we described, for the first time, the successful application of deep learning to *de novo* design for solving a Multi-Parameter Optimization (MPO) issue in an actual drug discovery project. Using the initial dataset of the project, with 881 molecules measured on 11 biological assays, we built 11 QSAR models and used them in combination with our deep learning-based AI *de novo* design algorithm. We were able to automatically generate 150 virtual compounds predicted as active on all 11 objectives. 20 molecules were selected as the most promising, and 11 were synthetized and tested. Interestingly, the 11 AI-designed compounds that were synthesized and tested displayed functional groups that were either rare in the initial dataset or never tried earlier in the project. Ultimately, one of the 11 AI-designed molecules met all the objectives of the project at the same time, suggesting that this method can propose innovative new molecules to solve MPO

1980: *WABOT-2 was built at Waseda University. This inception of the WABOT allowed the humanoid to communicate with people as well as read musical scores and play music on an electronic organ. (Reproduced from [1])*

problems, via its ability to identify favorable modifications, even with few data points to learn from [7].

With our experience in this and around 40 other projects completed or in progress here at Iktos, we have been able to identify some key points for a successful application of AI in drug discovery projects. Here they are:

1) One key thing to have in mind, AI needs data to feed upon, and the higher the quality of the input data, the higher the probability of obtaining good results. Since the beginning of the QSAR era with Hansch and Fujita [8], we know that the quality of the input data is one of the major requirements for obtaining good results, and with AI it is no different. Be sure you are collecting and storing the highest quality data you can. Good data produces trustable models. We are often asked: how many data points do you need to apply your AI technology to a given project. There is no definitive answer to that question (it varies from case to case, depending on the diversity or consistency and the level of "contrast" in the initial data set), but one thing is certain, the more, and the higher the quality, the better. Sometimes we are asked whether AI can help for undruggable targets with no known 3D structure, binding site or ligands. Clearly, this is a hard case for AI, as for anybody else! Conversely, AI can definitely help getting the best out of existing data and accelerate the optimization process.

2) Know when to trust your models, and when not to trust your models. Sometimes even with good data, models are not able to correctly predict the activity of molecules. Models built to predict the pIC50 of pyrrole molecules in a given target may not be the best to correctly predict the pIC50 of pyrimidine molecules in the same target. In other words, understand your applicability domain (AD) [9], an important tool for careful use of QSAR models. The AD for a chemical space is a theoretical region comprising both the model descriptors and modeled response which allows estimating the uncertainty in the prediction of a particular compound based on how similar it is to the training compounds used to build the model [9].

3) Synthetic accessibility is key to testing hypotheses. Even good models, built on quality data, respecting the AD, can make mistakes. Ultimately, they are just models. Thus, while selecting the molecules after an AI-generation, it is important to focus on the molecules with the easiest synthetic routes. In the end, the more molecules you are able to synthesize and test, the higher the probability you will identify active compounds.

4) User experience is key to allowing chemists the opportunity to take advantage of promising new technologies. Techniques such as docking, external (commercial) models, retrosynthesis software *(i.e.* our retrosynthesis technology https://spaya.ai), are frequently used to (re)score the molecules. An intuitive user experience is critical to making sure these techniques are used. Combined with a complex IT infrastructure to run everything efficiently and effectively, the barrier to using new technologies should be lowered as much as possible to ensure adoption.

5) Collaborate! Designing new drugs is a complex task and requires different capabilities like medicinal chemistry, machine learning, computational chemistry and more recently AI. Being able to make all those expertises collaborate efficiently and smoothly is challenging. Having access to a collaborative platform is key for success. Indeed, chemists are the best person to set up a generative AI because of their knowledge of the project and SAR (Structure Activity Relationship) and computational chemists are the best to build models. At Iktos we have built Makya (makya.ai) a platform which allows chemists and computational chemists to make the most of AI by generating easy to make molecules focusing on the team's expectations in a very simple and efficient manner.

6) Novelty comes with risk! It is important to balance the desire for new and novel ideas while understanding the limitations of the AD. In the previous example, where models constructed using pyrrole molecules may not correctly predict the activity of pyrimidine molecules, this balance is key. You might be interested in ring systems other than the pyrrole, but you'll need to acknowledge that the models have less predictive power outside of the AD.

7) Iterate! Success in getting the perfect molecule may not come at once, despite AI. It is often needed to run several AI-enabled Design Make Test (DMT) cycles before converging to optimized molecules meeting the project's success criteria. This comes as a consequence of the points raised above: the models are usually not perfect, especially if you are interested in generating novelty, but hopefully they will get better as you enrich them with new data points generated through an AI-guided process. What we have seen in our most recent successful experiences is that AI often enables substantial acceleration in improving the overall Multi-Parametric Optimization (MPO) profile of the molecules, over several DMT cycles, compared to standard human-driven approaches. But this requires trusting the technology over several iterations, rather than expecting a perfect solution at the first shot.

8) There is no magic in AI. Sometimes there is no solution in the project's chemical space. Instead of identifying the solution, in some cases with our AI technology, we were able to help our clients conclude that, according to our models, no molecule will meet all the expected criteria at the same time. This insight has enabled them to make the decision to stop the project (or revert to a more early stage back-up series) and focus resources elsewhere.

We are witnessing the beginning of AI being applied to drug discovery. The technologies being developed have a high potential, but they require significant effort to generate value in real-life settings. Have these key points in mind while collaborating on a drug discovery AI project will help you to avoid pitfalls and increase your rate of success.

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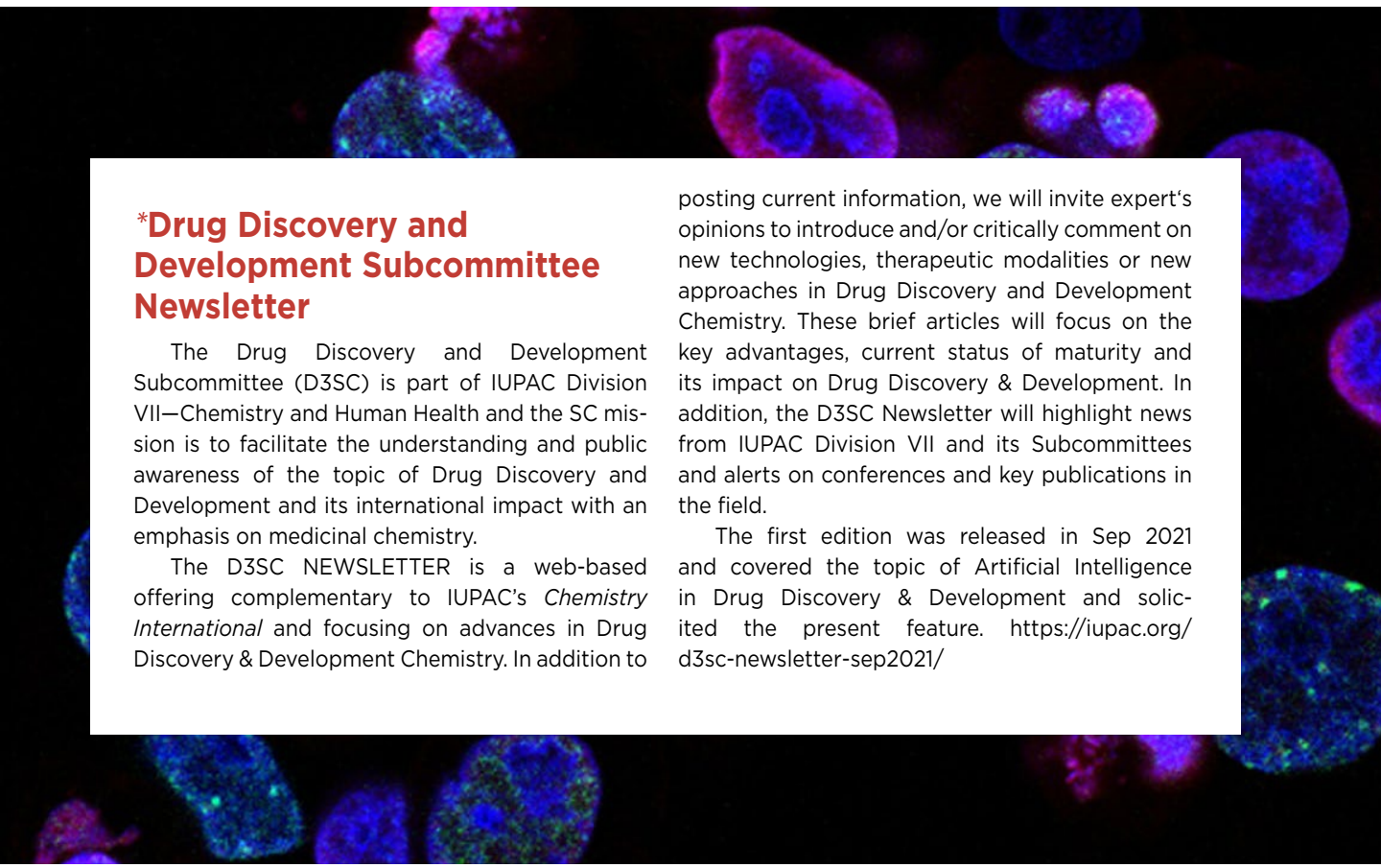
<yann.gaston.mathe@iktos.com>; Iktos, https://iktos.ai/



*Drug Discovery and Development Subcommittee Newsletter

The Drug Discovery and Development Subcommittee (D3SC) is part of IUPAC Division VII—Chemistry and Human Health and the SC mission is to facilitate the understanding and public awareness of the topic of Drug Discovery and Development and its international impact with an emphasis on medicinal chemistry.

The D3SC NEWSLETTER is a web-based offering complementary to IUPAC's *Chemistry International* and focusing on advances in Drug Discovery & Development Chemistry. In addition to posting current information, we will invite expert's opinions to introduce and/or critically comment on new technologies, therapeutic modalities or new approaches in Drug Discovery and Development Chemistry. These brief articles will focus on the key advantages, current status of maturity and its impact on Drug Discovery & Development. In addition, the D3SC Newsletter will highlight news from IUPAC Division VII and its Subcommittees and alerts on conferences and key publications in the field.

The first edition was released in Sep 2021 and covered the topic of Artificial Intelligence in Drug Discovery & Development and solicited the present feature. https://iupac.org/d3sc-newsletter-sep2021/

Tiny nanopesticides promise big gains to farmers

by Sophie Schmidt

New research has helped bring nanopesticides—tiny capsules capable of big impact—one step closer to regulatory approval.

Farmers are some of the biggest innovators in our country—whether it's embracing new technologies, adapting to a changing and variable climate, feeding a growing population with less arable land than ever before, or combatting evasive agripests.

It's no surprise that novel nanopesticides, tiny capsules that deliver chemicals targeted to the leaves or the roots of plants, have piqued the interest of the agricultural community in the past five years or so.

Nanopesticides not only promise to help farmers combat diseases and pests more effectively, but also reduce the environmental footprint of agriculture, which are both crucial aspects of sustainable agriculture.

Nanopesticides could help reduce the environmental footprint of agriculture by offering the same or improved plant protection from a lower rate of chemical application.

Nanopesticides: more with less

The beauty of their unfathomably small size (a hundred nanometres—or about a hundredth of the size of a single sheet of paper) is that nanopesticides have a disproportionately high surface area-to-volume ratio, making them highly efficient at delivering only a tiny volume of pesticide to plants in a targeted manner.

They're also capable of controlled release, with the active ingredient released slowly or in some cases, when most needed. Their nanocage or capsule (so-called nanocarrier) structure helps protect the precious chemical, making it more effective for a longer time. The net effect? The same or improved plant protection from a lower rate of application.

The potential of nanopesticides to improve the environmental footprint of farming is huge —both reducing the amount of toxins put in the environment, and bolstering yields by minimising losses.

So what has stopped nanopesticides from storming the market? A lack of a clear and reliable regulatory framework—that helps clearly identify the consequences to both human and environmental health—has, up until now, limited the approval of these products by regulatory agencies.

Tiny particles, big dreams

For CSIRO researcher Dr Rai Kookana, 30 years of research into contaminants and pesticides has just culminated in a very satisfying result—as a co-author of a new paper in Nature Nanotechnology that provides guiding principles for the regulatory evaluation of nanopesticides.

The paper was developed under a project funded by the International Union of Pure and Applied Chemistry (IUPAC) and led jointly by Kookana and Dr Linda Johnston (National Research Council, Canada).

Drawing from their international contacts around the world, the project team worked in close collaboration with industry and government (regulatory agencies) to develop a comprehensive framework for assessing potential human health impacts of nanopesticides.

This approach will help overcome potential barriers for regulators and industry globally, taking into account, for example, differing international regulatory requirements as well as community concerns about nanopesticides.

The project team, including Rai Kookana, Wendy Bruce, Shareen Doak, Linda Johnston, Melanie Kah, Vladimir Gubala, student observer, Hemda Garelick, Jordan Dinglasan, Reinhilde Schoonjans, Andrea Haase. Photo taken during Workshop on Nanopesticides Project in London (2019).

Many researchers, if prompted, can point to a pivotal moment in their childhood that piqued their research interest. Growing up on a farm in India during the 1970s was Kookana's moment.

Kookana witnessed first-hand the impact that earlier pesticides like Aldrin and Dieldrin had on the environment and public health. These were used on crops like corn and cotton and experienced a production boom after World War II.

These chemical compounds were eventually outlawed under the Stockholm Convention on Persistent Organic Pollutants (POPs) due to their toxic properties, resistance to degradation and ability to bioaccumulate in the environment. But this treaty was only finalised in 2001.

POPs, as well some other toxic conventional pesticides were proven or suspected in some cases to have devastating impacts on biodiversity, including decimating global populations of honeybees, birds, and other wildlife, and causing chronic health conditions in humans. Their legacy continues to be unearthed to this day.

Enter nanopesticides

In Australia and many other countries, improved regulation and monitoring of new pesticide products

has minimised some of the more acute risks (such as those posed by POPs), and has generally led to improved environmental and health management. However, farmers have continued to battle problems with modern pesticides, such as chemical resistance, leaching into the environment and safety to human health.

Dr Melanie Kah at the University of Auckland is the lead author of this paper, as well a long-term collaborator of Kookana and former distinguished Visiting Scientist at CSIRO.

"In the past two decades, the research community started looking to chemical alternatives including nanopesticides, which offer a safer and more promising future in their ability to target weeds, worms, mites, ticks, bacteria, and fungi," says Kah.

Dr Linda Johnston at International Union of Pure and Applied Chemistry (IUPAC), a co-author of the paper, is an expert in quantifying the nature and characteristics of nanoparticles in relation to their potential impact on human health.

"Nanopesticides, like other alternatives, are subject to rigorous safety testing to prevent unintended consequences," says Johnston.

In Australia, the Australian Pesticides and Veterinary Medicines Authority (APVMA) has been at the forefront of this initiative. It's important to note that some types of nanopesticide products are rapidly coming onto the market and have started gaining traction with farmers.

"One of the big drawcards of nanopesticides is the protection they offer to plants as well as to the non-target organisms in the environment. This is primarily because of their greater effectiveness and lower toxicity," explains Kookana.

"They are also known for their improved uptake by plant and reduced wash-off during a rain event."

"At the same time, some of their unique properties mean that they may pose a different set of risks to humans and the environment, and as such, demand their own safety chemical safety frameworks," adds Kah.

Risk and rewards

While nanopesticides sound highly promising, they also carry risk, as they are considered potentially toxic. Image: Ella Maru Studio.

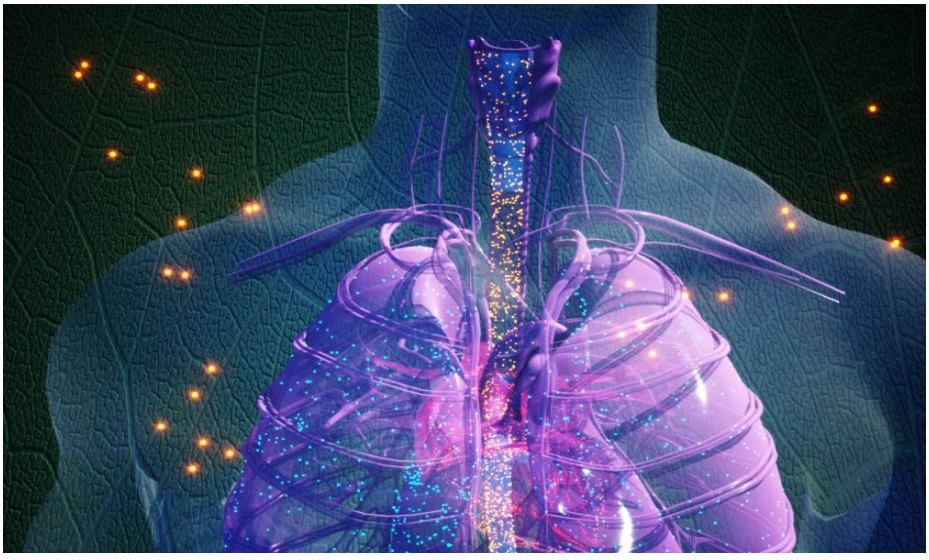
While nanopesticides sound highly promising, they also carry risk, for example, potential exposure to dangerous chemicals that are able to be absorbed into organ tissue and bloodstreams, or across placental barriers.

And while they have many environmental benefits, like targeted delivery, and reducing environmental degradation, their nanomaterial structure is considered to be "potentially toxic", according to Johnston.

It's further complicated by the slow-release system of some types of nanopesticides, a result of their nanocarrier mechanism. Nanocarriers involve coating the useful pesticide ingredient within a protective shell coating.

This shell allows for the biologically active pesticide chemical to be released into the environment under specific conditions (such as light, temperature, or pH), improving its efficacy against the pest and disease as well as protecting from degradation and leaching.

A framework for ecological risk assessment for nanopesticides has already been published, but some



While nanopesticides sound highly promising, they also carry risk, as they are considered potentially toxic. Image: Ella Maru Studio.

The project team, including (from left) Rai Kookana, Wendy Bruce, Shareen Doak, Linda Johnston, Melanie Kah, Vladimir Gubala, student observer, Hemda Garelick, Jordan Dinglasan, Reinhilde Schoonjans, Andrea Haase. Photo taken during Workshop on Nanopesticides Project in London (2019).

key knowledge gaps remained around what impacts they might exert on humans. That's where this new framework comes in.

"One of the key takeaways in the framework is that not all nanopesticides are created equal," says Kah.

"While some products may have exceptional properties, others may not, or may not (or may not retain them for a long time). The range of products that we have to deal with in developing this framework was eye-opening."

What the framework promises

The new framework study, led by the University of Auckland, focusses on human health risk assessments for nanopesticides, as well as nanofertilisers.

Kookana emphasises that that the framework doesn't attempt to provide an exhaustive list of the effect of nanopesticides on humans, or frame nanopesticides as the 'silver bullet' of agrichemicals.

The hope is it will be used as a starting point for understanding and addressing the concerns about nanopesticides.

The paper provides a decision tree and pathway to risk assessment, keeping in mind the different stages of human exposure—at mixing and loading, application and post-application, with each stage involving different dilutions and forms of the pesticide, or exposure opportunities.

The framework also helps industry to understand what questions the risk assessor has in mind and what data and information need to be provided to satisfy the regulatory requirements.

"Our study is an important step towards an approach for nanopesticides that can be accepted by regulatory agencies when assessing their toxicological impacts," says Kookana.

"It highlights the potential for nanotechnology and also points out the collective challenges that the scientific community, industry and government agencies face."

With this sound science now publicly available, Kookana believes that regulators and industry will be able to take the next step forward in realising the full potential of this innovation.

More information

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Sophie Schmidt <Sophie.Schmidt@csiro.au> is a communications advisor at the Land and Water business unit of CSIRO based in Hobart, Australia.

https://iupac.org/project/2017-035-2-600

Asymmetric Organocatalysis—A Game Changer

This year's Nobel Prize in Chemistry was awarded to Benjamin List and David MacMillan "for the development of asymmetric organocatalysis." IUPAC congratulates the laureates for their achievements.

Benjamin List is co-author of the readily available special topic paper "Organocatalysis Emerging as a Technology" published in the IUPAC journal *Pure and Applied Chemistry* <https://doi.org/10.1515/pac-2021-0501> (AOP 13 July 2021). This paper is part of a collection reviewing emerging technologies within the IUPAC Top 10 project which showcases the transformative value of Chemistry, informing the general public of the potential of the chemical sciences to foster the well-being of Society and the sustainability of our Planet. Organocatalysis was one technology highlighted in 2019 (See *Chem Int* Apr 2019; https://doi.org/10.1515/ci-2019-0203).

David MacMillan received the Thieme-IUPAC Prize in 2006, a Prize awarded since 1992 to scientists under 40 whose independent research deals with synthesis in the broadest context of organic chemistry. This includes organometallic chemistry, medicinal and biological chemistry, designed molecules, or materials, which have had a major impact in synthetic organic chemistry. It is awarded every two years and usually presented at the IUPAC International Conference of Organic Synthesis ICOS.

Chemists have always been inspired by nature. A few years back, researchers dreamt of a new kind of catalysts that, like most natural enzymes, would not require the use of expensive metals. "Organocatalysis" was born in the late 1990s and has not stopped growing. According to Paolo Melchiorre, one of the leading experts in the field, organocatalysis was successful because "[It] was quite democratic, everyone could have access to it without needing expensive reagents or a glovebox, which allowed many young researchers to start their independent careers, and quickly assembled a community of international experts that become a great incubator of ideas for catalysis without metals."

Following the announcement by the Royal Swedish Academy of Science, Peter Somfai, member of the Nobel Committee, has claimed that this year's award "is a game changer. Like a new chess piece that is very, very powerful."

https://iupac.org/asymmetric-organocatalysis-a-game-changer/

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Professors Balzani and Oganessian to Receive the First UNESCO-Russia Mendeleev International Prize in the Basic Sciences

Professor Vincenzo Balzani (Italy) and Professor Yuri Oganessian (Russian Federation) will be awarded the first UNESCO-Russia Mendeleev International Prize in the Basic Sciences. The decision was made on the recommendation of an eminent international jury chaired by Professor Jean-Pierre Sauvage, winner of the 2016 Nobel Prize in Chemistry.

Vincenzo Balzani, Emeritus Professor of Chemistry, University of Bologna, is recognized for the lasting impact of his outstanding scientific achievements in basic chemical sciences and his career-long efforts to promote international cooperation, science education and sustainable development. Professor Balzani pioneered inorganic photochemistry and supramolecular photochemistry. He has also made great contributions to science education and to reflection on science as a driver to achieve the Sustainable Development Goals, and on the relationship between science and society, science and peace.

Yuri Oganessian, Professor and Scientific Director at the Flerov Laboratory of Nuclear Reactions, Joint Institute for Nuclear Research, in Dubna, is recognized for his breakthrough discoveries that extend the Periodic Table of Chemical Elements and for his promotion of the basic sciences at global scale. Professor Oganessian's work played a leading role in the synthesis and study of new chemical elements of the periodic table. He has driven major developments in international scientific cooperation that led, *inter alia,* to the discovery of superheavy elements; the one with atomic number 118 was named after him as Oganesson. The laureates will receive the Prize at a ceremony at UNESCO Headquarters, Paris on 15 November, during the 41st session of the Organization's General Conference.

> "I want to express my warmest congratulations to the two winners, Professor Balzani and Professor Oganessian. Their achievements portray the inestimable value of the basic sciences to the advancement of international scientific cooperation, the building of our collective knowledge and to sustainable development following the footsteps of Dmitry Mendeleev. We need to continue increasing their large diffusion in the society at a time when the world and UNESCO are moving towards Open science" –Audrey Azoulay, UNESCO Director-General

"Russia historically pays special attention to the development of fundamental sciences. This arduous research does not bring quick results, but is the basis of many innovative achievements and modern technologies. Breakthrough discoveries are made possible by the fortitude and persistence of scientists and research teams. Someone's scientific courage and passion for exploration stands behind every invention, every new technology. The Prize named after the great Russian scientist Dmitry Mendeleev is an incentive

and an honorable reward for researchers who make discoveries for the benefit of all mankind" –Valery Falkov, Minister of Science and Higher Education of the Russian Federation

Established as a follow up of the International Year of the Periodic Table of Chemical Elements in 2019, the UNESCO-Russia Mendeleev International Prize in the Basic Sciences was created to foster scientific progress, science popularization and international cooperation in the basic sciences. The Prize honours the remarkable scientific heritage of Dimitri Mendeleev, father of the Periodic Table, whose work was fundamental to the development of chemistry, physics, biology, aeronautics, hydrodynamics, meteorology and astronomy as well as what is now termed sustainable development. Dmitri Mendeleev's version of the periodic table of 1869 contained gaps in places where he believed unknown elements would fit, thereby, challenging the generations to come to follow in his footsteps for the progress of science and the betterment of humankind. Since then, the Periodic Table has been continuously supplemented as scientists identify and synthesize new elements, mainly through international scientific cooperation.

The Prize is to be awarded annually to two individuals for their breakthrough discoveries or outstanding innovations driving, or with potential to drive, socio-economic transformation and development of human societies, and for their dedicated promotion of basic science. Each laureate receives a monetary award of USD $250,000, a gold medal, and a diploma.

Reproduced from https://en.unesco.org/news/professors-balzani-and-oganessian-receive-first-unesco-russia-mendeleev-international-prize

Paul Anastas wins the Volvo Environment Prize 2021

Paul Anastas, a Yale professor and pioneer in developing non-hazardous chemicals, wins the 2021 Volvo Environment Prize, one of the world's most respected scientific environmental awards. The research of Paul Anastas "is revolutionizing the chemical industry, a key contribution to meeting the sustainability challenge," says the Prize Jury.

Everything we touch, see and feel is chemical, whether it's furniture, clothes, medicine, or electronics. For the past two centuries, chemistry has been creating technological miracles, increasing the human quality of life. But its performance has also led to unintended consequences of pollution, waste, and toxicity.

Paul Anastas, widely known as the "father of green chemistry," set about to change this early in his career as a staff chemist in the US Environmental Protection Agency (EPA). He co-founded the Green Chemistry Institute and later served as an advisor in the White House and chief scientist at EPA. Professor Anastas is currently Director of Yale University's Center for Green Chemistry and Green Engineering.

"Green chemistry is not about sacrifice," says Paul Anastas. "The new products of green chemistry not only perform as well, they almost always perform better than the incumbent technologies. It's because, historically, our way of converting one chemical into another has been rather brutish and ugly. We heat, beat and treat these substances, often making them more toxic. That increases the risk of them reacting with our bodies and the biosphere."

Instead, Paul Anastas' research has focused on how nature does it. He and his students have developed methods for generic molecular design for reduced toxicity and waste reduction. In addition, Paul Anastas has developed The Twelve Principles of Green Chemistry, a framework widely used by industry and universities. He has also championed the development of green chemistry networks operating in more than 30 countries, resulting in numerous actions, such as creating new bio-based plastics. Or the redesign of manufacturing to reduce waste, which could have substantial environmental benefits since 90 percent of all materials that go into manufacturing wind up as waste immediately.

But the ultimate challenge is CO_2, the primary driver of climate change. Paul Anastas is optimistic: "What's going on now is brilliant green chemistry that converts CO_2 to useful materials, such as buildings or bridges. Large quantities of CO_2 going into materials is part of shifting the equation. It's one of the great challenges that green chemistry is meeting, and this award honors all the green engineering practitioners around the world."

The Volvo Environment Prize has for 32 years been awarded annually to people who have made outstanding scientific discoveries within sustainability. Three of the laureates have later been awarded the Nobel Prize. The Prize was celebrated on 1 Dec 2021 with a live streaming prize ceremony and seminar: https://www.environment-prize.com/ceremony/2021/

https://www.volvogroup.com/en/news-and-media/news/2021/oct/news-4101555.html

2022 Franzosini Award—Call For Nominations

The Subcommittee on Solubility Equilibrium Data (SSED) established the Franzosini Award to be made to a maximum of two young scientists working in the areas of solubility and homogeneous equilibrium data. The awardees must attend the International Symposium on Solubility Phenomena and Related Equilibrium Processes (ISSP), the biannual conference organized by the SSED.

The next 20th International Symposium on Solubility Phenomena and Related Equilibrium Processes (ISSP20) will be hosted by Simão Pinho in the Instituto Politécnico de Bragança, Bragança, Portugal, and is scheduled 4-9 September 2022.

The Nominations deadline for the Franzosini awards is **31 May 2022.**

For an history of the Award, see <https://iupac.org/what-we-do/awards/franzosini-award/>

https://iupac.org/2022-franzosini-award-call-for-nominations/

Grand Prix de la Fondation de la Maison de la Chimie—2022 call for nominations

The prize is intended to reward original work in chemistry to the benefit to mankind, society, or nature. The GRAND PRIX will be awarded for the eighteenth time in 2022, to one or several persons, irrespective of nationality. The prize will carry a monetary award of 35,000 Euros.

All entries must imperatively be presented through a learned society or a national or international scientific o**rganisation without any direct link with the nominee. Entry forms, together with a report detailing the arguments for the no**mination, must be returned to the Fondation de la Maison de la Chimie by **30 April 2022.**

All entries will be submitted to the jury members for examination. After due deliberation, the jury members will choose the laureate by a majority vote.

The Chair of the Jury is the incumbent President of the *Fondation de la Maison de la Chimie*, the other members being appointed by the Board of the Foundation.

The laureate will be invited to deliver a lecture on their work at an award ceremony that will take place at the Maison de la Chimie during the first quarter 2023.

https://actions.maisondelachimie.com/les-prix-de-la-fondation/grand-prix-de-la-fondation/

Mei-Hung Chiu elected on the ISC board

Last October, a new Governing Board has been appointed to lead the International Science Council (ISC), an international non-governmental organization that works to provide a global voice for science. The Governing Board is a central decision-making body of the Council, which was formed in 2018 by the merger of the International Council of Science (ICSU), representing the natural sciences, and the International Social Science Council (ISSC).

At the 2nd ISC General Assembly, which took place online 11-15 October 2021, ISC Members elected four Officers of the Governing Board and ten Ordinary Members to join the incoming President of the ISC, Peter Gluckman, who takes up his presidency at the conclusion of the 2021 General Assembly.

The ten Ordinary Members of the Governing Board elected for the next three years are: Karina Batthyány; Françoise Baylis; Geoffrey Boulton; Melody Burkins; Mei-Hung Chiu; Pamela Matson; Helena Nader; Walter Oyawa; Maria Paradiso; and Martin Visbeck.

IUPAC supported Mei-Hung Chiu's candidacy and is pleased to see her elected in this new position. Chiu is an elected member of the Bureau and Executive Committee of IUPAC since 2016. Prior she was Chair of Committee on Chemistry Education for four years. Mei-Hung Chiu is a Distinguished Professor at the Graduate Institute of Science Education, National Taiwan Normal University.

The membership of the ISC Governing Board reflects the multi-disciplinarity of the Council's membership base, as well as regional and gender diversity. Amongst its duties, the ISC Governing Board provides strategic leadership and develops priority activity and business plans for approval by the General Assembly, as well as monitoring the implementation and performance of such plans. The Board oversees the scientific activities and other operations of the Council and reports to the General Assembly, as well as proposing budgetary outlines and the scale of annual dues to be paid by Members.

https://council.science/current/news/new-governing-board-2021/

2022 IUPAC-Solvay International Award For Young Chemists—Call For Applicants

The IUPAC-SOLVAY International Award for Young Chemists is intended to encourage outstanding young research scientists at the beginning of their careers. The awards are given for the most outstanding Ph.D. theses in the general area of the chemical sciences, as described in a 1000-word essay. The award is generously sponsored by Solvay.

In 2022 IUPAC will award up to five prizes. Each prize will consist of a USD 1000 cash award and up to USD 1000 towards travel expenses to attend the 2023 IUPAC Congress in The Hague (18-25 Aug 2023; see iupac2023.org). In keeping with IUPAC's status as a global organization, efforts will be made to ensure fair geographic distribution of prizes.

The awards will be presented at the 2023 IUPAC Congress. Each awardee will be invited to present a poster on his/her research and to participate in a plenary award session, and is expected to submit a review article for publication in *Pure and Applied Chemistry.*

Complete applications must be received at the IUPAC Secretariat by **15 February 2022.**

https://iupac.org/2022-iupac-solvay-international-award-for-young-chemists-call-for-applicants/

SDGs for the Benefit of Society—Video from IYCN symposium, August 2021

The United Nations Sustainable Development Goals (SDGs) are a direct call to action, encouraging governments and citizens around the world to actively preserve the planet and its inhabitants for the greater success of mankind. A symposium held last August during the 2021 IUPAC Congress, organized by IYCN and including speakers from around the world, focused on the impact that different organizations and individuals have on the betterment of society while working on the SDGs.

The symposium was set to inspire researchers with different backgrounds to consider how they too can contribute to this effort. The recordings now made available is to sustain that reflection and also highlight that work towards the SDGs can take many forms.

The IYCN symposium on the UN-SDGs for the Benefit of Society held last IUPAC|CCCE 2021, is available to watch on the IYCN Youtube channel at https://bit.ly/3DrrMNd

INCHI Outreach

Last November, the InChI TRUST started the release of a newsletter, called InChI OUTREACH. The goal is to share new information about the InChI Project, the InChI Trust and the usage of the tools and technologies that are being created, updated, and maintained. A release 4 to 6 times per year is being planned. Please send any comments, questions, or suggestions to Outreach Director, Rudy Potenzone (rudy@inchi-trust.org).

To join InChI OUTREACH Mailing List, visit https://iupac.org/inchi-outreach/

An interview with Tsuyoshi Minami

Professor Tsuyoshi Minami of the University of Tokyo, Japan, is the first person to be awarded the IUPAC Emerging Innovator Award in Analytical Chemistry—an award that recognizes outstanding work undertaken by researchers who are at an early stage of their independent career.

Here he speaks with Vera Koester of ChemistryViews about his current research based on analytical and supramolecular chemistry, and how internationality and interdisciplinarity shaped him.

You have worked in the US, in the UK, and also, of course, in Asia. Did you experience differences between the people or in the labs?

Yes, during my Ph.D. I studied at the University of Bath in the UK as a visiting research student. Later, I was a postdoc and research assistant professor at Bowling Green State University, Bowling Green, OH, USA.

Coming to the UK was the first time I was outside of Japan, so it was exciting coming from what is maybe a rather isolated island to this European island.

Especially in the US, it was very international with students from all around the world. After my research stay in the US, I joined a device laboratory at Yamagata University as an assistant professor. There, I was not among chemists. All discussions took place without chemical structures. It was a tough time for me, but also very inspiring.

Through the precious experience in this device group, I decided to expand my group to further broaden my research field, and because of my international experience, I try to accept international students and researchers in my group at the University of Tokyo.

Currently we are struggling with the coronavirus, but I like to collaborate with colleagues from other universities and I have students from Europe, Asia, the Arabian countries, and the US in my lab. In fact, I am trying to help mix the cultures and integrate different students from different backgrounds and with different mindsets. I believe that such international collaborative research encourages students and young researchers, just as I was encouraged in my thinking in the UK and US.

What role do scientific societies such as the Japanese Chemical Society or IUPAC play in this?

They are very important. IUPAC in particular connects chemists worldwide. The Chemical Society of Japan is involved in IUPAC.

I would say that the Chemical Society of Japan is increasingly opening up to other countries and is becoming more international. Originally, they organized their national conference only in Japanese, but now they have started to include English presentations and sessions. They especially encourage students to present in English. So if foreign scientists want to attend, that is relatively easy now.

Read full interview in *ChemistryViews:* https://doi.org/10.1002/chemv.202100103

ChemistryViews is the online science news magazine of Chemistry Europe, an organization of 16 European chemical societies. It informs about what is happening in the global chemistry community and has a strong focus on the peo-ple behind the science. It covers new ideas, educates, and entertains.

In Memoriam

Remembering Professor Kozo Kuchitsu (1927-2021)

Professor Kozo Kuchitsu passed away on 22 March 2021. A full Obituary has appeared in *Chemical Physics Letters* **779,** 138791 **(2021) (https://doi.org/10.1016/j.cplett.2021.138791). Here, we would like to remember his tremendous contribution to IUPAC, Commission I.1, and the "Green Book."**

Professor Kuchitsu graduated from the Department of Chemistry, the University of Tokyo, in 1951 and received his Doctor of Science degree in 1958 under the supervision of Professor Yonezo Morino. He was appointed Assistant and then Associate Professor in the same department, and succeeded Professor Morino in 1969 at the Chair of Physical Chemistry, Department of Chemistry, the University of Tokyo.

Professor Kuchitsu joined the Physical Chemistry Division of IUPAC (Division 1), starting as an associate member of Commission 1.1 on Symbols, Terminology, and Units. He then became titular member and was elected Chairman of the Commission I.1 (1981-1985). Besides Commission I.1, Professor Kuchitsu also served as President (1993-1995) and Past President (1996-1997) of the Physical Chemistry Division.

Professor Kozo Kuchitsu (fifth from right) at an IUPAC meeting with the core group preparing the third edition of the Green Book. The meeting took place on 12-16 March 1999 at Hotel Europe, Engelberg, Switzerland. From left to right: Bertil Holmstroem (Sweden), Jeremy Frey (United Kingdom), Tom Cvitas (Croatia), Herb Strauss (USA), Martin Quack (Switzerland), Kozo Kuchitsu (Japan), Franco Pavese (Italy), Michio Takami (Japan), Juergen Stohner (Switzerland), and Roberto Marquardt (France) with a view of Mount Hahnen in the back.

Cover of the Japanese translation of the Green Book, Third Edition, RSC Publishing, Cambridge, UK (2007). The translation was completed by joint efforts of AIST (National Institute for Advanced Industrial Science and Technology) and the CSJ (Chemical Society of Japan) subcommittee on Units and Symbols (published by Kodansha, Tokyo, April 2009).

Among his many contributions to IUPAC, he was one of the five founding authors of "Quantities, Units and Symbols in Physical Chemistry," known as "the IUPAC Green Book." (first edition; 1988); as well as a co-author of the second (1995) and third editions (2007). Long after his official appointment at Commission I.1, he kept working on the Green Book and its related publications. Especially in the 2000s, he was instrumental in preparing the Japanese translation of the third edition as well as of its compact ten-page version, which was a translation of "A Concise Summary of Quantities, Units and Symbols in Physical Chemistry" by Jürgen Stohner and Martin Quack.

The meetings with Professor Kuchitsu were always marked by his great kindness; he discussed complex issues with genuine interest, patiently listening to others, and carefully considering their opinions. He was greatly appreciated for his deep insight on wide-ranging subjects, his enthusiasm, as well as his attention to detail, and the extraordinary amount of work that he carried out tirelessly, even in his eighties.

Professor Kuchitsu profoundly shaped Commission I.1 and the "Green Book," for which he had a special affection. We will remember him for his thoughtfulness, his profound scientific knowledge, and his generous and kind personality.

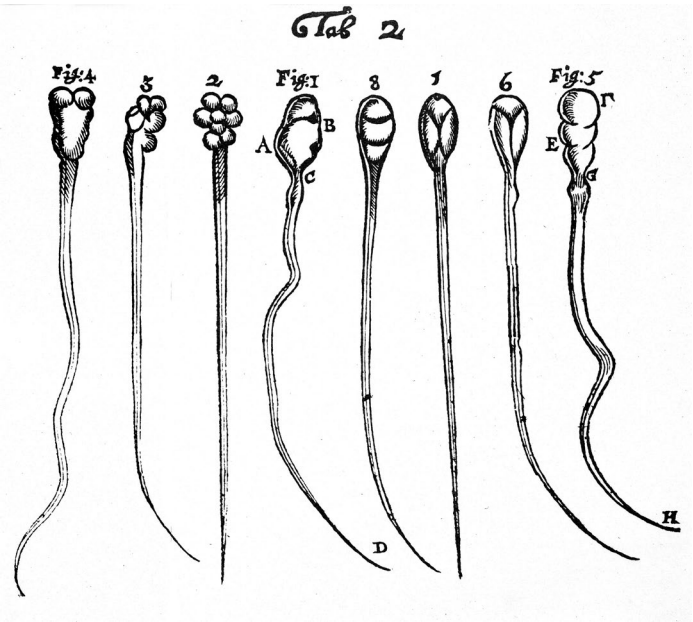
Royal Society of Chemistry Provides Guidelines for Censorship to its Editors

by Anna Krylov, Gernot Frenking, and Peter Gill

Anton van Leeuwenhoek [1] was a founder of microbiology. By perfecting lens grinding, he created microscopes capable of 200x magnification. Leeuwenhoek was the first to observe blood cells and microorganisms. He communicated his observations to the Royal Society, which published them in its *Philosophical Transactions.* Leeuwenhoek was also the first to observe spermatozoa in semen, a breakthrough in understanding sexual reproduction [2]. However, he was hesitant to communicate his findings, concerned that they might be offensive. He prefaced his report: "If your Lordship should consider that these observations may disgust or scandalise the learned, I earnestly beg your Lordship to regard them as private and to publish or destroy them as your Lordship sees fit [2]." His Lordship—the president of the Royal Society—did opt to publish van Leeuwenhoek's observations in *Philosophical Transactions* in 1678 [3]—thus begetting the field of sperm biology.

Things could have played out differently for Leeuwenhoek in 2021. Per recent Guidelines [4] of the Royal Society of Chemistry, a professional society publishing more than 50 chemistry journals [5], editors must now "consider whether or not any content (words, depictions or imagery) might have the potential to cause offence."

The document [4] begins: "We have a shared responsibility to guard against all forms of discrimination or exclusion. We expect all staff, authors, reviewers and editors to cooperate with measures introduced to ensure inclusion and non-discriminatory conduct. Our aim is for all published material to be respectful, accurate and relevant. The aim of this guidance is to help you *to identify and prevent the publication* of inappropriate content in our journals and books, and to encourage you to reflect on how inappropriate content can impact members of the community and readers around the world." The Guidelines [4] continue, "Words, depictions and imagery have the potential to cause offence, therefore we need to consider how content might be perceived by others. There can be a disparity between the intention of an author and how their content might be received—*it is the perception of the recipient that determines offence, regardless of author intent.* This highlights the need for scrutiny and awareness at all stages from content creation to publication." (Emphasis ours).



Sperm from rabbits (Figs 1-4) and dogs (Figs. 5-8), drawn by draughtsman of Antoni van Leeuwenhoek in 1677, published in 1678. (Image retrieved from Wikimedia Commons)

An accompanying memo clarifies: "Offence is a subjective matter and sensitivity to it spans a considerable range; however...it is the perception of the recipient that we should consider, regardless of the author's intention." That is, the offence is understood in terms of the feelings of the offended, not whether there is a plausible reason to be offended; this is at odds with the "Free Speech and Academic Freedom" report by the UK Department of Education [5], which states: "Potential for offence caused by speech should not in itself be used to prevent lawful freedom of speech" (p. 34).

What sort of inappropriate content should editors be on the lookout for? The Guidelines [4] provide a list of 15 "indicators" of inappropriate content, including "Harmful, hateful"; "Harassment: unwanted [content] that makes others feel intimidated or humiliated"; "Material...that presents explicit/exploitive, obscene or degrading text, pictures, illustrations"; "Any content that could reasonably offend someone on the basis of their age, gender, race, sexual orientation, religious or political beliefs, marital or parental status, physical features, national origin, social status or disability"; and "Likely to be upsetting, insulting or objectionable to some or most people." The authors of the Guidelines [4] could have saved some ink and shortened the list to either of the last two, as each is sufficiently broad to justify censoring anything in chemistry and beyond.

One might wonder, how likely would a chemistry paper be to contain such inappropriate content? After all, chemistry is blissfully distant from such "contentious" areas as human biology, heredity [6], and sexual reproduction [7]. Yet recent examples show that even writing about highly technical matters can be a minefield of "offences." As one of us recently documented in "The Peril of Politicizing Science" [8], content that is "objectionable to some" includes names of scientific discoveries and equations, such as the "Shockley-Queisser limit" and "Newton's Laws"; technical terms, such as "quantum supremacy," "master password," and "dummy variable"; and a slew of plain English words [9]. For example, "normal" allegedly "makes most people feel excluded." [10] So much for "normal pH" and "normal distribution" [11]. Some scholars—including an associate vice president of Mount Royal University in Canada—are offended by English grammar and are calling for the rejection of capital letters as a "symbol of hierarchy" and oppression [12]. Following the Guidelines, are RSC editors now to prevent publication of "pH", "pKa", and "[M]"?

Censorship—"the suppression or prohibition of any parts of books, films, news, etc. that are considered obscene, politically unacceptable, or a threat to security"—is already a reality in scientific publishing. Today censorship is administered not by repressive governments but by Twitter vigilantes, or, more generally, "outrage mobs"; an outrage mob is defined as "a group or crowd of people whose goal is to sanction or punish the individual, individuals, or organization they consider responsible for something that offends, insults, or affronts their beliefs, values, or feelings." [13]

In 2020, *Angewandte Chemie* removed a published paper from their website in response to the demands of an offended mob [14]. In 2021, a paper the *Journal of Hospital Medicine* about the perils of tribalism in scientific discourse [15] was retracted and republished along with an apology [16] for this "microaggression"—apparently, the world "tribalism" belongs to the list of "oppressive", "culturally appropriative" language [10,17]. The *Journal of Intelligence* explicitly states on its website that it will not consider manuscripts that may "lead to or enhance political controversies." [18] More examples can be found in a recent study by Stevens, Jussim, and Honeycutt [13].

This work also explores current mechanisms of censorship and suppression of scholarship. Importantly, it highlights the responsibility of authorities in resisting "outrage mobs" calls for punishment and suppression of ideas: "Although outrage mobs often trigger the punishment process, in Western democracies, mobs no longer actually burn witches at stakes. For most punishment to occur in academia, some authority has to agree to implement the mob's punishment. …Mobs do not get papers retracted; that is the decision of editors and editorial boards. Thus, the key turning point in whether an academic outrage mob is effective at punishing an academic for their ideas is usually the action of authorities." Hence, it is imperative for our leadership to resist the mobs and defend the institutions they are entrusted with against the ideological subversion.

The Guidelines were created by the RCS Committee of Inclusion and Diversity [19] as a new addition to their "A framework for action in scientific publishing," developed to address alleged systemic and individual biases [20]. RSC has also issued a "Joint commitment for action on inclusion and diversity in publishing" [21], already endorsed by many other publishers, pledging to "engage all relevant stakeholders to improve outcomes on inclusion and diversity, at all stages of the publishing process." In their response to our Letter to *Chemistry World*, RSC clarifies that the Guidelines were "created in partnership with external experts" and "dovetail with existing policies and decision-making processes." [22] The question that remains unaddressed is how the goals of inclusion and diversity will be advanced by censorship of scientific publications.

Censorship is antithetical to the scientific enterprise. The publishers of the Royal Society of Chemistry should focus on its mission, facilitating the communication of high-quality chemistry research, and stay true to the purpose of the Royal Charter—"the general advancement of chemical science and its application." [23] Rather than turning Twitter censorship into policy, scientific publishing leadership worldwide should defend the core principle of science—the free exchange of ideas.

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Anna I. Krylov, Professor of Chemistry, Department of Chemistry, University of Southern California, USA; https://orcid.org/0000-0001-6788-5016; krylov@usc.edu; Gernot Frenking, Professor of Chemistry, Philipps-Universität Marburg, Marburg, Germany; https://orcid.org/0000-0003-1689-1197; frenking@staff.uni-marburg.de Peter M. W. Gill, Professor of Chemistry, School of Chemistry, University of Sydney, Sydney, New South Wales, Australia; https://orcid.org/0000-0003-1042-6331; p.gill@sydney.edu.au

Metrological and quality concepts in analytical chemistry (IUPAC Recommendations 2021)

David Brynn Hibbert, Ernst-Heiner Korte, and Ulf Örnemark
Pure and Applied Chemistry, 2021
Vol. 93, no. 9, pp. 997-1048
https://doi.org/10.1515/pac-2019-0819

Metrology, being the science of measurement and its application, covers the experimental production and the use of quantity values in all fields of science and engineering, including chemistry and, not least, analytical chemistry. The metrological concepts to be applied in all sciences are defined in the 3rd edition of the International vocabulary of metrology—Basic and general concepts and associated terms (VIM) (bipm.org); however, various fields have specialized tasks and typical laboratory procedures to meet the metrological challenges in their fields. This requires us to identify and define dedicated concepts to ensure consistent application and terminology and, therefore, these Recommendations aim at providing such concepts and terms to complement the VIM in the field of analytical chemistry.

These Recommendations result from updating the third edition of the IUPAC Orange Book and provide concepts for Chapters 1 and 13 in the forthcoming fourth edition, "Compendium of Terminology in Analytical Chemistry."

https://iupac.org/project/2012-007-1-500

A unified pH scale for all solvents: part I—intention and reasoning (IUPAC Technical Report)

Valentin Radtke, Daniela Stoica, *et al*
Pure and Applied Chemistry, 2021
Vol. 93, no. 9, pp. 1049-1060
https://doi.org/10.1515/pac-2019-0504

The definition of pH, its measurement and standard buffers, is well developed in aqueous solutions. Its definition in solvents other than water has been elaborated for a couple of solvents and their mixtures with water. However, the definition of a universal pH scale spanning all solvents and phases, not to mention standard procedures of measurement, is still a largely uncharted territory. UnipHied is a European collaboration and has the goal of putting the theoretical concept of an earlier introduced (2010) unified pH_{abs} scale on a metrologically well-founded basis into practice. The pH_{abs} scale enables the comparability of acidity between different phases. This article draws the connection of the concepts of unified acidity and secondary pH measurement.

Structure-based nomenclature for irregular linear, star, comb, and brush polymers (IUPAC Recommendations 2020)

Jiazhong Chen, Edward S. Wilks, Alain Fradet, Karl-Heinz Hellwich, Roger C. Hiorns, Tamaki Nakano, Claudio G. dos Santos, and Patrick Theato
Pure and Applied Chemistry, 2021
Vol. 93, no. 9, pp. 963-995
https://doi.org/10.1515/pac-2020-0103

Between 1984 and 2012, IUPAC published several documents containing recommendations for the nomenclature of a wide variety of polymer types such as regular linear single-strand, irregular single strand, organic regular double-strand, and cyclic organic macromolecules, non-linear macromolecules and macromolecular assemblies, and quasi-single-strand inorganic and coordination polymers. More recently a document on source-based nomenclature for single-strand homopolymers and copolymers was published in 2016, and a document on nomenclature for dendrimers and hyperbranched polymers was published in early 2019. However, structure-based nomenclature for certain types of branched polymers with three or more blocks of identical constitutional repeating units (CRUs) (three-arm star, four-arm star or brush, *etc.*) has not yet been fully addressed by the IUPAC.

This document provides recommendations for structure-based nomenclature of polymers comprising a linear single strand with two or more blocks of identical CRUs and branched strands (star, comb, and brush-like) containing three or more blocks of identical CRUs connected by a central non-repeating junction unit. This document also revises some of the rules given in the document for regular linear single-strand molecules, in particular, rule 22 on polymer chains as substituents.

https://iupac.org/project/2019-036-1-800

Feasibility of multifunction calibration of H+-responsive glass electrodes in seawater (IUPAC Technical Report)

Daniela Stoica, Bárbara Velasco Anes, Paola Fisicaro, and Maria Filomena Camões

Pure and Applied Chemistry, 2021
Vol. 93, no. 12, pp. 1487-1497
https://doi.org/10.1515/pac-2020-0202

Seawater pH values are of the highest relevance in marine chemistry studies, not only through being acidity indicators but also due to the control provided by H^+(aq) over the various simultaneous equilibria occurring in seawater. Although the concept of $pH = -\lg a_{H^+} = -\lg(m_{H^+}\,\gamma_{H^+}/m^0)$, where m_{H^+} is the relative (molality basis) activity, γ_{H^+} is the molal activity coefficient of the hydrogen ion H^+ at molality m_{H^+}, and m^0 is the standard molality, was introduced in 1910 and reaffirmed on successive occasions by relevant bodies, different conceptual definitions and alternative measurement procedures have been adopted and are in use by some, namely among oceanographers, often leading to confusion. This leads to major difficulties with the use of data, *e.g.*, on what concerns comparison of results in space and time. Primary pH values, the highest quality level in terms of the metrological chain, have been assigned to primary reference pH buffer solutions of low ionic strength, by a primary method based on measurements of the Harned cell potential in association with the Nernst equation, as well as on the adoption of extra-thermodynamic model assumptions for electrolyte solutions. Although equivalent types of recommendations dealing with standards and procedures based on metrological traceability are still lacking for higher ionic strength media, as it is in the case of seawater, reference Tris–Tris·HCl buffer solutions in artificial seawater have been suggested for use in the calibration of pH meter systems. In this work, Tris–Tris·HCl buffer saline solutions of three different molality ratios have been assigned reference values and multi-point calibration of pH meters in terms of either pH or pH^T is thus possible and supports measurement of their respective values under routine conditions at a high metrological level.

IUPAC Provisional Recommendations

Provisional Recommendations are preliminary drafts of IUPAC recommendations. These drafts encompass topics including terminology, nomenclature, and symbols. Following approval, the final recommendations are published in IUPAC's journal *Pure and Applied Chemistry* (PAC) or in IUPAC books. During the commentary period for Provisional Recommendations, interested parties are encouraged to suggest revisions to the recommendation's author. https://iupac.org/recommendations/under-review-by-the-public/

Terminology for Chain Polymerization

Chain polymerizations are defined as chain reactions where the propagation steps occur by reaction between monomer(s) and active site(s) on the polymer chains with regeneration of the active site(s) at each step. Many forms of chain polymerization can be distinguished according to the mechanism of the propagation step (*e.g.,* cyclopolymerization—when rings are formed, condensative chain polymerization—when propagation is a condensation reaction, group-transfer polymerization, polyinsertion, ring-opening polymerization—when rings are opened), whether they involve a termination step or not (*e.g.*, living polymerization—when termination is absent, reversible-deactivation polymerization), whether a transfer step is involved (*e.g.*, degenerative-transfer polymerization), and the type of chain carrier or active site (*e.g.*, radical, ion, electrophile, nucleophile, coordination complex). The objective of this document is to provide a language for describing chain polymerizations that is both readily understandable and self-consistent, and which covers recent developments in this rapidly evolving field.

Corresponding Author: Graeme Moad <graeme.moad@csiro.au>

Comments by 31 March 2022

Chemistry Teacher International Enters Fourth Year

by Jan Apotheker

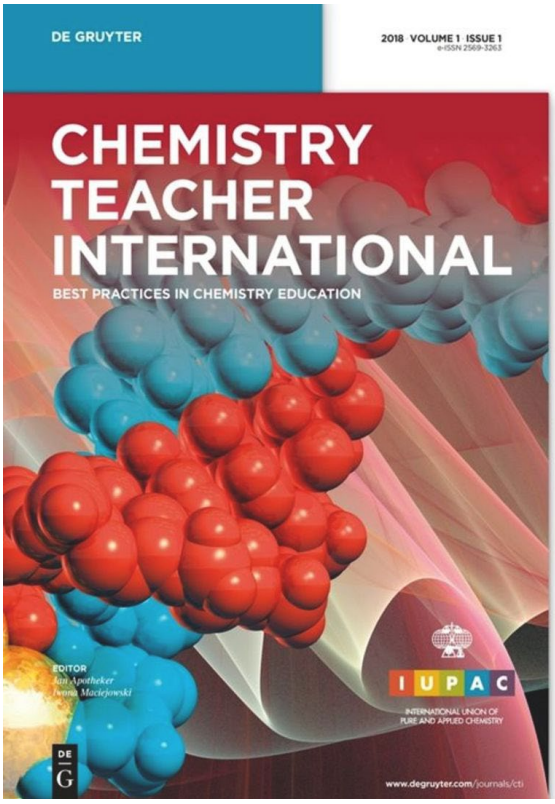
The IUPAC journal *Chemistry Teacher International (CTI), Best practices in Chemistry Education (*ISSN:2569-3263), is now in its fourth year of existence. In 2019 issues 1.1 and 1.2 were published, and in 2020 issues 2.1 and 2.2. In 2021 four issues were published, including two special issues; one on polymer science with Division IV (Polymer Division); and one on green chemistry together with CHEMRAWN (Committee on Chemical Research Applied to World Needs), Division VI (Chemistry and the Environment Division), and COCI (Committee on Chemistry and Industry). Four issues are planned for 2022. In this article we report on the first three years of the journal's existence—the rationale for its establishment, the composition of the editorial board, its funding model, authorship, and readership.

Rationale

The journal was initiated by the Committee on Chemistry Education of IUPAC, in cooperation with the Division of Chemistry Education of EuChemS. Both committees agreed that a truly international journal was needed, one that was easy to access for teachers. For the development of education, the exchange of experiences—positive and negative—is essential. The description of good practices by teachers for teachers in a more international setting should broaden the scope of teachers, beyond developments in their own country. Since travel abroad for teachers is normally very limited, an online, freely accessible journal would help inspire teachers. Both committees decided an international journal was needed for articles focusing on:

- Good practice in chemistry education at all levels
- Reports about developments in chemistry education
- Bridging the gap between research and classroom practice (Herrington & Daubenmire, 2016)
- Papers presented in conferences about chemistry education such as
  - ICCE
  - ECRICE
  - NICE
  - ACRICE
  - EUROVARIETY
- Reports on educational activities of IUPAC divisions and standing committees.

There is only a limited number of international journals (about 20) dedicated to science—and or



chemistry—education research (Kreke *et al.,* 1998; Towns & Kraft, 2012). By now there may be a few more. Most of these journals have a subscription model and are mainly focused on research in science education.

In 2016 Keith Taber (Taber, 2016) wrote an editorial in Chemistry Education Research and Practice (CERP), titled "What is wrong with 'practice' papers." In the article he explained why several types of papers are not published in CERP. More specifically he explained and argued what chemistry education research is and what it is not. He went on to explain why good practice papers should not be published in CERP. Basically, his idea was that reports on good practices, in general, do not add to the scientific knowledge and educational knowledge as such.

The Committee on Chemistry Education agreed that good practices are not necessarily chemistry education research. In some cases, they might be, but not as a general rule. That does not mean publications on good practices are not important. Reports about good practices can play an important role in improving education. An article about a way in which a flipped classroom was used, that also tries to explain why this worked in that particular situation, may inspire another teacher to try something similar in his or her own situation.

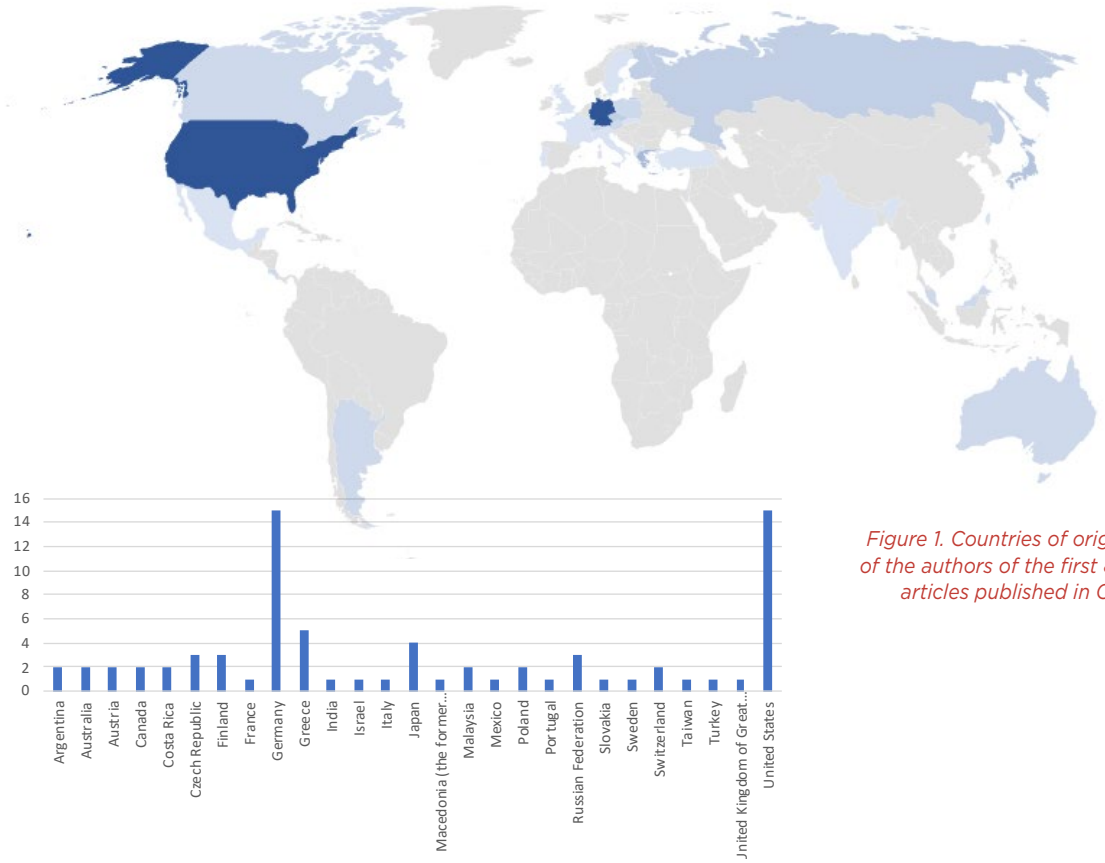


Figure 1. Countries of origin of the authors of the first 82 articles published in CTI

Journals publishing good practices in secondary education are mainly national teacher journals, like *The Science Teacher* published by NSTA; *Education in Science*, published by the ASE in the UK; *Chemie &Schule*, published in Austria; *Chemkon*, published in Germany; *NVOX*, published in the Netherlands; and *La chimica nella scuola*, published in Italy. Up to now there were very few international journal publishing good practices in chemistry education.

Since most teachers in secondary schools do not have access to journals with a subscription model, it was decided to let *CTI* be an open access journal, available to everybody with an internet connection. That means no subscription fees, but instead an Author Processing Charge (APC). For the first two volumes the fee was paid by DeGruyter (publisher) and IUPAC. The APC was set at € 375, and was implemented since July 2021. In order to stimulate publications from around the world, there is a reduction scheme (50% or 100% reduction), based on the economic situation of countries. Members of IUPAC receive a 33% reduction. Apart from that the editorial board can invite authors to publish and waive the APC.

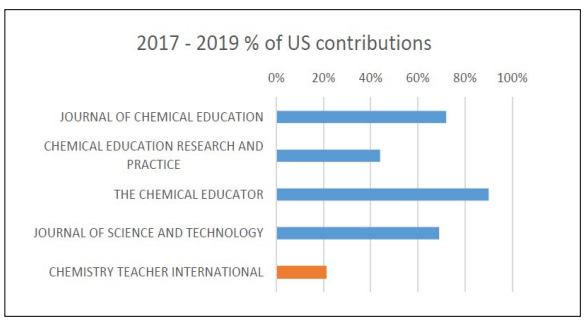


Figure 2. Article source in several journals on chemistry education

Origin of articles received

From the start, the journal has had no problem attracting articles from an international group of authors. In figure 1 the country of origin of the first 82 articles is given. By now (November 2021) more than 100 articles have been received.

Recently an article discussing research on education in Ethiopia and Indonesia was received. Especially for teachers in Africa it is important to have an international forum, where they can exchange

Name and email	Institution	Country	Region
Jan Apotheker J.H.Apotheker@rug.nl	University of Groningen	The Netherlands	Editor in chief, CCE (Europe)
Rachel Mamlok, rachel.mamlok@weizmann.ac.il	Weizmann Institute	Israël	Vice-editor in chief, Division on Chemistry Education (Middle-East
Suzanne Boniface, suzanne.boniface@vuw.ac.nz	Victoria University of Wellington	New Zealand	Australia/ New Zealand
Mei-Hung Chiu, mhchiu@gapps.ntnu.edu.tw	National Taiwan Normal University	Taiwan	Asia (Network for Inter-Asian Chemistry Educators)
Marietjie Potgieter, marietjie.potgieter@up.ac.za	University of Pretoria	South Africa	Africa (African Conference on Research in Chemistry Education)
Ian Butler, ian.butler@mcgill.ca	McGill University	Canada	North America
Iwona Maciejowska, iwona.maciejowska@uj.edu.pl	Jagiellonian University in Krakow	Poland	Europe (European Conference on Research in Science Education, EuroVariety)
Alejandra G. Suárez, asuarez@fbioyf.unr.edu.ar	National University of Rosario	Argentina	Latin America
Ethel Orlando Ethel.rios1@upr.edu	University of Puerto Rico	Puerto Rico	Representative CPCDS

Table 1. Editorial board of CTI

information about their educational research and developments.

To demonstrate the international character of *CTI* the article source of some research journals is given in figure 2.

It's clear that there is no dominance from one particular country in the source of articles, indicating *CTI* is truly an international journal, encompassing all regions of the world. The educational board that was formed reflects this idea. The composition is given in table 1.

The editors are not only responsible for the review process (each paper is reviewed by two external reviewers), but also play a role in soliciting papers within their region. Based on the success of the first two years *CTI* has been accepted in SCOPUS and EBSCO-host, two major search engines. It means *CTI* will receive an impact index within Scopus. *CTI* has submitted a request to be accepted within the Social Science Citation Index as an emerging journal.

Readership

Over the first two years some data have been collected about the use of *CTI.* These are given in figures 3 and 4. These data

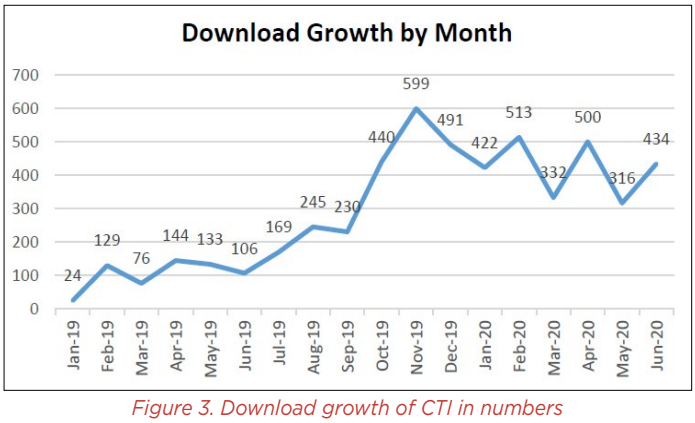


Figure 3. Download growth of CTI in numbers

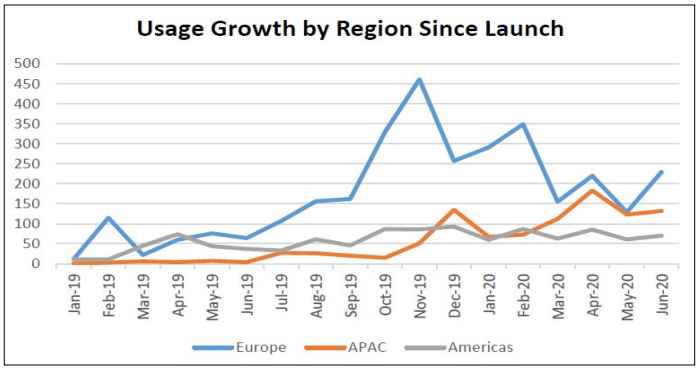


Figure 4. Usage growth by region

Authors	Title
Catherine L. Moad and Graeme Moad (Moad & Moad, 2020)	Fundamentals of reversible addition–fragmentation chain transfer (RAFT)
Ali Bagheri, Suzanne Boniface, Christopher M. Fellows (Bagheri et al., 2021)	Reversible-Deactivation Radical Polymerisation: chain polymerisation made simple
Stanislaw Penczek, Julia Pretula and Stanislaw Slomkowski (Penczek et al., 2021)	Ring-opening polymerization
Nurul Fatahah Asyqin Zainal, Jean Marc Saiter, Suhaila Idayu Abdul Halim, Romain Lucas and Chin Han Chan (Zainal et al., 2020)	Thermal analysis: basic concept of differential scanning calorimetry and thermogravimetry for beginners
Daniela Held, Peter Kilz (Held & Kilz, 2021)	Size-exclusion Chromatography as a Useful Tool for the Assessment of Polymer Quality and Determination of Macromolecular Properties
Suhaila Idayu Abdul Halim, Chin Han Chan and Jan Apotheker (Abdul Halim et al., 2021a)	Basics of teaching electrochemical impedance spectroscopy of electrolytes for ion-rechargeable batteries – part 1: a good practice on estimation of bulk resistance of solid polymer electrolytes
Suhaila Idayu Abdul Halim, Chin Han Chan and Jan Apotheker (Abdul Halim et al., 2021b)	Basics of teaching electrochemical impedance spectroscopy of electrolytes for ion-rechargeable batteries – part 2: dielectric response of (non-) polymer electrolytes
Tamaki Nakano, Adriana Pietropaolo and Masahiro Kamata (Nakano et al., 2021)	Chirality analysis of helical polymers
Volker Abetz, Torsten Brinkmann and Mustafa Sözbilir (Abetz et al., 2021)	Fabrication and function of polymer membranes
Denis M. Zhilin and Andrij Pich (Zhilin & Pich, 2021)	Nano- and microgels: a review for educators
Christine K. Luscombe, Uday Maitra, Michael Walter, Susanne K. Wiedmer (Luscombe et al., 2021)	Theoretical background on semiconducting polymers and their applications to OSCs and OLEDs
Masaru Matsuo, Rong Zhang, Yuezhen Bin (Matsuo et al., 2021)	An understandable approach to the temperature dependence of electric properties of polymer-filler composites using elementary quantum mechanics
Jiří Vohlídal (Vohlídal, 2020)	Polymer degradation: a short review

Table 2. Content special issue Polymer Science

indicate that the readership of *CTI* is growing. It is also clear that marketing is needed in order to increase the readership.

Special Issues

The editorial board has decided to publish at least one special issue per year. These special issues focus on a specific theme. In June 2021 a special issue was published with Polymer Science as a central theme. The content of that special issue is given in table 2.

For the next special issue, a call was sent out requesting papers concerning the theme: "Examples of the use of the principles of Green Chemistry and Sustainable Development in the design of industrial processes for secondary chemistry and for introductory chemistry courses. "Many chemistry curricula now feature green chemistry. The curriculum in the Netherlands is an example (Apotheker, 2018). In introductory chemistry courses in higher education more and more attention is given to the principles of green chemistry (Hjeresen *et al.,* 2000), as well as the ideas of sustainable development (*UN Sustainable Development Goals*, n.d.). This includes design principles like "cradle to cradle," and "cradle to grave" as well as life cycle analysis (Braungart & McDonough, 2002).

The number of concrete examples to illustrate these principles that are used in education at this moment is

limited, even though there are many recent examples. Within chemistry education it is important for students to understand the role that chemistry plays in society. One of these roles is to apply chemical knowledge to design processes that implement the principles of green chemistry and help in sustainable development. In order to demonstrate the role of chemistry, more information for teachers is needed so they can use this information and share with their students.

Later in 2022 a special issue on chemistry and cultural heritage will be published. As argued above it is important for students to recognize the role of chemistry in society. Articles about the use of chemistry by indigenous people are expected, as well as articles about the use of chemistry in the restoration of works of art (Figure 5).

Contribution to IUPAC

Chemistry Teacher International has made a flying start, and continues to attract enough articles to be able to published at least 4 issues a year. It is clear that *CTI* will contribute to the development of chemistry education internationally. *CTI* clearly fills a gap between chemistry education research and the activities in the classroom. *CTI* still needs to grow further and work is needed in the future to make sure it stabilizes and reaches a large group of teachers with an international orientation.

For IUPAC, *CTI* is a journal in which the divisions and standing committees can showcase their activities to an important group. Chemistry education, both in secondary schools as well as in introductory courses is an ideal platform to demonstrate the important role of chemistry in society, and the role IUPAC has within the chemistry community. The special issues of *CTI,* but also articles in general issues, can be used to highlight IUPAC's activities.

The special issues so far have been supported by different IUPAC divisions and standing committees. The editorial board welcomes ideas and initiatives to reach out to the educational community.

Figure 5. Still Life: vase with 12 Sunflowers, van Gogh (Neue Pinakothek) Van Gogh used a chromate based paint: the yellow color is slowly turning brown due to reduction of Chromium(VI) to chromium(III). Understanding the chemistry of the process helps in the restoration.

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Jan Apotheker <j.h.apotheker@rug.nl> is CTI Editor-in-chief and past Chair of the IUPAC Committee on Chemistry Education; he is retired lecturer in Chemistry Education from the University of Groningen in The Netherlands.

Online Chemistry Simulations to Intrigue, Engage and Attract 21st Century Science Students

by Linda Sawson

Undoubtedly the Covid-19 pandemic has revealed how little we have utilised computers and the internet for science teaching. Prior to the crisis, computers and the internet had been used by the majority for data spreadsheets, as word processors, and as a means of rapid communication.

As we look towards a post pandemic "new normal" it is right that we should address this issue by forging an ambitious and innovative marriage between the internet and science teaching. Simulators for Teaching Ltd., (Sim4t), formed in 2011 by a team of experts in scientific instrumentation and education has been at the forefront of innovation: We produce online software that simulates scientific instrumentation and experiments for chemistry and general science students in universities, colleges, and schools.

Enabling Educators

Sim4t has enabled educators to complement in-person teaching with simulations: for example, the School of Chemistry at University College Cork was looking for cost effective ways for advancing their laboratory classes but in a new and dynamic way, so simulation experiments were ideal. Similarly, the Department of Chemical Sciences at the University of Limerick, a user since 2018, had to design five undergraduate laboratory experiments as part of a new module. They have subsequently managed to advance how they teach and connect with over 30 additional chemistry students to their existing laboratory cohort, per semester, using Sim4t software, thereby improving teaching efficiency.

Significantly, this year, the opportunity to break the Covid-19 lockdown by providing online Sim4t experiments for students studying remotely has been seized upon by institutions in Romania, Italy, and the UK.

Flexibility

The key word in terms of how an institution may use Sim4t technology is *flexibility*:

- As a replacement for laboratory classes; classes can be expensive due to instrument and building costs, and staff time. Simulation offers a full online experiment for a fraction of the cost of a real laboratory.
- The software can be used as a pre-laboratory exercise to help students use their actual laboratory time more efficiently or give them some "extra laboratory time" by using the simulator to follow up on things introduced in a formal laboratory class.
- The online system can be used for distance learning and by part-time students and thereby overcome logistical problems associated with delivering education to this group.
- The software can be used to promote self-study and independent learning amongst students and provide efficiencies in both staff time and how laboratory facilities are used.
- The choice is up to each individual institution.

So, what does the online portal offer?

Simulators for the Web (Sim4Web)

The Sim4t secure online portal, known as Simulators for the Web (Sim4Web), is based on a UV-Visible Absorption spectrometer simulator. Currently, we offer seven experiments covering topics from an "Introduction to UV-Visible Absorption Spectroscopy" through "Qualitative and Quantitative Analyses" and onto "Chemical Kinetics." Users must register to access the Sim4Web secure platform via an e-mail address and password. There are two types of user defined by the system: supervisor and student, respectively.

Sim4Web allocates different privileges and access to documentation depending on the user status. As a supervisor, one can create an experimental session and invite students onto that session. A supervisor can also run an experiment for themselves: A typical Home Screen is shown in Figure 1. Navigation through the software is achieved via the menu list on the left-hand side of the screen working down through from top to bottom allowing access to the virtual materials, glassware and instrumentation necessary to perform repeated runs of an experiment.

Documents

Documentation for each experiment is accessed via the "Documents" submenu shown in Figure 1. This includes a complete experimental procedure which guides the user through operation of the simulator and the experiment, detailed lecture notes covering the theory of the topic and model answers (for supervisors only).

Qualitative and Quantitative Analyses

Experiment 1 in the Sim4Web catalogue is "The Beer-Lambert Law and Identification of an Unknown Mixture" and introduces the concepts of *qualitative* and *quantitative* analyses.

Figure 1. The Home Screen

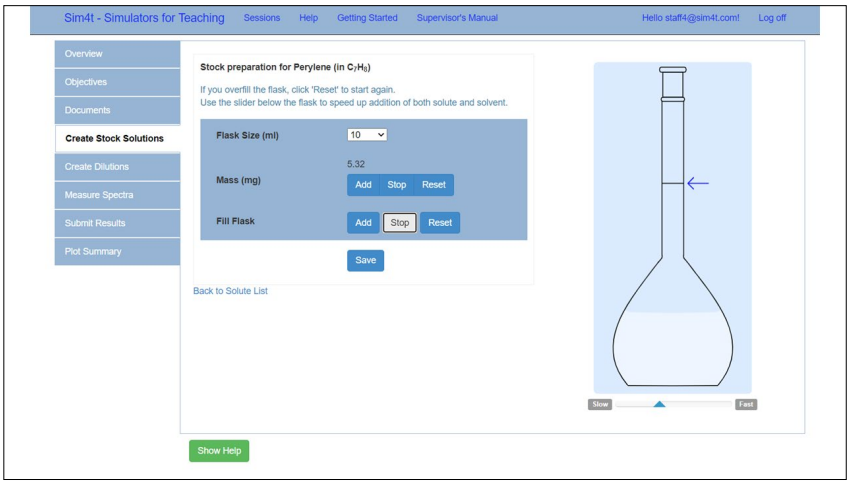


Figure 2. The Virtual Flask

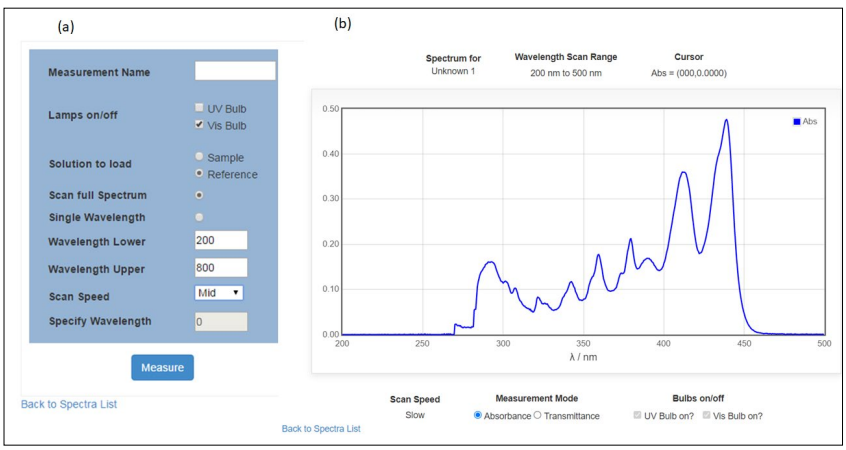


Figure 3. The Spectrometer Simulator

The first part of this exercise, involves preparing virtual samples and recording UV-Visible spectra for naphthene, anthracene, and perylene, respectively, in toluene solution. Beer-Lambert plots are then constructed for each aromatic species and the molar absorption coefficient (□), determined. In the second part of the experiment, unknown samples, allocated by the supervisor to each individual student, are investigated. Given the information derived in part one, UV-Visible spectroscopy will be used qualitatively to identify the species, and then quantitatively to determine the amount of each component present in the unknown sample.

The Virtual Flask

The virtual flask module (shown in Figure 2, for perylene) allows repeated attempts at sample preparation of a stock solution from the "Create Stock Solution" menu. The desired flask size is selected via a drop-down menu and virtual chemicals can be weighed out and solvent added up to the graduated mark via the slider control under the flask. Similar modules allow dilutions of a stock solution to be created via the "Create Dilutions" submenu.

The Spectrometer Simulator

Once the virtual samples have been prepared, they can be run on the spectrometer simulator accessed via the "Measure Spectra" submenu. The spectrometer set up screen is shown in Figure 3a). This menu allows selection of the measurement mode: either a full scan or single wavelength readout. In the full scan mode, the wavelength range can be defined in addition to the scan speed.

A solvent reference must be run prior to each spectroscopic sample measurement. The spectrometer scan window for an unknown mixture is shown in Figure 3b). Data can be displayed in either Absorbance or Transmittance mode with a cursor available to generate point intensity readings at a given wavelength.

Learning Outcomes

The experiment provides practice in sample preparation and solution dilutions in addition to operation of the spectrometer simulator.

Chemical Reaction Kinetics

Two experiments covering chemical kinetics are currently offered via the Sim4Web platform, both based on the reaction of crystal violet (CV) with sodium hydroxide (NaOH). One experiment allows the empirical determination of the rate law (described

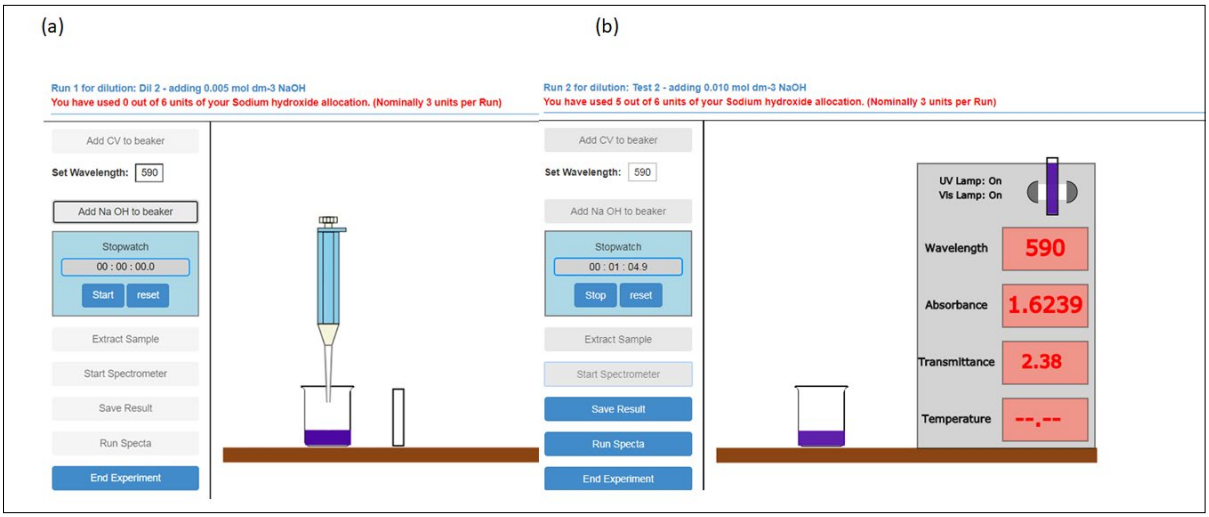


Figure 4. The Wet Bench

in the following section) while the second concerns the temperature dependence of the reaction and Arrhenius behaviour.

CV is an intensely coloured triarylmethane dye, that transforms into a colourless product on reaction with NaOH. Consequently, the absorbance of a reaction mixture containing CV and NaOH will be proportional to the concentration of unreacted dye still present in solution. The reaction of CV and NaOH can therefore be monitored and the kinetics studied by measuring the absorbance of the mixture as a function of time. By using the Beer-Lambert law, if □ for CV is known, the concentration of CV can subsequently be derived as a function of time.

The rate of the reaction or rate law between CV and NaOH can be written:

$$\text{Rate} = k\,[OH^-]^x\,[CV]^y \qquad \text{(eq. 1)}$$

where k is the rate constant (or rate coefficient) for the reaction, x is the order with respect to OH^-, and y is the order with respect to CV. In this experiment, students are tasked with determining, experimentally, the value of x and y. In order to do this, the reaction (and the kinetics) is simplified by using a vast excess of NaOH: it can therefore be assumed, that the concentration of hydroxide ion does not change through the course of the reaction even though all of the CV may have been used up. Consequently, the $[OH^-]$ term in the general rate law is constant and can be grouped with k as in equation 2:

$$\text{Rate} = \{k\,[OH^-]^x\}\,[CV]^y \qquad \text{(eq. 2)}$$

where $k' = k\,[OH^-]^x$ (k' is termed a *pseudo* rate constant or the *observed* rate constant.)

The rate equation can, therefore, be written:

$$\text{Rate} = k'[CV]^y \qquad \text{(eq. 3)}$$

This approximation simplifies the reaction and allows k' and y to be determined experimentally by carrying out two reactions: in the first kinetic run the concentration of NaOH is half that used in the second experiment. For both reactions, the $[OH^-]$ is vastly in excess of that of CV.

Once k' has been derived it is possible to determine k and x since the concentration of NaOH is known in both experiments.

This experiment is composed of 2 parts: initially students must make up a stock solution of CV and then prepare a series of dilutions to allow □ to be determined.

The second part of the experiment is concerned with using an absorption spectrometer simulator to monitor the kinetics of the reaction by using a virtual wet bench as shown in Figure 4.

By clicking "add CV to beaker" a virtual pipette releases 9 cm^3 of a 10^{-5} mol dm^{-3} CV dye solution into a beaker (see Figure 4a). The desired wavelength (□) of interest can then be selected by clicking "Set Wavelength." (This should be the same □ that was used to derive □ in Part A of the experiment).

The reaction is initiated by clicking "add NaOH to beaker" wherein a virtual pipette releases 1 cm^3 of a 0.05 mol dm^{-3} NaOH solution into the beaker containing the CV dye. (The effective concentration of NaOH in the reaction is, therefore, 0.005 mol dm^{-3}.) The clock must be started immediately the transfer has been made. A sample of the reaction mixture is extracted via a virtual pipette and transferred to a cuvette.

By clicking the "Start Spectrometer" button, the sample is loaded into the spectrometer (as in Figure 4b) and an absorbance reading taken as soon as possible, noting the time of the measurement. The absorbance readings should then be converted into concentrations using the Beer-Lambert law and the value of □ for CV in aqueous solution determined in Part A. (Enough 0.05 mol dm^{-3} NaOH solution has been allocated by the software to perform a further two kinetic runs if desired).

The software allows a second kinetic experiment to be run following the same procedure as outlined above but using a 0.1 mol dm^{-3} NaOH solution.

Data Treatment

The students must first work out the concentration profile of CV during the course of the reaction using the □ value determined in Part A. The data should subsequently be plotted to determine whether the reaction is zero, first or second order.

Learning Outcomes

The experiment provides practice in sample preparation and solution dilutions in addition to operation of the spectrometer simulator. The kinetics segment of the experiment offers experience in quick and careful addition of a reactant to start a reaction while carefully coordinating the start of the stopwatch and extraction of a sample for analysis. Practice in careful monitoring and recording of the absorbance as a function of time forms the latter practical aspects of the experiment.

How to treat data and plot graphs correctly to derive meaningful physical constants from the gradient is also a learning outcome form this experiment.

What do Students Think?

Perhaps it is appropriate at this point, to leave the final word to the students themselves:

A recent survey, commissioned by Sim4t, revealed that over 97% of student respondents liked the accompanying documentation (*i.e.,* lecture notes, experimental procedures, and user manuals) and found it extremely helpful.

Furthermore, 95% of the pool said that the combination of the virtual flask module and the spectrometer simulator was very useful for their studies and that they would like to have online chemistry simulations to complement their current science programme.

In Summary

Sim4t provides a cost effective, fully interactive, online learning system (Sim4Web) which will allow institutions to provide innovative and engaging material, effectively deliver distance learning, widen access to science education for all and improve teaching efficiency in the 21st century educational market.

For more information about the simulations and products that Sim4t offer please go to the company website: www.sim4t.com
visit the Sim4t YouTube channel:
https://www.youtube.com/channel/UCezS564e-gpKuvqJEQjJRAg
or e-mail: l.swanson@sim4t.com

Green Chemistry Postgraduate Summer School

by Mirabbos Hojamberdiev, Aurelia Visa, Fabio Aricò, and Pietro Tundo

The 13th Green Chemistry Postgraduate Summer School was held for the first time in a hybrid way, both online and in-person in Venice 4-9 July 2021, as a result of the ongoing restriction related to the Covid-19 pandemic and some limitations on travelers' mobility.

The Summer School is an international initiative organized and managed by the Green Sciences for Sustainable Development (GSSD) Foundation (www.gssd-foundation.org), a non-profit Foundation based in Venice, Italy. In 2021, it was held in collaboration with IUPAC Interdivisional Committee of Green Chemistry for Sustainable Development (ICGCSD), Ca' Foscari University of Venice, and the Italian National Commission for UNESCO Roma. It was generously sponsored by various organizations, including the Organization for the Prohibition of Chemical Weapons (OPCW), PhosAgro, RSC (UK), and GreeNovator.

For those attending in person, the event took place in the classrooms of Ca' Foscari University of Venice. The event was chaired by Pietro Tundo, President of GSSD Foundation and Chair of ICGCSD. The Organizing Committee included Fabio Aricó from Ca' Foscari University, Mirabbos Hojamberdiev from Uzbekistan, and Aurelia Visa from Romania. The Summer School was also supported by Elena Alfine and Emilia Pasta (administration), Paula de Waal (ZOOM Manager), and Giacomo Rossi and Michele Ruta (website managers). The website www.greenchemistry.school provided the latest information on application for students, selection results, abstract submission, poster presentation, programme, entry visa-related information, lectures, etc., and was the key platform to communicate effectively with lecturers and students.

Figure 1. The Organizing Committee: from left, Mirabbos Hojamberdiev, Fabio Aricó, Aurelia Visa, and Pietro Tundo

The Summer School was internationally followed and widely advertised by IUPAC, which issued press releases daily (https://iupac.org/brief-from-ssgc2021/)

In total, 170 applications from postgraduates were received and 130 were considered eligible to attend the Summer School after a rigorous selection conducted by nine members of the International Scientific Committee by strictly followings the set criteria: CVs, publications, recommendation letters from their supervisors, motivation letters, *etc*. From these 130 selected postgraduate attendees coming from 39 different countries, 15 PhD students attended in-person in Venice. From the 34 lecturers from all over the world, 10 participated in-person and delivered their lectures in Venice.

The program of the Summer School included 13 scientific lecture sessions and 8 poster sessions on the following main topics:

1. Exploitation of renewable resources,
2. New reaction pathways,
3. Energy saving,
4. Food safety,
5. Climate Change damages mitigation,
6. Education, and
7. Health.

In the morning before scientific sessions, various sponsors and institutions also delivered their talks. After each scientific lecture session, 30 minutes were given for questions and answers mixing input from both online and in-person participants.

Welcome Address and Opening Remarks

The welcome address and opening remarks were delivered by

- Pietro Tundo;
- Salvatore Orlando, Director of the Department of Environmental Sciences, Informatics and Statistics (DAIS);
- Christopher Brett, IUPAC President and Professor of Chemistry at University of Coimbra, Portugal;
- Andrey Guryev, CEO of PhosAgro, Russia; Natalia Tarasova, Director of the Institute of Chemistry and Problems of Sustainable Development, Mendeleev University of Chemical Technology of Russia; and
- Sandra Averous-Monnery, Programme Officer at the United Nations Environment Programme (UNEP)

Figure 2. Some of the in-person postgraduate attendants with Organizing Committee

The detailed day-by-day program is documented in a full report available under https://www.greenchemistry.school/programme/ and in the daily brief at https://iupac.org/brief-from-ssgc2021/

Poster Awards

In total, 79 posters were received, and the postgraduate attendants were given the opportunity to present their research over multiple sessions; 13 posters were presented in-person. The Jury, chaired by Neil Coville, Emeritus professor of University of the Witwatersrand, Johannesburg, South Africa, had the challenging task to review all the posters both online and in-person and was struck by the originality and scientific relevance of the research presented. Ultimately, 11 posters were awarded: four of them in-person were awarded 500 € each by PhosAgro; they were (in alphabetical order):

- **Felipe Sanchez Bragagnolo**, Faculty of Agricultural Sciences, São Paulo State University, São Paulo, Brazil: *A green approach to valorize soy agro by-products*
- **Monika Horvat**, University of Ljubljana, Faculty of Chemistry and Chemical Technology, Slovenia: *Selective Oxidative Cleavage Of C-C Double Bond By Hydrogen Peroxide*
- **Mohammed Kadhom**, Department of Environment, College of Energy and Environmental Science, Alkarkh University of Science, Iraq: *Improving the Performance of TFN Membranes by Incorporating UiO-66 and MIL-125 MOFs Nanoparticles Used for Water Desalination*-
- **Manar M. Taha**, Energy Materials Laboratory, School of Sciences and Engineering, The American University in Cairo, Egypt: *Controlled Fabrication of Mesoporous Electrodes with Unprecedented Stability for Water Capacitive Deionization Under Harsh Conditions in Large Size Cell*

Seven online poster award winners were (in alphabetical order):

- **Luca Filippi**, Karlsruhe Institute of Technology (KIT), Karlsruhe, Germany: *Fully renewable NIPUs via thiol-ene polymerization*
- **Stephanie A. Fraser**, University of KwaZulu-Natal, South Africa: *A novel solvent-based approach towards luminescent cellulose paper*
- **Giulia Rando**, Department ChiBioFarAm, University of Messina, Italy: *Pillararene-Based PES blended polymers: Design, Preparation and Sustainable Applications*
- **Caterina Rovegno**, Department of Chemical, Pharmaceutical and Agricultural Sciences, University of Ferrara, Italy: *Efficiency improvements of CO_2 utilization: the case of styrene carbonate synthesis in microdroplets conditions*
- **Solange M. Selzer**, Physical Chemistry Department, Faculty of Chemistry Science, Universidad Nacional de Córdoba, Argentina: *Study of Toxicity and Cellular Uptake of Magnetic Nanoparticles With Different Coatings*
- **Gabriele Soriano**, Department of Chemical Sciences, University of Naples Federico II, Naples, Italy: *Plant metabolites as stimulants and/or inhibitors of parasitic plant seed germination*
- **Yanru Zhang**, Institute of Chemistry, Chinese Academy of Sciences, P.R. China: *Synthesis of Higher Carboxylic Acids via the Hydrocarboxylation of Alcohols with CO_2 and H_2*

Closing Remarks

The closing remarks were given by Christopher Brett, IUPAC President, who expressed his thanks to the organizers; and by Marco Bella, Member of Parliament of the Italian Republic in the Chamber of Deputies and Professor at La Sapienza University of Rome. Bella underlined the crucial role of a better university education and the need to create a better world not producing "more", but rather producing "better." At the end, Aurelia Visa delivered relevant statistics associated with countries, gender, scientific output, awards, grants, etc. about this Summer School attendance. It was announced that the 14th Green Chemistry Postgraduate Summer School will be held online/live and in-person 3-8 July 2022 in Venice, Italy.

Conclusion

The experience from the past 13 editions of the Summer School on Green Chemistry, held from 1997 to 2021 with more than 1000 postgraduate students attending, tells us that young chemists are interested in Green Chemistry and understand the important role of Green Chemistry in building a sustainable society. Green Chemistry is a good key for students to look around scientific disciplines and decide how and where to go forward using Green Chemistry principles. From the outcomes of this latest hybrid Summer School, we learned how to manage the future Summer Schools in a hybrid format, giving a very valuable opportunity to the postgraduate students from emerging nations, who cannot afford travelling to attend in person. This Summer School represents a turning point for a new kind of outreach and capacity building, considering the high quality of scientific contributions, the Green Deal, and a fast scientific progress in developing countries. Our ultimate goal is to make the Summer School a permanent event to be held every year in Venice, Italy. Thanks to the involvement and active participation of outstanding lecturers, partners, and sponsors, we hope to achieve this goal in the near future.

Acknowledgments

The Summer School was organized and managed by the Green Sciences for Sustainable Development Foundation (www.gssd-foundation.org), a non-profit organization based in Venice, Italy, in collaboration with IUPAC, Ca' Foscari University of Venice, and the Italian National Commission for UNESCO Roma. The Summer School was also endorsed by the Ministero della Transizione Ecologica, UNESCO-UNITWIN "Green Chemistry Excellence from Baltic Sea to Mediterranean Sea and Beyond, European Chemical Society, Associazione Italiana per la Ricerca Industriale, The World Academy of Sciences (TWAS), and Patrocinio Regione del Veneto, and Citta' di Venezia. The Summer School was financially sponsored by the Organization for the Prohibition of Chemical Weapons (OPCW), PhosAgro, the Royal Society of Chemistry, and GreeNovator.

Mirabbos Hojamberdiev <hmirabbos@gmail.com> is from Uzbekistan-Japan Innovation Center of Youth, Uzbekistan and Technische Universität Berlin, Germany; Aurelia Visa is from the Romanian Academy, "Coriolan Drăgulescu" Institute of Chemistry, Romania and a member of the IUPAC Interdivisional Committee on Green Chemistry for Sustainable Development (ICGCSD); Fabio Aricó from Ca' Foscari University of Venice, Italy; and Pietro Tundo is President of Green Sciences for Sustainable Development Foundation and Chair of ICGCSD.

https://www.greenchemistry.school/

Congress of the Slovak & Czech Chemical Societies

by Milan Drábik

The 73rd Annual Congress of the Slovak & Czech Chemical Societies, held 6-10 September 2021 in High Tatras, Slovakia, attracted nearly 400 participants who presented and discussed the large scope of topics and achievements of chemistry research in Slovakia and Czech Republic. The program comprised an exclusive plenary lecture by Pavol Čekan on Development of quantitative and multiplex diagnostic technologies and application, and several invited lectures, lectures, and posters.

As an on-going tradition, the organisers were eager to award IUPAC Poster Prizes to the best posters and as before, they proceeded with the challenging task of reviewing and judging all the submissions. The IUPAC Poster Prize is aimed to PhD students and chemists younger than 40 years, thus poster presentations of 107 young colleagues (from among the total number of more than 200 posters) have been monitored and evaluated with the aim to choose two posters and authors to be awarded. Members of the ad-hoc monitoring and evaluating committee have been Jan John, president of Czech Chemical Society, Eva Víglašová, guarantee of the poster sessions of the Congress, Pavol Čekan, and Milan Drábik, chair of Slovak National Committee of IUPAC. After two evenings of viewing posters and discussions with authors, the committee decided to award and present the certificates to:

- **Klaudia Kvaková,** PhD student at Institute of

Organic Chemistry and Biochemistry of the Czech Academy of Sciences, Prague, Czech Republic: *Fluorescent Nanodiamonds Modified With Biocompatible Polymers*

- **Elena Kupcová,** university teacher at Department of Chemistry of the Matej Bel University, Banská Bystrica, Slovakia: *Sample Pre-Treatment and Determination of* Polycyclic aromatic hydrocarbons *Mixture in Different Types of Matrices*

Klaudia Kvaková explains the theme of her research and poster: Sentinel node(s) (SN) mapping became the standard procedure used in cancer diagnostics. However, agents commonly used to map the nodes have several major drawbacks. Fluorescent nanodiamonds (FNDs) are biocompatible materials that exhibit unique optical properties enabling their visualization in biological systems and thus could replace the now commonly used agents. Here we focus on the preparation of FNDs labelled with D-mannose for SN visualisation. It has been also shown that these particles interact specifically with macrophages, which are retained in the lymphatic nodes providing their clear imaging contrast.

Elena Kupcová gives insight into the theme of her research and poster: Polycyclic aromatic hydrocarbons (PAH) are very persistent organic contaminants found not only throughout the whole spectrum of environment such as soil or water, but are also carefully monitored in the food. The poster presents analytical methods applicable to the determination of 18 PAHs in water, soil and meat samples; the data acquired by three extraction methods (Soxhlet extraction, solid-phase extraction, liquid-phase microextraction) and two chromatographic methods (high-performance liquid chromatography coupled with fluorescent and UV detection, gas chromatography coupled with mass spectrometry) are compared.

The 53rd International Chemistry Olympiad in (Virtual) Japan

by Nobuhiro Kihara

The International Chemistry Olympiad (IChO) is an annual competition for talented students who are interested in chemistry. Nations around the world send a delegation of up to four students at the secondary school level along with two pedagogically professional mentors. In a usual IChO, the participating students are tested on their chemistry knowledge and skills in a five-hour laboratory practical examination and a five-hour written theoretical examination.

The IChO program is intended to stimulate students' interest in chemistry through solving creative chemical problems that are both practical and theoretical. It also aims to promote international contacts in chemistry, friendships between young chemists of different nationalities, cooperation among pupils, and exchange of scientific experiences in chemistry. The first IChO was held in the former Czechoslovakia in 1968, and the event has been held every year since then. The delegations that attended the early events were mostly countries of the former Eastern Bloc, and the event was not held outside the Bloc until 1980 when it was held in Austria.

All participants are ranked according to their individual scores, and no official team scores are given. Gold medals are awarded to the top 10 % of students, silver medals are awarded to the next 20 % of students, and bronze medals are awarded to the next 30 % of students. Honorable mentions are awarded to the top 10 % of non-medalist students.

The IChO is composed of three key elements:

Examination

Chemistry is an experiment-based science, with every theory coming out of the laboratory. Therefore, both theoretical and practical examinations play important roles in the IChO.

Japan held the 53rd IChO in July 2021. It was originally planned to follow the 2020 Olympic and Paralympic Games in Tokyo. We anticipated that popular interest in chemistry would be enhanced by a scientific Olympiad being held after the excitement of a sporting Olympiad. When we heard the first reports of COVID-19 early in 2020, it appeared to be a minor concern. Despite the virus being thought of as causing a new kind of cold, we knew that the common cold is inactive in summer when the IChO was to be held. However, shortly after the pandemic spread across the globe, it became evident that COVID-19 was active

in summer, too. The 2020 Olympics and Paralympics were postponed for one year, and so was the IChO in Japan. Instead, in 2020, the 52nd IChO was held remotely for the first time and organized in Istanbul, Turkey <https://icho2020.tubitak.gov.tr/>

Communication

Talented students from all over the world come together to take part in the IChO. Conversation, cooperation, and communication with each other provide a great opportunity for promising youngsters to enjoy international experiences and to make friends with other participants via their common interest, chemistry.

Culture

The venue chosen for the 53rd IChO, the Kansai area, is 500 km from Tokyo and was the ancient capital where according to Japanese legend, the first government of Japan was established 2681 years ago. Several places were to be visited, including not only very old temples but also state-of-the-art scientific institutes.

In the middle of January 2021, the Organizing Committee (OC) of the 53rd IChO met with the Steering Committee (SC) via Zoom. Two proposals were discussed: one for an in-person Olympiad and one for a remote event. Unfortunately, it was already clear that all the elements of the IChO described above could not be included in an in-person IChO during the COVID-19 pandemic, due to difficulties in travelling and the need for social distancing.

The first priority being of course the safety of all participants, it was ultimately decided to hold the 53rd IChO as a remote event. The SC approved a remote IChO at its second meeting at the end of February. In this remote IChO, the competition only involved theoretical problems, and the students attended the examination from their own countries. Most of the elements essential to the IChO would be lost in the remote IChO, which was very disappointing. Even in a remote format, however, the important features of IChO must be maintained as much as possible. The participating students must have extraordinary experiences. Therefore, the Organizing Committee incorporated several activities and communication tools into the 53rd IChO to cover these important features:

Examination

In order to reinforce the importance of laboratory work, the practical tasks prepared for the 53rd IChO were made open, despite not being officially approved by the International Jury meeting for the 53rd IChO. The Organizing Committee prepared videos in which all tasks were demonstrated with explanations and published the videos as one of the activities during the event.

The OC would be delighted if those who are inspired by the demonstrations prepare and submit their original videos in which they attempt the practical tasks and discussions. Reports on the tasks will also be highly welcome.

Communication

OC prepared a virtual reality (VR) space for communication. When participants accessed the VR space, their avatars were created. Everyone could participate in events and activities via their avatars. In the VR space, there were venues in which avatars could enjoy close conversations, cooperation, and communication with others.

Culture

IChO participants were offered virtual visits to several locations, including Nara City, Osaka City, Kyoto City, and Himeji Castle. However, the OC added some that are very interesting to experience but not suitable for in-person visits due to hazards, sensitivity, space limitations, or language difficulties. SPring-8, a large synchrotron radiation facility that delivers the most powerful synchrotron radiation currently available, is one of the most interesting places in the Kansai area for the participating students of the IChO in particular. However, it is very difficult to visit SPring-8 as an activity in the IChO due to space limitations inside SPring-8 and the sensitivity of its advanced instruments. A workshop for preserving cultural assets, for example, repairing an image of Buddha, is another interesting place where modern chemistry is applied to very old subjects, although it is again very difficult to physically visit such a workshop because of the sensitive work, space limitations, and language difficulties. In the 53rd remote IChO, the participants virtually visited these highly restricted locations to experience more interesting cultural tours than would otherwise be possible.

The opening ceremony started at 15:00 JST on 25 July. The participants could access the ceremony via either the VR space or the usual video streaming. Over 200 participants entered the VR space to enjoy the realistic ceremony.

The first version of the theoretical problems was published at 21:00 JST on 25 July. It should be noted that 21:00 JST is almost the only time window to permit cooperation all over the world: 21:00 JST is 24:00 for the easternmost country, New Zealand, and 9:00 for the westernmost country, Costa Rica. Therefore, most of the programs were scheduled at 21:00 JST.

The OC sought comments on the problems from mentors, revised the problems according to the

comments, then proposed a second version of the problems for finalization to the international jury meeting, the body that decides matters regarding the IChO that bind both participants and organizers. The jury meeting started at 21:00 JST on 26 July and finished around 2:00 JST on 27 July. The OC revised the problems according to the decisions of the jury meeting and published the official final version at 9:00 JST on 27 July. Next, the mentors started to translate the official English version into the individual local languages for their students. All delegations finished their translations by 9:00 JST on July 28.

It should be noted that 60 hours elapsed from the publication of the first version of the problems to the deadline for translation. Of course, contact between mentors and students after the publication of the problems was clearly prohibited in the competition guidelines. If a mentor wanted to cheat, for example, passing on the problems and solutions to his or her students, we could not prevent it. However, the OC trusted in the professionalism and the pride of mentors. If a mentor had said to their students, "Hey, I'll tell you the problems and solutions, then you'll all get gold medals," they would lose the respect of their students. As expected, there were no suspicious results in the scores obtained, confirming that the IChO community is strong and ethically healthy.

The translated versions of the problems were made available to the invigilators at 9:00 JST on 28 July. The invigilators downloaded and printed out the problems for the students by the starting time of the examination. The invigilators are a crucial component of the remote examination. The OC asked country delegations to appoint invigilators who are independent of the mentors, have no relationship with students and have no other activity in the 53rd IChO. Invigilators were to be socially well-established persons such as school principals and should not be a parent or a relative of a student. For the same reason, the examination location should be a public place such as a school, and the OC requested that each country choose a single location.

Unfortunately, restrictions on movement were severe in some countries during the period for the 53rd IChO. Further, some students had to quarantine because their close relatives were infected by COVID-19. In such urgent circumstances, the OC allowed these students to take the examination in their homes, invigilated by their parents. The relevant delegations were asked to guarantee the fairness of the examination, and all delegations worked hard to make the students' homes suitable as examination locations.

A total of 309 students took the examination, while three students were absent. All examination locations were inspected beforehand via Zoom and were monitored and recorded throughout the examination via Zoom.

The earliest examination started at 12:00 JST on 28 July in New Zealand, the easternmost country, and the last examination started at 24:00 JST in USA and Costa Rica, the westernmost country. The examination time was 5 hours. Participating students were not allowed to use any communication devices or computers during the period 19:00 to 24:00 JST to avoid any ill-intentioned communication via the Internet or social media. All these requirements were controlled by the invigilators.

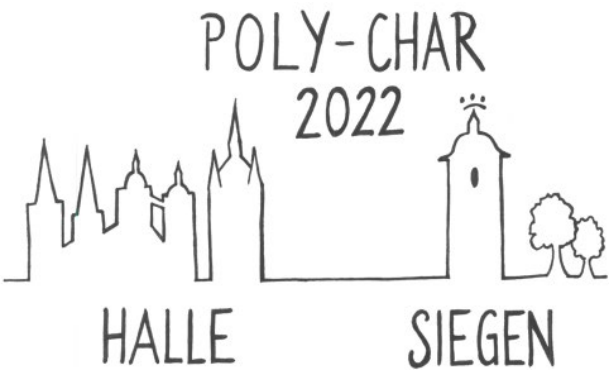
After the examination, the invigilators sorted the answer sheets by page numbers, scanned them to prepare PDF files for each student, and submitted them to the OC. After all answer sheets were received, the OC started marking.

After arbitration of the marking, the scores of all students were finalized, and the medals were allocated. The final results were announced in the closing ceremony at 21:00 JST, on 2 August, which was held also in VR and later published as a streaming video. Even after the closing ceremony, the participants could still enjoy virtual tours in VR.

After several events over the period of 11 days, the 53rd IChO was successfully completed. The 53rd IChO was financially supported by IUPAC, which we gratefully acknowledge. This support from IUPAC was used to subsidize participation fees for some countries that were facing economic difficulties. This year, there were several countries experiencing economic difficulties due to the COVID-19 pandemic.

At the end of this report, we wish to again congratulate all participating students. Some received medals, and some did not. However, they all tried their best to tackle the same chemical problems. When these youngsters meet again as the leaders in the field of chemistry, will they talk about the days of the 53rd IChO? We will be deeply honored if the 53rd IChO becomes one of the career milestones marked by the excellent chemists of the future.

Nobuhiro KIHARA was vice-chair of Executive Committee and vice-chair of Science Committee for IChO2021; he is professor at the Department of Chemistry at Kanagawa University, Japan



POLY-CHAR [Halle|Siegen] 2022

POLY-CHAR [Halle|Siegen] 2022 will take place as an all-digital online meeting and aims at building bridges in polymer materials science by spanning the gap between the COVID-pandemic affected to the post-COVID period that we hopefully all witness very soon. In particular, the meeting shall bridge the previous meetings in the longstanding series with annual conferences and associated short courses, specifically POLY-CHAR [Venice], which eventually had to be held as digital meeting with a one year delay in 2021, and the upcoming POLY-CHAR [Auckland] 2023.

POLY-CHAR [Halle|Siegen] 2022 is scheduled for 22-25 May 2022, with a short course on polymer characterization on 22 May, followed by the conference program with lectures and posters on 23-25 May. The online program features, in addition to numerous contributed and invited talks, plenary lectures by leading scientist in the field—prize winners as well as brilliant researchers in the early stages of their careers.

The annual forum brings together researchers, including senior professors, young scientists, students, and experts from industries as well as from academia. Scientists involved in experiments, theory, and computer simulations can work together to achieve a systemic understanding of connections between structures, interactions, and properties of polymers. Thematically POLY-CHAR [Halle|Siegen] 2022 encompasses all areas of polymer-related research with dedicated highlight sessions on *Polymers for Circular Economy* as well as *Polymers for Health,* including biopolymers in nutrition and health.

From the beginning one of the important aims of this conference is to put a special emphasis on international collaboration, promotion of young scientists and collegial environment. Hence it gives a forum also to young scientist to present their results and meet with distinguished scientists from all over the world.

Contact **Sven Henning**, <sven.henning@imws.fraunhofer.de> Fraunhofer Institute for Microstructure of Materials and Systems IMWS, 06120 Halle (Saale), Germany or **Holger Schönherr <**schoenherr@chemie.uni-siegen.de>, University of Siegen, Department of Chemistry & Biology & Research Center of Micro and Nanochemistry and (Bio)technology (Cμ); Physical Chemistry I,57076 Siegen, Germany.

https://poly-char2022.org/

MACRO 2022, the 49th World Polymer Congress

Come join one of the world's largest gatherings of polymer scientists and engineers to share the latest advances. MACRO 2022 will be held from 17-21 July 2022 in Winnipeg, Canada

The abstract portal is now open to receive abstracts for oral presentations and posters for the following themes:

1. Polymer synthesis and kinetics
2. Polymer physics and characterization
3. Polymers for biomedical engineering
4. Polymers for nanotechnology
5. Smart and functional polymers
6. Polymers from renewal resources and biodegradable polymers
7. Polymer engineering and rheology
8. Polymers for energy and environmental applications

In addition, we welcome abstracts for the following two special technical sessions:

- Porous Polymers
- The Fate of Polymers in a Changing World

Please visit https://www.macro2022.org/call-for-abstracts/ to submit abstracts.

We continue to base our planning on an in-person conference. However, in the event the addition of a virtual component to MACRO 2022 is justified, all accepted abstracts will be honoured.

We look forward to your contribution to make MACRO 2022 an engaging event.

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