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A Year of Young Elements

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INTERNATIONAL UNION OF
PURE AND APPLIED CHEMISTRY

Sustaining Active Learning in Virtual Classroom ►

Blockchain Technology ►



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

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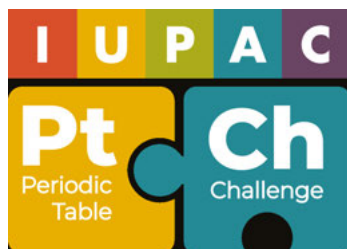
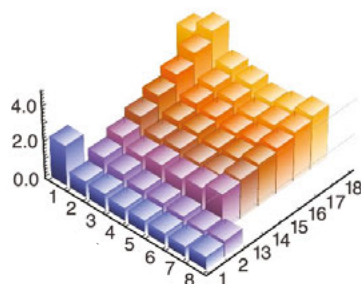
Cover: In 2019, in celebration of the 100th anniversary of IUPAC and the International Year of the Periodic Table, IUPAC and International Younger Chemists Network (IYCN) created the Periodic Table of Younger Chemists honoring a diverse group of outstanding younger chemists from around the world who embody the mission and core values of IUPAC and highlight the diversity of careers, creativity, and dedication of the young chemists leading the community into the next century. See feature page 3.

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IUPAC during COVID-19

by Colin Humphris

I have just been listening to an intriguing debate that is underway in the UK. The theme was how to come out of lockdown, to both restart the economy and protect public health whilst the SARS-

CoV-2 virus is still out there. Effective treatments and vaccines have yet to be proven. I am sure similar discussions are underway in many countries across the world. It underlines the anxieties and uncertainties we all face with regards our health, our families and friends, our finances and our work. This is at a time when the international chemistry community is mourning the premature passing of friends, colleagues and loyal servants.

IUPAC is not immune to this uncertainty. It is having to adjust to working during the pandemic and considering how it can remain effective in the future. As Treasurer it won't surprise you to know that I worry about the financial implications for the Union. There is an expectation of a deep recession and only a slow return to a semblance of normality. The new "Normal" may be very different. Governments are taking on substantial debt to protect their economies. This will need to be repaid potentially limiting future funding for science.

It is however also clear that there will be opportunities as we design and implement new ways forward at a time of disruptive change. The good news is that the reports to Bureau in April underlined a very high level of activity throughout the Divisions and Committees, working virtually through various digital media.

Bureau highlighted a number of issues that are worthy of debate and I want to encourage all chemists to contribute to this:

- This is a time when analytical standards, unambiguous nomenclature and reliable, critically evaluated data will be invaluable for diagnostics and testing, supporting vaccine development and ensuring the maintenance of standards throughout key supply chains including food. Bureau agreed a work group to identify how IUPAC can best assist the UN bodies in the front line including the World Health Organisation (WHO).
- Many international conferences and meetings have been cancelled or postponed this year. Some are already proceeding virtually. In the future, people

may be reluctant to attendance of international meetings in person, have difficulty finding travel insurance, and cheap, convenient flights. How should such meetings be redesigned to make them more worthwhile, to make physical presence far more valuable than simply attending virtually? Alternatively, how can we enhance virtual meetings to provide better networking opportunities and ways to develop relationships that are otherwise lost.

- The return to practical research work needs to be safe. There is experience out there and IUPAC may be able to help by facilitating sharing of this and proven practice in other sectors. Webinars are being suggested on this subject.

During the biennium 2018-19 IUPAC made an operating loss of US \$350k and adjustments were already in place to address this unsustainable position including the extensive use of virtual meetings. I am however anticipating further:

- Pressure on subscriptions as governments economise and reprioritise their expenditure. Chemists should continue to encourage their National Adhering Organisations to support IUPAC and also consider joining IUPAC themselves through the Affiliate Membership Program (AMP) or for industry through the Company Associate (CA) program.
- Loss of publishing income as a result the postponement of conferences and delays in publishing of their proceedings in *Pure and Applied Chemistry (PAC)*. We need to be creative to ensure a steady flow of content for *PAC*.
- Increasing costs of travel as the airline industry restructures.

We will be seeking additional income through sponsorship of activities such as the Periodic Table Challenge 2.0. We are proceeding with the creation of the Centenary Endowment Fund to support our strategic priorities. We fortunately also have a Review Team whose work is already underway. Their objectives are to recommend:

1. Directions for the scientific work of the union going forward, and how to structure the Union to achieve its scientific objectives.
2. Ways of working that would reduce costs and improve efficiency.

The Covid-19 pandemic provides additional context, impetus and urgency to the team's work. Please look out for opportunities to contribute to the Review or offer feedback, and please stay safe. 

Reflecting on a Year of Elements

by Lori Ferrins, Christine Dunne, João Borges, and Fun Man Fung

The Periodic Table of Younger Chemists (PTYC) arose from a group of aspiring scientists in attendance at the 2017 World Chemistry Leadership Meeting in Sao Paulo, Brazil. This project was a celebration of the 100th anniversary of IUPAC and the International Year of the Periodic Table. IUPAC and the International Younger Chemists Network (IYCN) joined forces to create the PTYC and honor rising stars in chemistry from around the world. Beginning in July 2018 and ending in July 2019 at the World Chemistry Congress, we unveiled and honored a diverse group of 118 outstanding younger chemists who embody the mission and core values of IUPAC. The resulting Periodic Table highlights the diversity of careers, outreach participation, and dedication to the chemistry community of those leading us into the next century of IUPAC.



Jovana Milic
Scientist, École
Polytechnique Fédérale de
Lausanne, Switzerland



Xuefeng Jiang
Professor, East China Normal
University, China

Dubnium: "This platform uniquely recognizes the contributions of young scientists beyond research excellence, including the commitment to education, international collaborations, and fostering diversity. I wish there were more initiatives that highlight these aspects in the development of young professionals as I believe that, if this was the case, we would be living in a better world!"

Sulfur: "I am proud to represent sulfur, having established **3S** (Smell-less, Stable and Sustainable) green sulfuration with a set of new sulfurating reagents and corresponding methodologies. I am an active contributor to IUPAC via organic chemistry achievements and outreach to the community of scholars and industry

and benefited from the activities of IUPAC through academic exchange with other members in the global younger chemist community."

Each month for a year, there was immense collaboration and discussion regarding the achievements of the *hundreds* of nominees. To say this was a challenging task would not be giving it the true credit all the elements deserve. Everyone who was nominated was exceptional, including those who were nominated and not awarded an element. We were, and continue to be, impressed by the depth, breadth, and ambition of the younger chemists within the chemistry community.

This project was designed to open a line of communication to cross borders, tackle sustainability issues, and collaborate across labs, cultures, and professions. We are only as strong and capable as those we surround ourselves with and this group of 118 younger chemists is primed and ready to uphold the task of spearheading the development and leadership for the future of their respective chemical societies, and the one we all share together: IUPAC.

Cobalt: "I have developed long standing networks within the global chemistry community. Through these networks, I have found supportive research collaborators and funding opportunities that have served to support not only my own career but that of my students as well."

Argon: "Being selected as an element communicated that recognition and appreciation of my "little" contribution to the advancement of Chemistry. It has also catalysed my involvement with IUPAC activities. I am exploring avenues of making more impact."

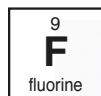
Cynthia Ibeto
Senior Lecturer, University of
Nigeria Nsukka, Nigeria



Sadhna Mathura
Lecturer and Academic
Coordinator, University of the
Witwatersrand, South Africa



A Year of Young Elements

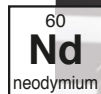


Fun Man Fung
Assistant Director (Education)
& Chemistry Instructor, National
University of Singapore

Fluorine: "I had not heard about the IYCN until I was introduced to the PTYC. I chanced upon the PTYC on Twitter when researching ways to celebrate IYPT2019 at my local university. Sensing that it was a great opportunity to promote chemistry and science, I forwarded these to my friends and colleagues in Japan and Taiwan, whom I served together with on the International Chemistry Olympiad (IChO)

Steering Committee. I discovered more about the IYCN through the website and learned that I shared a similar philosophy! I was incredibly happy to learn that such a volunteering group exists that espouse mentorship for the younger chemists in the world."

The celebration of the PTYC through its collaboration with IYCN and IUPAC, was so important to highlight the strength of the young chemists around the world. We quite literally bonded over this shared connection which crossed international borders. The strong network fostered by the close-knit collaboration of IUPAC and IYCN, under this unifying project, has done an impeccable job in connecting like-minded leaders to unite and shape our futures together.



Marian Asantewa Nkansah
Senior Lecturer, Kwame
Nkrumah University of
Science & Technology, Ghana

Neodymium: "I was in Paris for my first IUPAC Congress in 2019. Participation opened me up to the structure of IUPAC and how it runs. I was invited to join the Chemistry and Environment Division of IUPAC. As part of the process, my application to be an Affiliate of IUPAC has been accepted. I am looking forward to contributing at the Division level."

Rubidium: "My knowledge on the role and worldwide impact of

IUPAC on our daily lives' dates to my basic and high school studies in which my interest in the Chemical Sciences flourished. I became familiar with IUPAC as the world recognized scientific organization on chemical nomenclature and terminology. More recently, I wanted to increase my involvement and contribute to IUPAC's goals by addressing the 2030 United Nations Sustainable Development Goals, as well as by sharing my passion and spreading scientific knowledge on the interdisciplinary field of chemistry and its impact via science outreach and public engagement activities.

In 2018, when I heard about the IYCN, which is an affiliated organization of IUPAC that connects, supports and advocates for chemists who are in the early stage of their career, I learnt different ways to contribute towards fulfilling the IUPAC goals. In fact, I promptly identified myself with the vision, mission, aims, projects, and activities launched by IYCN which led me to expressing my willingness to join the growing network.

I became familiar with the IUPAC100 PTYC launched by IUPAC and IYCN, in celebration of the 100th anniversary of IUPAC and the 2019 International Year of the Periodic Table and was selected as the representative of the element Rubidium for embodying the mission and core values of IUPAC. Such recognition enabled me to connect with, and learn from, many younger chemists' element awardees from across the globe at the 47th IUPAC World Chemistry Congress (47th IUPAC WCC). This was my first ever IUPAC WCC, which allowed me to significantly strengthen my bonds with IUPAC, proudly acting as a "young ambassador" of the organization and contributing to aid in fulfilling its noble goals and shaping the future of chemistry worldwide.

IUPAC2019 also featured the IYCN General Assembly in which I was honored to represent Portugal as a delegate and had the opportunity to actively and effectively contribute to redefine the mission and vision of IYCN. The IYCN General Assembly was a very enriching meeting in which I was fortunate to meet, interact, and learn from many younger chemists from countries worldwide. The General Assembly also raised my willingness and desire to keep on fighting (and volunteering) toward supporting, connecting, advocating,



João Borges
Research Fellow,
University of Aveiro, Portugal

A Year of Young Elements

and empowering young chemists to progress and fulfill their career goals.

Everyone has a voice within IUPAC, and we should all contribute toward its shared mission with IYCN by aiding in the development of a common language for chemistry."



Lori Ferrins

Research Assistant Professor
Northeastern University,
United States of America

Nickel: "Being named "Nickel" in the PTYC introduced me to IUPAC and all of the opportunities that it presents. Attending my first General Assembly was an enriching experience, giving me a chance to explore many of the projects that IUPAC champion. As a result of these experiences, I have developed a keen interest in IUPAC, and I look forward to contributing to projects in the future."



Victor Sabanza

Undergraduate Student,
University of La Rioja, Spain

Meitnerium: "As an undergraduate student, being here is an outstanding honour. However, the most impressive fact is that I was selected for sharing my passion for Chemistry and the Periodic Table with younger students. I believe inspiring other people and being inspired by others is key to science."

This project is just the beginning of not only empowering younger chemists within the IUPAC community but also a continued collaboration between IUPAC and IYCN. The bonds made throughout 2019 will continue to grow and we intend to nurture this network of outstanding younger chemists with several initiatives.

We are working to develop a webinar series, featuring presentations from the awardees of the periodic table. We want to give the outstanding younger chemists an opportunity to talk about their research and contributions to the chemical science community. This series would then culminate in a face-to-face meeting at the IUPAC congress in 2021 (iupac2021.org/).

The collaboration and in-person leadership development at the IUPAC World Chemistry Congresses will continue to be cultivated in the years to come. The IUPAC 2021 WCC in Montreal, Canada will be the first opportunity for the legacy of the PTYC to continue. We hope to provide a platform in which the awardees can share their research, career developments, and future outlook for the IUPAC community. By continuing to honor these outstanding chemists we will be able to show how the power of a diverse community, in collaboration with IYCN, can impact not only IUPAC, but also the greater scientific community. Our crystals are just beginning to form, and we are so excited to see them grow. In April 2020, a new IUPAC project highlighting the activity and engagement of the Periodic Table of Younger Chemist awardees with the IYCN and IUPAC has been initiated. See project 2020-012-2-020 (<https://iupac.org/project/2020-012-2-020>) for details and updates.

Lead: "There are many talented young chemists in the world, and to be selected as one of the 118 elements was an honor; we are a symbol of the diversity of careers globally. I see the PTYC as an opportunity to keep in touch for future projects and collaborations and I am curious to see where our paths might cross again."



Torsten John

Ph. D. Candidate
Leipzig University, Germany

Congratulations to all the elements, and welcome to the IUPAC family! 🌐

<https://iupac.org/100/pt-of-chemist/>

Sustaining Active Learning in Virtual Classroom

by Fun Man Fung, Wei Heng Chng, Hui Ru Tan, and Magdeline Tao Tao Ng

Considering the SARS-CoV-2 outbreak and the suspension of many physical face-to-face (F2F) lessons due to the #StayHome measures, many educators have been mandated by schools and institutions to put their teachings online. Many are asking: “How do I lead my online class without losing student engagement?” and “How do I know if my students are understanding the lesson content in real-time?” [1] Despite the unprecedented disruptions to mankind, we need not be paralysed by the COVID-19 situations that besiege us as tertiary institution academics. Being educators, we should embrace this tumultuous crisis as an avenue to blaze a trail in online learning. As the coronavirus threat continues to crescendo, we have found glimmers of hope in some success to sustain active learning in our online classes.

Achieving Engagement with Students Remotely

Students may be distracted by any simultaneous household hustling in their homes. Hence, as we transitioned from physical F2F to online lessons, we faced the challenge of maintaining a similar level of engagement. We found that a three-pronged approach—maintain students-teachers interactions; plant regular checkpoints with live responses; and facilitate real-time collaboration amongst learners—were helpful to actively engage learners during the online lessons. In the next three subsections, we will share how the three aspects can be achieved using the various online platforms that we have experimented with.

Maintain Students-Teachers Interactions

Synchronous learning is more engaging than asynchronous learning [2]. Synchronous learning usually adopts the usage of webinar tools such as Zoom, Google Hangout Meet, and Microsoft Teams. We used Zoom because it was linked to our learning management system at the National University of Singapore (NUS).

There were around 170 students and each lesson lasted for 90 minutes. The lessons were led by a teaching team that comprised a lecturer and teaching assistant (TA). To promote interactions with the teaching team, we encouraged students to engage on the chat-box. In every class, a TA moderated the live chatbox and could clarify students' doubts instantly. If there were many questions raised on a similar point, the TA would sound to the lecturer to clarify before moving on with the lesson. Despite losing the physical interactions, we observed that students asked more questions using the online chatbox [3]!

Plant Regular Checkpoints with Live Responses

Real-time responses were valuable in helping us understand students' grasp of the knowledge. These live responses enabled us to tailor the subsequent lessons to suit students' level of understanding of the concepts and keep them engaged. To obtain real-time responses from students, we planted unannounced checkpoints using short quizzes and polls. We found success with PollEverywhere (PollEv). We used PollEv to administer quizzes/polls and obtain real-time responses from students. Apart from PollEv, other interactive platforms such as Mentimeter, Kahoot!, and



Physical face-to-face lesson conducted before school closure (left) and online face-to-face class lesson (right)

Pigeonhole Live are also extremely handy in inserting such checkpoints.

Facilitate Real-time Collaboration amongst Learners

Whilst lessons are now conducted online, this does not mean the end of collaborative learning and group discussion! Breakout rooms, a built-in Zoom function, was used to divide the class into smaller groups of seven students at designated junctures. During this period, the teaching team visited the breakout rooms and facilitated the group discussions. In these breakout rooms, we encouraged the students to unmute their microphones so that they could discuss more efficiently with their peers. Screen sharing also facilitated collaborative learning. A typical group discussion lasted between three to five minutes, although additional time could be given when necessary. To encourage exchange of ideas within the class, an assigned leader from each group would share the key points of their discussions on Padlet, an online “whiteboard” the class can view publicly.

Team Teach!

One highlight of our unique lesson delivery has always been team teaching [4]. Team teaching is an element that piques students' interest. It exposes students with multiple perspectives on the subject matters and encourages students to critically evaluate each perspective [5]. Everyone in the teaching team could freely chime in their opinions on the subject matter. In addition, we invited guest lecturers to provide their expertise from another fresh perspective. We observed that students were highly engaged and were actively asking questions to our guest lecturers.

Conclusion

As we move away from physical F2F lessons due to such extraordinary times, educators can celebrate the use of technology in fostering an active online learning environment. By effectively using available online platforms, engaging lessons can be delivered while achieving meaningful interactions among the teaching team and students. There is no magic pill! We encourage educators to explore and iterate on various methods to make online learning more active in your own ways.

Acknowledgements

We appreciate the other team members including Prof. Robert Kamei, MD and Christian Chonardo for their support in shaping up a highly engaging online classroom with cinematic effects. We are grateful to NUS Libraries for their continuous support. 🏠



Working with a guest lecturer is a great way to bring a new perspective into a lecture. A host and TA can still help facilitate a lesson with proper social distancing.

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Fun Man Fung, <fun.man@u.nus.edu>, orcid.org/0000-0003-4106-3174, Department of Chemistry, National University of Singapore. Wei Heng Chng, NUS Graduate School for Integrative Sciences and Engineering, National University of Singapore and Department of Pharmacy, National University of Singapore. Hui Ru Tan, NUS Graduate School for Integrative Sciences and Engineering, National University of Singapore and Department of Food Science & Technology, National University of Singapore. Magdeline Tao Tao Ng, NUS Libraries, National University of Singapore.

Footnote.

On 3 April 2020, Fun Man Fung took part in a webinar titled “Tools to Thrive Remotely.” The session, organized by the International Younger Chemists Network (IYCN) in collaboration with European network EYCN, was part of a global conversation engaging CHEMISTS FIGHTING COVID-19. Recordings are available from <https://iupac.org/chemists-fighting-covid-19-a-global-conversation/>. Fun Man is part of a IUPAC project which aims to highlight the activity and increase the engagement of the Periodic Table of Younger Chemist awardees with IYCN and IUPAC (<https://iupac.org/project/2020-012-2-020>)

Blockchain Technology

Uses in Research and Communication

by Bonnie Lawlor

I first heard of blockchain technology at a conference in 2017 when Christopher Wilmer, Assistant Professor at the University of Pittsburgh and Managing Editor of *Ledger*, [1] gave a presentation on the technology. While he did mention Bitcoin and other cryptocurrencies with which the technology was originally associated, Wilmer's talk explained how his journal uses blockchain for proof-of-publication. He commented that as a data-storage mechanism, "blockchains are well-suited to be used in scholarly publishing because they are extremely resilient, tamper-proof, practically indestructible databases; there is no single point of failure or cost of operation; and there is an incontrovertible proof-of-publication date, even across countries and institutions whose incentives are not aligned (which is sometimes a point of contention for scientists racing to discover cure/new theorem/etc.)" [2].

Fast forward a year later and the momentum of blockchain's adoption was beginning to become apparent. At the 2018 NFAIS Annual Conference it was announced that a pilot project was soon to be initiated for the development of a protocol where information about peer review activities (submitted by publishers) would be stored on a blockchain. This would allow the review process to be independently validated, and data to be fed to relevant vehicles to ensure recognition and validation for reviewers—more about this later.

By that time I had become totally fascinated by the technology and the fact that it was being used outside of the financial realm—and equally curious to learn more about the technology—what it was and how it could be used as part of the process of scientific research and communication. So what is Blockchain Technology?

What is Blockchain Technology?

According to a recent report from the National Institute of Standards and Technology (NIST), "Blockchains are immutable digital ledger systems implemented in a distributed fashion (*i.e.*, without a central repository) and usually without a central authority. At its most basic level, they enable a community of users to record transactions in a ledger public to that

community such that no transaction can be changed once published." That same publication concluded that "The use of blockchains is still in its early stages, but it is built on widely-understood and sound cryptographic principles. Moving forward, it is likely that blockchains will be another tool that can be used to solve newer sets of problems..." [3].

The technology has the potential to dramatically improve the storage and tracking of such things as intellectual property/patents, health records, social security information, land titles, international borders, stocks/bonds/debts, and money (*i.e.*, Bitcoin). Blockchain technology is a bit of a dichotomy. On the one hand it is *not* a new technology; rather it is an innovative way of using existing technologies such as asymmetric key encryption, hash values, Merkle trees [4], and peer-to-peer networks [5]. But on the other hand, it can be perceived as an emerging technology as its uses are just beginning to be tested worldwide across diverse industries (life sciences, food safety, entertainment, healthcare, government, ethical trading, *etc.*) with some successes and some failures.

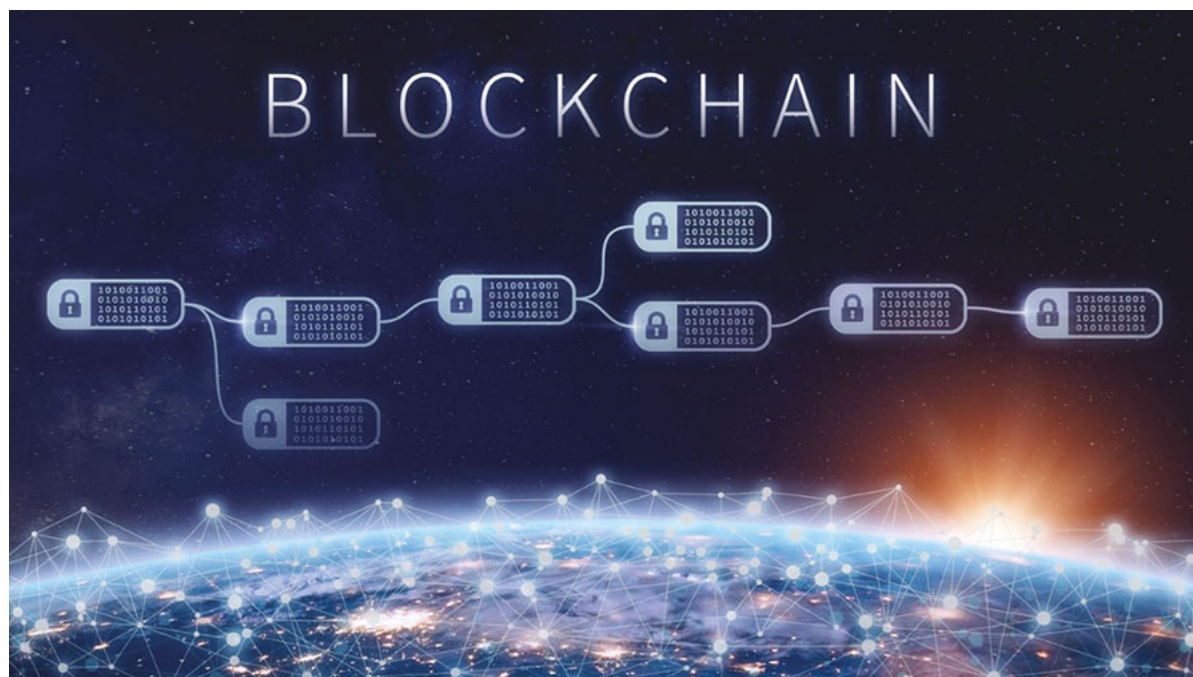
Why has this technology gained momentum in its adoption? According to an article in a recent issue of *MIT Technology Review*, it is because the technology itself "...is all about creating one priceless asset: Trust" [6]. The article talks about the history of the double-entry book-keeping method that dates back to the fourteenth century. It was established as a reliable record-keeping tool and became an integral part of the business culture. The downside was that it also allowed financial institutions to become powerful middlemen in global finances—something that continues to this day.

The fact is that "trust" is needed in all fields that are "controlled" by middlemen, including scientific communication. And blockchain technology—basically a list of transactions—is believed to hold the promise of trust even for non-financial "transactions." The following will give you a taste of some current blockchain applications in the area of scientific research.

Blockchain and the Researcher's Workflow

Research Funding

My initial curiosity about the technology drove me to attend a conference on blockchain for scholarly publishing in 2018 [7]. One of the presentations was on using the technology to manage the first step in the research process—funding. Knowbella Tech (see: www.knowbella.tech), is an organization that has a patented system and methodology for providing a decentralized



platform for connecting scientific researchers with funding sources via blockchain technology (see U.S. patent filing number 62/555,989). This platform was described as one that: 1) focuses on connecting members of an open-science community; 2) connects researchers with collaborators and/or funders; 3) generates decentralized electronic contracts; and 4) tracks the progress of research projects and directs payment of funds in awarded tranches.

They use “smart contracts” to manage grants. “Smart contracts” were defined as a computer program that is stored and runs on the blockchain. The contract defines a set of rules and procedures that relate to a binding agreement between parties just like a traditional contract, but unlike its paper counterpart, it can automatically enforce these obligations. An example of one of the smart contract rules with regards to a grant can be when the grant starts, ends, *etc.*, and it was noted that smart contracts can improve grant funding by changing the funding model for Open Science. As researchers are well aware, there are many steps in the grant process, including application submission and review, the selection step, background checks, and ongoing management of the grants that are awarded. KnowbellaTech believes that the use of blockchain both simplifies and speeds-up the process. It also enables scientific collaboration around the globe, allows researchers to share their research immediately, and gives grant funders and applicants direct access to one another.

Managing the Research Process

Another presentation was from ARTiFACTS, a company launched in March of 2018 that is using blockchain technology to build a ledger for research (see: <https://artifacts.ai/>). They have their own distributed ledger system (blockchain) that individual researchers can use, *free of charge*, to upload their research findings as they go through the research process from the very beginning all the way through to final publication. By doing so researchers have ultimate proof of their work and when it was done (entries are time-stamped). They can protect and manage their intellectual property while facilitating knowledge sharing, if and when they want to share; and they can get credit at any point for any type of research output—they do not have to wait until their research results are actually published.

ARTiFACTS also provides access and services for the institutions who support and partner with researchers such as universities, funders, publishers, and corporations engaged in research. Importantly for publishers, they make the supplementary research outputs of a paper accessible from the publisher’s platform by delivering the metadata and links connecting these research outcomes to a publishers’ digital production and dissemination systems. The objective is to ultimately create a “deep historical archive of published and discovered findings” that will be accessible to the broader scientific community [8]. It should be noted that in 2019 ARTiFACTS entered into an agreement with the

Max Planck Society and the Bloxberg consortium [9], to create a network infrastructure that is hosted by prominent research institutions spanning multiple countries. The network continues to expand as of this writing as new institutions decide to participate [10]. ARTiFACTS is a growing venture worth following.

Publishing

There were some interesting and theoretical proposals put forth at the conference regarding both the use of blockchain to allow individuals to “publish” their own research findings as well to participate in the creation of a universal citation index. Jason Griffey, at the time an Affiliate Fellow at Berkman Klein Center for Internet and Society, Harvard University, noted that a core attribute of blockchain is the fact that it is a decentralized system and therefore the roles of “middlemen” such as librarians and publishers are at question, for power will no longer reside in traditional places. He noted that currently good provenance is accomplished by the use of metadata that reflects the chain of ownership of files and physical objects. Such use facilitates the tracking of files over time, and it is pretty much under the control of the publishers. But enter blockchain and there now becomes the potential for users to create and control their own identity along with the capability for distributed verification. He described it as a “universal library card” that allows information consumers to own their identity and move between information systems. The “card” would be the means of authentication. Griffey mentioned a year-long project funded by the U.S. Institute of Museum and Library Services (IMLS) that has the goal of gaining a better understanding of blockchain technology and imagining its potential for small and large, urban and rural libraries and their communities (see: <https://ischoolblogs.sjsu.edu/blockchains/>). The site has a link to videos that not only explains blockchain technology, but also discusses potential applications—definitely worth a look.

Richard Ford Burley, Deputy Managing Editor, *Ledger*, spoke on the features and drawbacks of centralized citation indexes (e.g. the *Science Citation Index*®), ultimately asking whether or not incentives can be leveraged to create a decentralized citation ledger using blockchain technology. He noted that the *SCI*® is now part of the Web of Science owned by Clarivate Analytics, a large commercial information provider that must be concerned about their bottom line. Therefore, he asserted, economics must come into play when that organization decides what material does or does not get indexed in their services. He said that

he understands that journal selectivity is perceived as a necessity for ongoing financial sustainability, but questioned whether it is necessary in light of today’s technology—specifically blockchain. He then went on to describe how a decentralized citation index built on a blockchain might work, with authors themselves inputting the necessary information—not employees of a large organization. He views the potential benefits are that such a system would eliminate the pressure on start-up and smaller journals; create a more accessible ecosystem for data curation businesses; and perhaps offer the potential for more targeted curation for social ends. However, he did say that there are potential issues, for example, dishonest scholars and journals would require mitigation by curators; spam attacks would require “captcha”-like proof-of-humanity or other mitigation techniques; and there would be the need to implement the blockchain and a create a new cryptocurrency or use an existing one such as bitcoin to reward participants. Burley closed by saying that there is a lot of work that would need to be done toward creating a stable, decentralized citation ledger, but such a venture offers very real promise for the future.

Another speaker, Lambert Heller, Head of Open Science Lab, TIB, German National Library of Science and Technology in Hannover, reinforced Griffey’s and Burley’s vision. He discussed how advanced peer-to-peer (P2P) architectures will set new standards for how scientists support scholarly works and interactions. Heller believes that blockchain offers a route to a true scholarly commons and that use of decentralized networks to share data and publications could make research more open, efficient, and fair. He referred conference attendees to read one of his articles covering some ideas from his presentation, with further links that is available at <https://bit.ly/blockchain-commons>. Let’s see if anyone follows-up on this vision of the future.

Peer Review—a Blockchain “Failure?”

While on the topic of publishing it is important to note that the recent initiative for the use of blockchain to improve the peer review process that I mentioned earlier suffered a setback. This publishing industry initiative was implemented in mid-2018 to make the peer review process more transparent and trustworthy. The project was led by Digital Science and phase one participants were Cambridge University Press, Springer Nature, Taylor and Francis, Katalysis, ORCID, and Karger, along with the Wellcome Trust who served in an advisory capacity. For fourteen months

they piloted the suitability of blockchain technology to solve urgent challenges in the peer review process. A test of a minimal viable product that was developed with Katalysis validated that blockchain could indeed facilitate the safe exchange of peer review data between publishers and other parties in the scholarly ecosystem. However, during that same time period other efforts were being developed and a meeting was held on 5 September 2019 with representatives from more than twelve organizations, including ten publishers. The net outcome of their discussions was the decision that focusing on existing initiatives would be a more efficient and cost-effective path towards making the peer review process more transparent, efficient, and recognizable and that the study of the use of blockchain should be discontinued. I personally was disappointed as I thought the project held promise, but the rationale for aborting the project was convincing (see: <https://www.blockchainpeerreview.org/2019/11/determining-the-future-of-the-blockchain-for-peer-review-initiative/> for details).

The Future of Blockchain

When I attended the conference in 2018 Blockchain technology was “at the peak of inflated expectations” since most of the initiatives discussed were very new (see the Gartner Technology Hype Cycle) [11]. By October of 2019 the technology had begun sliding into the “trough of disillusionment,” with predictions that it would be another five to ten years before it would have a transformational impact [12].

Yet, Blockchain continues to be a buzzword and an area of focus around the globe and my personal opinion is that it should not be ignored—even by IUPAC. Can/should the technology be applied to tracking IUPAC Recommendations or the critical evaluation of data or the changing terminology in the Color Books? What potential value does it hold, if any, for IUPAC and its member organizations? The scientific community is not ignoring blockchain. Take a look at what the Pistoia Alliance is doing in this area to ensure that the pharmaceutical industry takes an informed approach to the technology (see: www.pistoiaalliance.org/tag/blockchain).

I remain both enthusiastic and optimistic about the technology, but I have learned over the past two years that I need to temper my enthusiasm and keep in mind some of the pearls of wisdom that were sprinkled throughout the 2018 blockchain conference:

- Blockchain is *not* a solution in search of a problem; while worth exploring, implementation is not for

everyone. Do your homework first!

- Blockchain is a potential disruptor for the information economy (indeed for all industries); therefore publishers—the middlemen between authors and information consumers—need to take this technology *very* seriously and use it to their advantage.
- Blockchain has been built on prior technologies, many of which are still essential. It is important to know what has gone before and to continue to build upon the strongest technologies.

When looking at blockchain there are two quotes whose individual messages need to be carefully balanced. These are:

“We are stuck with technology when what we really want is just stuff that works”[13].

And

“We tend to *overestimate* the effect of a technology in the short run and *underestimate* the effect in the long run”[14].

My personal advice: *do not under estimate the potential of blockchain technology in the long run!* Those of you who know me know are well aware that I love horse racing, and I assure you that if Blockchain Technology were a horse, I would bet on it! In my opinion, it is a technology that should not be ignored (for a primer on blockchain technology see: IBM’s 2nd edition of *Blockchain for Dummies* that is freely-accessible at: <https://www.ibm.com/blockchain/what-is-blockchain>. 🐎)

Note:

With their permission, this article is based upon the overview of the 2018 blockchain conference that the author wrote for *Information Services and Use* [15]. The entire issue is open access and contains many interesting articles written by speakers at the conference.

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Extending electronegativities to superheavy Main Group atoms

by Paul J. Karol

IUPAC recently published recommendations on rules for oxidation states within which was an endorsement of the electronegativity scale, called configuration energies, conceived by Allen and constructed from available calculated results. In conjunction with the International Year of the Periodic Table and the recognized extension of the Periodic Table through the end of its seventh period, it seemed timely to broaden those simple electronegativity calculations to include Main Group superheavy elements.

Introduction

Electronegativity, although not experimentally measurable, nevertheless is one of the most useful and central concepts to chemistry, starting primarily in introductory courses at college and pre-college levels, our target audience here. Its use in predicting and/or understanding chemical reactive behavior is well-appreciated. With the Periodic Table now covering the complete collection of elements within the range of atomic numbers Z from 1 to 118 [1,2], it seems heuristically reasonable to explore the newest regime. Theoretical orbital energy calculations already available [3,4] facilitate this venture that can actually be extended with a good degree of confidence to $Z = 120$.

Pauling Electronegativities

The Gold Book [5], IUPAC's Compendium of Chemical Terminology, refers to electronegativity as a concept introduced by L. Pauling [6] measuring the qualitative property that a chemist calls electronegativity as "the power of an atom to attract electrons to itself." With the above empirical definition, electronegativity is an atom-in-molecule property, not an invariant property of the atom but a property dependent on the atom's environment in the molecule, on the number and types of atoms attached to it, on the atom's oxidation state. Recently, Rahm *et al.* have proposed extending the concept to include the external influence of compression [7]. Pauling's electronegativity values for the *Main Group* elements are illustrated in Figure 1. The periodic trends going across rows and down groups (columns) are evident and underly the usual discussion about electronegativity behavior.

Other Electronegativity Schemes

Other approaches espousing the view that electronegativity is a property of atoms in molecules also give multiple values for an atom, taking into account the oxidation state and molecular environment including the influence of solvation. Since the Gold Book also has entries on group electronegativities or substituent electronegativities, it seems reasonable to refer to atomic electronegativities (or perhaps to intrinsic electronegativities) when focusing on a property characteristic of a free atom. In that regard, as emphasized by the recent endorsement by IUPAC in their codification of oxidation states [8,9], the electronegativity hypothesis introduced by Allen and collaborators is advantageous and produces very reasonable values in qualitative agreement with other assignment venues although the transition elements are problematic and the inner transition elements were not addressed. Up-to-date comprehensive reviews of electronegativity have been published recently by Politzer and Murray [10] and by Rahm *et al.* [7,11,12], each of which acknowledge both the simplicity and accuracy of the Allen electronegativities for *Main Group* elements but definitely not for the transition and inner transition elements. Cao *et al.* [13] review the role of electronegativity as one of the main determinants of chemical behavior. Our particular argument here is not to sponsor nor review any particular scheme but rather to employ the one that seems both successful and uniquely applicable to extending the Periodic Table at this time and one that has been embraced by IUPAC [8,9].

Pauling Electronegativity Scale							He
H 2.20							
Li 0.98	Be 1.57	B 2.04	C 2.55	N 3.04	O 3.44	F 3.98	Ne
Na 0.93	Mg 1.31	Al 1.61	Si 1.90	P 2.19	S 2.58	Cl 3.16	Ar
K 0.82	Ca 1.00	Ga 1.81	Ge 2.01	As 2.18	Se 2.55	Br 2.96	Kr
Rb 0.82	Sr 0.95	In 1.78	Sn 1.96	Sb 2.05	Te 2.1	I 2.66	Xe
Cs 0.79	Ba 0.89	Tl 1.62	Pb 1.87	Bi 2.02	Po 2.0	At 2.2	Rn
Fr 0.7	Ra 0.9	Nh	Fl	Mc	Lv	Ts	Og
eka-Fr	eka-Ra						

Fig. 1: Pauling electronegativity values for Main Group elements. Colors are to guide the eye towards increasing electronegativity.

Allen Electronegativities

Attraction of an atom to its electrons is arguably quantified by the electron energies, negative relative to the binding threshold. Allen *et al.* [3,4] have logically identified an electronegativity scheme measuring the difficulty with which an atom yields its valence electron. The Allen scheme is not as fundamentally grounded as are many of the alternatives. It is quantitatively embodied in what they call the configuration energy (CE, symbol E_c): the average orbital energy of valence electrons in ground-state isolated atoms according to

$$E_c = \frac{n_s \varepsilon_s + n_p \varepsilon_p}{n_s + n_p} \quad (1)$$

in which n_s and n_p , respectively, are the numbers of s- and p-valence electrons in the ground state configuration for the *Main Group* elements we are restricting our considerations to here. Orbital energies for these electrons are indicated by ε_s and ε_p , respectively, and the latter are *j*-multiplet-averaged: $(2j+1)$. They approximate ionization energies.

In their publication, Allen *et al.* use experimentally determined spectroscopic electronic energies, ε , when available, as through the NIST Atomic Spectra Database (www.nist.gov/pml) tabulations. Alternatively, and in the cases of experimentally unknown energies, theoretical values for orbital eigenvalues determined by Dirac-Fock calculations can be employed. Allen *et al.* actually use Dirac-Hartree-Fock calculations acknowledging these compare very favorably with available Dirac-Fock results. Experimental (spectroscopic) and theoretical (Dirac-Fock) final orbital energy values differ only slightly, 1% or less in most cases as noted by Allen *et al.* [3,4] (*q.v.*). Theoretical Dirac-Fock values through $Z = 120$ have been published by Desclaux [14] and nowhere else to date. Table 1 has the calculated valence energies for *Main Group* elements from rows 6 and 7 of the Periodic Table, extending to the yet undiscovered s-block elements with $Z = 119$ and 120 beginning the eighth row. Unit of the energy is E_h (hartree) with ($1 E_h$ approximately 27.21 eV). The configuration energies are calculated according to eq. 1 from the ground state valence orbital configurations indicated in the first column. These are proportionately

Atom A.. $s^n p^m$	ε_s (calc) $/E_h$	ε_p (calc) $/E_h$	ε_s (spec) $/E_h$	ε_p (spec) $/E_h$	E_c	χ_A (theory)	χ_A (spec)
Cs.. s^1	0.2561	--	0.2865		0.2561	0.59	0.66
Ba.. s^2	0.3260	--	0.3830		0.3260	0.75	0.88
Tl.. $s^2 p^1$	0.8984	0.3763	0.9656	0.4019	0.7206	1.67	1.79
Pb.. $s^2 p^2$	1.1330	0.4766	1.1111	0.5008	0.8017	1.85	1.85
Bi.. $s^2 p^3$	1.3724	0.5739	1.288 ^a	0.5990	0.8905	2.06	2.01 ^a
Po.. $s^2 p^4$	1.6197	0.6715	1.474 ^a	0.692 ^a	0.9849	2.27	2.19 ^a
At.. $s^2 p^5$	1.8763	0.7707	1.685 ^a	0.787 ^a	1.1126	2.50	2.39 ^a
Rn.. $s^2 p^6$	2.1429	0.8723	1.872 ^a	0.8845	1.1875	2.74	2.60 ^a
Fr.. s^1	0.2654	--			0.2654	0.61	
Ra.. s^2	0.3325	--			0.3325	0.76	
Nh.. $s^2 p^1$	1.1762	0.3780			0.9101	2.09	
Fl.. $s^2 p^2$	1.4429	0.4827			0.9628	2.21	
Mc.. $s^2 p^3$	1.7150	0.5847			1.0368	2.38	
Lv.. $s^2 p^4$	1.9961	0.6874			1.1236	2.58	
Ts.. $s^2 p^5$	2.2878	0.7924			1.2204	2.81	
Og.. $s^2 p^6$	2.5913	0.9005			1.3232	3.04	
eka-Fr.. s^1	0.3177	--			0.3177	0.73	
eka-Ra.. s^2	0.3835	--			0.3835	0.88	

^a Values are approximations employed by the authors of Reference [4].

Table 1: Calculated (Dirac-Fock) and experimental (spectroscopic) s, p orbital energies, the resulting configuration energies (E_c , eq. 1), all in hartree. Electronegativities (EN, symbol χ_A) from calculations (theory) and spectroscopic measurements (spec) are scaled according to $\chi_A = 2.30016 E_c$.

Extending electronegativities to superheavy Main Group atoms

Allen Electronegativity Scale							
H 2.30							He 4.16
Li 0.91	Be 1.58	B 2.05	C 2.54	N 3.07	O 3.61	F 4.19	Ne 4.79
Na 0.87	Mg 1.29	Al 1.61	Si 1.92	P 2.25	S 2.59	Cl 2.87	Ar 3.24
K 0.73	Ca 1.03	Ga 1.76	Ge 1.99	As 2.21	Se 2.42	Br 2.69	Kr 2.97
Rb 0.71	Sr 0.96	In 1.66	Sn 1.82	Sb 1.98	Te 2.16	I 2.36	Xe 2.58
Cs 0.66	Ba 0.88	Tl 1.79	Pb 1.85	Bi 2.06	Po 2.27	At 2.50	Rn 2.74
Fr 0.61	Ra 0.76	Nh 2.09	Fl 2.21	Mc 2.38	Lv 2.58	Ts 2.81	Og 3.04
eka-Fr 0.73	eka-Ra 0.88						

Fig. 2: Periodic Table of all Main Group element Allen electronegativities. Values through Pb are from reference [4]. The superheavy ($Z > 103$) Main Group element electronegativities are from this work.

rescaled, as by Allen *et al.*, to electronegativities (EN) closely matching those of Pauling using the multiplicative factor 2.300 16. The preferred choice is to use the spectroscopically-determined values when available (through Pb) and the theoretical values for the rest. Complete results for *Main Group* elements are illustrated in Figure 2.

As with the previous scales, electronegativity increases from left to right across each row from alkali metal to noble element as is illuminated in Figure 3, monotonically in most cases. However, the monotonic drop in electronegativities proceeding down any group column reverses as the heavy elements are approached. This is most likely a reflection of relativistic effects in which the valence electrons are drawn in

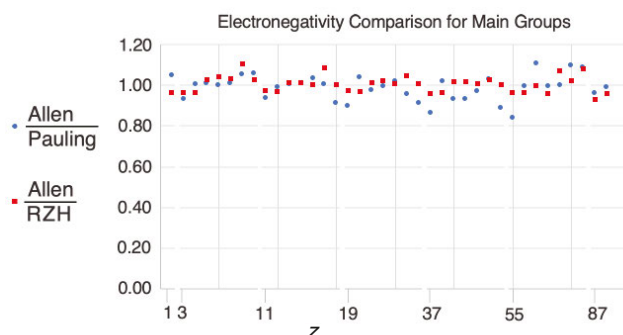


Fig. 4: Demonstrating how the Allen electronegativities concur with those of the commonly advocated Pauling electronegativities and with the Rahm, Zeng, Hoffmann (RZH) electronegativities established for Main Group elements obtained from Reference 12.

closer to the nucleus and are more difficult to “move”.

Figure 4 shows the relative value of each Allen electronegativity from Figure 2 compared to its Pauling electronegativity counterpart from Figure 1 for the *Main Group* elements exclusive the noble gases. Also displayed are the values from the very recent stratum advocated by Rahm *et al.* [11]. The concurrence lends credibility to the extension of calculated *Main Group* heavy element electronegativities advocated in this work and, pending future more sophisticated theoretical calculations, will not be expected to be significantly modified. Their likely use in anticipating the chemistry of new elements [15,16] is reasonable as we enjoy speculating on where the International Year of the Periodic Table leads us. 🌐

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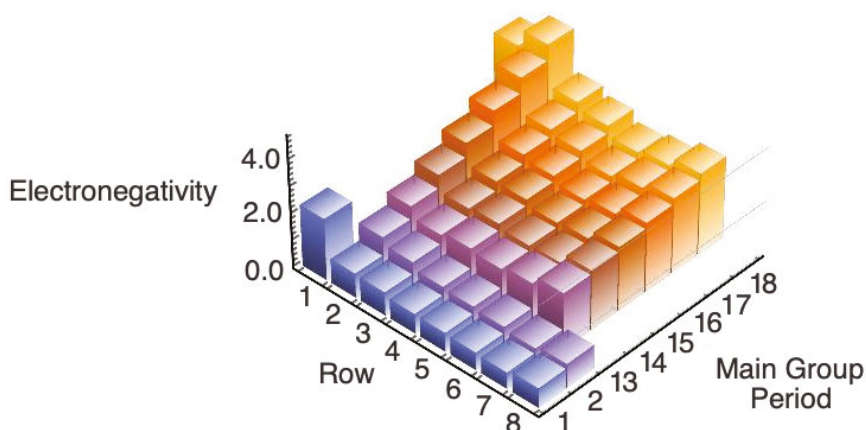


Fig. 3: Three-dimensional display of *Main Group* element Allen electronegativities in a Periodic Table format starting on the left, row 1, with hydrogen.

Extending electronegativities to superheavy Main Group atoms

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Paul J. Karol, <https://orcid.org/0000-0002-3555-6899>

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Bonnie Lawlor was Chair of IUPAC Committee on Publications and Cheminformatics Data Standards from 2014-2019 and is Secretary of *Chemistry International* Editorial Board.

Gender Gap in Science

A Global Approach to the Gender Gap in Mathematical, Computing, and Natural Sciences: How to Measure it, How to Reduce It?

by Mei-Hung Chiu and Mark Cesa

There continues to be a persistent gap between women's and men's participation, access, rights, pay, and benefits in the natural sciences, mathematics, and computing. The UNESCO Institute of Statistics reports that fewer than 30% of the world's researchers are women. Many scientists, mathematicians, computing experts, and policy makers are working to reduce this gender gap by way of a wide

range of initiatives. The International Science Council (ISC) funded a unique three-year project in 2017-2019 called, "A Global Approach to the Gender Gap in Mathematical, Computing and Natural Sciences: How to measure it, how to reduce it?" that has provided a wide-ranging view of the issues women face in the sciences and how these issues may be overcome.

This project involves eleven partner organizations. Seven of these are union members of the ISC. The two lead organizations for the project are The International Mathematical Union (IMU), through its Committee for Women in Mathematics; and IUPAC (see IUPAC project 2017-007-1-020). Other participating unions include the International Union of Pure and Applied Physics (IUPAP); the International Astronomical Union (IAU), the International Union of Biological Sciences (IUBS); the International Council for Industrial and Applied Mathematics (ICIAM); and the International Union of History and Philosophy of Science and Technology (IUHPST). The other four organizations are the United Nations Educational, Scientific and Cultural



A Global Approach to the Gender Gap in Mathematical, Computing, and Natural Sciences: How to Measure It, How to Reduce It?

Organization (UNESCO), through its project STEM and Gender Advancement (SAGA); Gender in Science, Innovation, Technology and Engineering (GenderInSITE); the Organization of Women in Science for the Developing World (OWSD); and the Association for Computing Machinery (ACM), through ACM-W.

Goals

The main goal of the project was to investigate the gender gap in STEM disciplines through three principal tasks, globally and across disciplines. These main tasks were: (1) a global survey of scientists; (2) a study of scientific publication patterns; and (3) a database of good practices to encourage girls and young women to enter STEM fields. The primary focus of the project was on the academic profession, but information was gathered as well regarding conditions in industrial employment. The overall objective was to identify and promote tools, behaviors and practices to foster equality between men and women working in science by providing data from which to draw conclusions, take actions, implement policies to attract and retain women in STEM fields, and develop and evaluate practical recommendations.

Findings

The Global Survey of Scientists

The Global Survey of Scientists aimed to measure the gender gap in science around the world by investigating issues relating to the education and upbringing of young women; their career choices; workplace conditions and family obligations; and rates of participation and retention of women in the sciences, computing, and mathematics by comparing the experiences of women and men. The survey was conducted in seven languages (Arabic, Chinese, English, French, Japanese, Russian, and Spanish). To prepare the questionnaire, three regional meetings, in Colombia, South Africa, and Taiwan, were held to review the draft questionnaire with a special focus on: collecting feedback on regional implications of topics, providing unambiguous wording, gathering input to ensure that the survey was appropriate for all regions and for disciplines, and developing an outline for the distribution plan.

The Global Survey of Scientists was launched on 1 May 2018 and closed on 31 December 2018. There were more than 32,000 respondents to the first question, and analyses were performed on nearly 25,000 responses, including from 2,698 chemists, that contained sufficient data. Responses came from 159 countries,

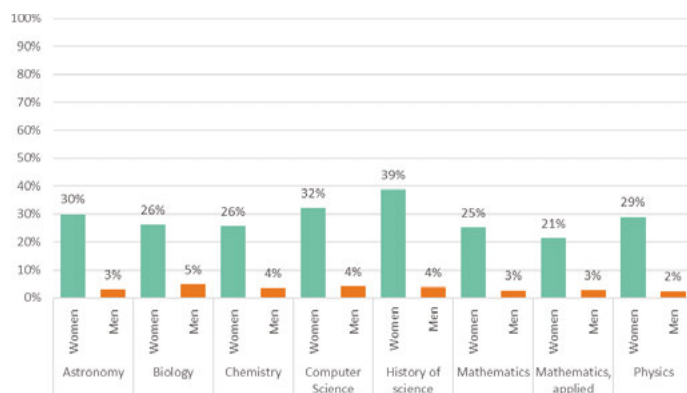
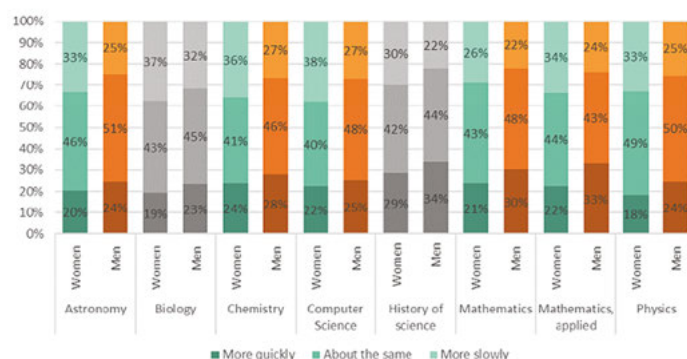
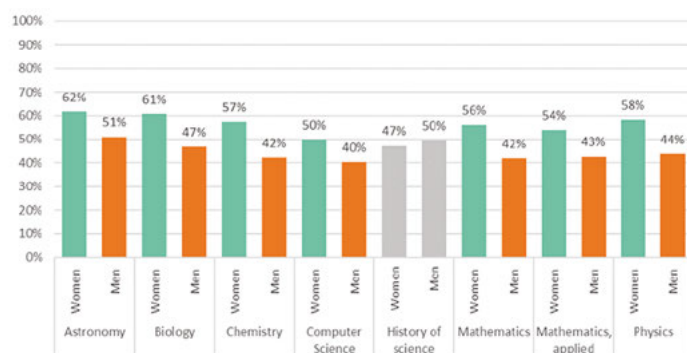


Figure 1. Respondents indicating they personally encountered sexual harassment at school or work, by discipline.



Grey indicates the differences are not statistically significant by gender on the 0.002 level.

Figure 2. Percentages of respondents comparing their career progression to their colleagues who completed their final degrees at the same time by discipline.

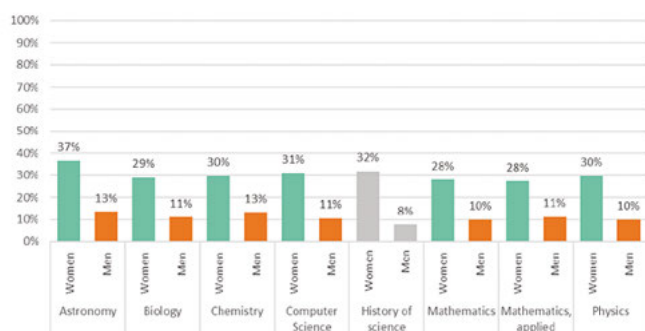


Each of these statistically significant relative differences (62% to 51%, or -1.2 times, in Astronomy, for example) understates the relative likelihood between women and men in the multivariate model which accounts for confounding factors including age, employment sector, geographic region, and level of development.

Grey indicates the differences are not statistically significant by gender at the 0.002 level.

Figure 3. Percentages of respondents indicating their career influenced their decisions about children, marriage, or a similar long-term partnership by discipline.

The Global Gender Gap in Science



Each of these statistically significant relative differences (37% to 13%, or ~2.8 times, in Astronomy, for example) understates the relative likelihood between women and men in the multivariate model which accounts for confounding factors including age, employment sector, geographic region, and level of development. Grey indicates the differences are not statistically significant by gender at the 0.002 level.

Figure 4. Percentages of respondents indicating their career or rate of promotion slowed significantly because they became a parent by discipline.

and women and men are almost equally represented in the final dataset. Data were analyzed using three basic statistical approaches: bivariate, multivariate, and qualitative analyses. Data were collected using “snowball sampling,” a technique in which existing respondents recruit others from among their colleagues, and partners in the project encouraged respondents in the partnering organizations, professional societies, and other relevant groups. Snowball sampling does not provide a statistically representative set of results, but they indicate trends among the respondents that were generally consistent across disciplines, geographical regions, and level of development.

In the final report of the Gender Gap project, results of the Global Survey of Scientists were reported

in a graphical form that illuminated the differences between women’s and men’s experiences across disciplines, geographical regions, level of regional economic development, education, and employment sector.

It was found that systematic differences between the experiences of men and women still exist, across all regions, all disciplines, and all development levels; chemistry was not an exception.

The final report contains a great deal of information across the sciences. For chemistry in particular, some examples of the major findings are discussed here.

More than six times more women than men in chemistry reported having personally encountered harassment at work or school (Figure 1). This trend was essentially the same across disciplines, geographic regions, and levels of economic development.

Compared with men, women in chemistry tended to report more frequently that the progression of their careers was significantly slower than that of their peers (Figure 2). Women in chemistry also tended to report in greater numbers than men that their careers were more strongly affected by their decisions regarding children, marriage or similar long-term partnership, and that their careers were slowed significantly when they became parents (Figures 3 and 4)

There were also significant findings that spanned disciplines, regions and levels of economic development. For example, women in the survey were less likely than men to report respectful treatment by coworkers. Also, women were more likely than men to report that they took interruptions in their studies, and that the interruption had a negative impact on their professional credibility. More female respondents than male respondents expressed that they felt discriminated against

Item	Gender Differences
Doctoral advisor support†	Respondents from Math programs were more likely to rate advisor support higher than respondents from other disciplines.
Respectful co-workers†	Respondents whose discipline was Physics were more likely to agree they had respectful co-workers than respondents from other disciplines.
Never experienced discrimination†	Respondents from Math and Physics were more likely to indicate they had never experienced discrimination than respondents from other disciplines.
Promotion slowed after children†	Respondents from Math were less likely to indicate their promotion slowed after becoming a parent than respondents from other disciplines.
No career change after children†	Respondents from Chemistry and Math were more likely to indicate their work or career did not change when they became a parent than respondents from other disciplines.

These gender differences are statistically significant at the $\alpha = 0.002$ level after accounting for potential confounding factors (age, discipline, geographic region, and level of development.)

†The dependent variable is ordinal, so we are unable to report a single odds ratio.

Table 1. Differences across disciplines.

The Global Gender Gap in Science

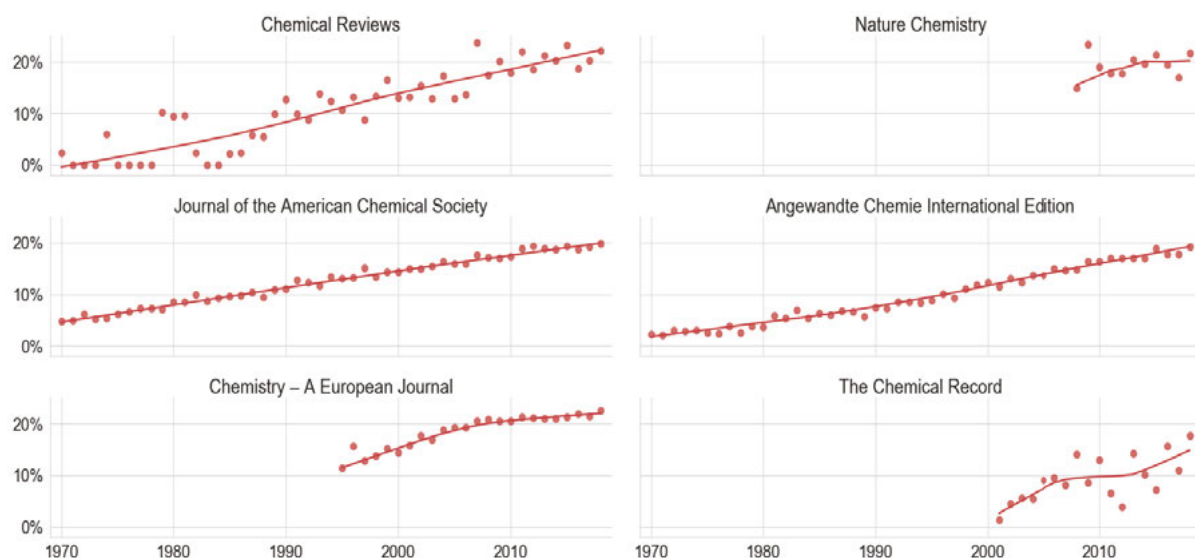


Figure 5. Trends in authorship by women in six major chemistry journals.

in the assessment or evaluation of their achievements because of their gender. Fewer women reported being treated fairly in their work environment, and women more frequently reported lower pay than that of their colleagues. Finally, the gender gap in science does not disappear with increasing levels of regional economic development, as defined by the Human Development Index, HDI. In some instances, a higher level of development was found to be correlated with more negative experiences by women in graduate program quality, and relationship with their graduate advisors.

Overall, these analyses provide compelling evidence that women and men do not have the same experiences in science, and that women's experiences are less positive than men's. There are gender differences in every area that was examined. In addition to findings from the survey regarding harassment and rates of career progression, the survey found: (See Table 1):

- Women are less likely than men to say that everyone is treated fairly in the educational system and in employment.
- Women report less positive relationships with their doctoral advisors, lower doctoral program quality, and more interruptions in doctoral studies than men.
- Women are less likely to report respectful treatment by co-workers than men.

Study on Publication Patterns

The analyses of publication patterns for women in mathematics, astrophysics, computer science and quantitative biology were based on data from three

bibliographic sources managed by scientific organizations, namely: 1) The SAO/NASA Astrophysics Data System for research in astronomy and astrophysics, zbMATH for pure and applied mathematics; and arXiv for physics and mathematics and computer science or quantitative biology. However, in chemistry, the researchers used data on the representation of women in a selection of chemistry publications. Data from Crossref was used to investigate the proportion of women in 6 prestigious chemistry journals that were suggested by IUPAC volunteers: *Chemical Reviews*, *the Journal of the American Chemical Society*, *Chemistry-A European Journal*, *Nature Chemistry*, *Angewandte Chemie International Edition*, and *The Chemical Record*. The proportions of women authorship in these journals has been increasing steadily over the past 20 – 50 years (below 5% in 1970 up to values in the vicinity of 20% in the 2010s), a pattern that is not always repeated in other scientific disciplines (Figure 5).

There are overall improvements in academic career development for women as measured by increases in numbers of publications authored by women, although on a different pace depending on discipline. In particular, theoretical fields and sub-fields show the slowest improvement in most of the metrics applied, which leads to interesting questions such as the role of collaboration for the achievement of equal opportunities. However, the proportion of women authoring papers in top journals has remained static in mathematics and theoretical physics, while it increased in astronomy and chemistry. A pattern of fewer women authors in theoretical disciplines and sub-disciplines was found

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while a larger presence of women was found in applied fields and with multiple authors. The rise of women representation in chemistry over the past five decades is perhaps the most noteworthy among the analyzed STEM disciplines. Even though the promising results were found, due to data limitation across the globe, much remains unexplained about how women chemical scientists on a global level.

Database of good practices

Various methods have been employed to gather information about initiatives for inclusion in the database, including holding conferences and conducting online searches. Countries in specific regions have been targeted through searches using the country name and a combination of key words (STEM, science, mathematics, gender, female, women, girls, mentor, role model, and workshop).

Creating the database has presented three challenges. The first challenge concerns the longevity of initiatives that are projects with finite funding (e.g., Horizon 2020 funded). Unless these projects have produced resources that can be found and used in future, they will not be included in the database. The second challenge is the difficulty in finding evidence of the effectiveness and impact of initiatives. The database of good practice currently includes 67 gender initiatives from more than 44 countries in all geographical regions of the world. Twenty-one initiatives come from Western Europe, followed by North America with 8 initiatives and Asia-Pacific with 7 initiatives. Among them, 24 initiatives relate to STEM education.

Finally, the final version of the database is to be hosted on the IMU/CWM website, and project partners will be able to make a link from their websites to the database.

Resources

Website: <https://gender-gap-in-science.org/>

Report: a book illustrated by a cartoonist is available on line at <https://doi.org/10.5281/zenodo.3697222>

Survey: the questionnaire in several languages is available at <https://statisticalresearchcenter.aip.org/global18>, for the list of all the questions in English, see <https://reurl.cc/yyzOxE>

Interactive tools: for publication patterns, see <https://reurl.cc/5gY30M>, for a preliminary version of the database, see <https://reurl.cc/gvKrLR>.

Good practice: a selection of initiatives for reducing the gender gap, see the Database at <https://www.mathunion.org/cwm/gender-gap-in-science-database>

[mathunion.org/cwm/gender-gap-in-science-database](https://www.mathunion.org/cwm/gender-gap-in-science-database)

Research papers: several research papers will be submitted by the teams in charge of the three tasks.

Dissemination material: a 8-page illustrated document with main ideas and recommendations can be found at <https://gender-gap-in-science.org/promotional-materials/>

Creation of a community: 7 ISC unions (IMU, IUPAC, IUPAP, ICIAM, IUHPST, IAU, IUBS) and 4 other organizations (UNESCO, ACM, OWSD and Gender in Site) collaborated successfully. The three regional workshops and the final ICTP conference involved 150 active scientists all over the world.

Recommendations

Based on the findings of the project, the following recommendations were discussed and approved at the final Gender Gap project conference at ICTP in Trieste, Italy, in late 2019:

For instructors and parents

- Avoid gender stereotyping and unconscious gender bias in interactions with female students and children.
- Avoid books and social media that reinforce the gender gap in science. Develop gender awareness in the classroom and encourage girls in their learning of STEM subjects.
- Encourage relevant single-sex activities to raise girls' self-confidence and possibilities for expressing themselves.

For local organizations

- Promote a respectful, collegial working atmosphere in your organization.
- Define best practices to prevent, report and address sexual harassment and discrimination in professional spaces.
- Address the impact of parenthood on the careers of women. Encourage provision of a research-only year after maternity leave or parental leave.
- Ensure transparency of statistics on salaries, course loadings, bonuses, hiring and promotion, observing progress or difficulties experienced by female academics. Encourage policies to help reduce gendered salary disparities.
- Welcome families and provide child friendly environments. Provide improved support systems for parents.
- Address gender equality in all institutional policies. Identify a person or a group in charge of

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gender equality inside the organization, looking at the gender balance in all kind of activities.

- In all outreach and educational programs, include the aim of reducing the gender gap.

For scientific unions

- Work collectively to change culture and norms to reduce the various aspects of the gender gap.
- Define and advertise best practices to prevent, report and address sexual harassment and discrimination in professional spaces.
- Recommend and disseminate in the scientific community proper accounting of child bearing/caring responsibilities (18 months per child recommended) when evaluating candidates in hiring and promotion processes.
- Actively promote the visibility of female scientists, in particular at conferences.
- Encourage the diversification of scientific awards, actively encouraging the nomination of women.
- Encourage the presence of women in editorial boards in your discipline and publish reports on the proportion of papers published by women.
- Welcome families in scientific activities.
- Create a committee for women and/or gender equality, with an assigned budget line.
- Actively promote gender balance at every level of your organization, including its leadership, its committees and also institutional events.
- In all outreach and educational programs and products, raise the awareness about the gender gap and include specific actions/events that aim at reducing the gender gap.

Next Steps

Plans are under way to continue the work of the Gender Gap project to complete work on the major project tasks in 2020. Work will continue on collecting additional resources for good practices, as well as making the raw data from the global survey available to unions and interested scientists in a manner that assures confidentiality. Several of the unions are

contributing financially and through volunteer participation. Finally, members of the Gender Gap project will discuss with the ISC its work on “Gender-transformative Science.” 

Note

This report was produced based upon the final report and booklet of the project. For details, please refer to <https://doi.org/10.5281/zenodo.3697222> and <https://gender-gap-in-science.org/promotional-materials>. Figures and drawings were taken from the final report.

Acknowledgement

Thanks to the representatives from the 11 unions and other PI/contributors to the tasks of the project, in particular, for the leadership from Marie-Françoise Roy. These people are Marie-Françoise Roy (IMU, lead 1), Mei-Hung Chiu (IUPAC, lead 2), Irvy (Igle) Gledhill (IUPAP), Francesca Primas (IAU), Nathalie Fomproix (IUBS), Jean Taylor (ICIAM), Catherine Jami (IUH-PST), and Jodi Tims (ACM). Task 1: Rachel Ivie, Mark Cesa, Laura Merner, Silvina Ponce Dawson, Susan White, and John Tyler; Task 2: Helena Mihaljević and Lucía Santamaría; Task 3: Merrilyn Goos and Regina Kelly. Also, thanks to Lea Castor for the drawings in this article.

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2. UNESCO (2016). *The SAGA Science, Technology and Innovation Gender Objectives List (STI GOL)*, SAGA Working paper 1. Paris. Isbn:978-92-2-100-154-3. url: <https://unesdoc.unesco.org/ark:/48223/pf0000245006>

Mei-Hung Chiu is a professor at National Taiwan Normal University and a member of the IUPAC Executive Committee. Mark Cesa was president of IUPAC from 2014-2015.



The 2020 Bright Science Award in Materials Sciences goes to Marc Hillmyer

Royal DSM, a global science-based company in Nutrition, Health, and Sustainable Living, announced that it has awarded Professor Marc Hillmyer, from the Chemistry Department at the University of Minnesota Twin Cities, the 2020 Bright Science Award in materials sciences. The jury selected Professor Hillmyer because of the scientific breadth and depth of his work and its relevance to the advancement of biobased and circular materials.



Over the past few decades, linear economic consumption of material resources has left the world facing a series of defining, complex and interdependent environmental challenges. It's this concerning landscape that underpins the Bright Science Award in materials sciences. This award is for scientists who have made major contributions to fundamental or applied research in the field of sustainable materials and whose work is instrumental in helping businesses involved in materials industries adopt more sustainable strategic directions.

Hillmyer's scientific work, which combines deep knowledge of polymer synthesis and polymer properties, contributes to the development of recyclable and biobased performance polymers. Hillmyer's scientific breakthroughs also include controlled nano-porosity in materials made from sacrificial block copolymers as well as the hierarchical self-assembly of multifunctional block copolymers into, for example, multicompartment micelles with three distinct physicochemicalities as used in nanolithography. Such breakthroughs, often achieved in collaboration with industrial advisors, are crucial for the transformation toward a bio-based and circular economy.

The DSM Bright Science Awards Program includes yearly awards for PhD graduates as well as awards

for experienced scientists such as Professor Hillmyer. Every even year, the award for experienced scientists is related to materials sciences. In odd years, its related to life sciences. The award is accompanied by a cash prize of €25,000—which should be allocated to the award winners' research group to ensure that we all continue to benefit from bright science. The 2020 Bright Science Award in materials sciences was organized by DSM in partnership with IUPAC.

<https://iupac.org/the-2020-bright-science-award-in-materials-sciences-goes-to-marc-hillmyer/>

The 2020 Hanwha-Total IUPAC Young Scientist Award goes to Athina Anastasaki and Changle Chen

The Hanwha-Total IUPAC Young Scientist Award (formerly Samsung-Total Petrochemicals - IUPAC Young Scientists Award) is dedicated to outstanding young scientists (under 40 years) and is sponsored by a grant from the aforementioned company. The prize was first awarded on the occasion of MACRO 2004 (Paris) and is granted biennially on the occasion of the IUPAC World Polymer Congress. The awardees are selected from the nominees by a Committee of the IUPAC Polymer Division. In the year 2020 the award will be presented at Macro2020+ and there are two awardees (*ex aequo*) namely: Athina Anastasaki, Department of Materials, ETH Zurich, and Professor Changle Chen, Department of Polymer Science and Engineering, University of Science and Technology of China.

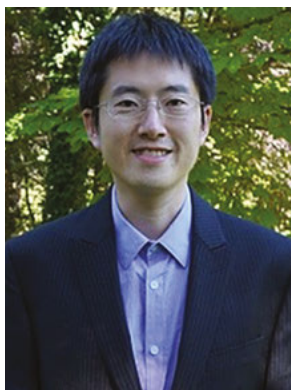
Anastasaki was born in Greece and obtained her B.S. in Chemistry from the National and Kapodistrian University of Athens. She subsequently joined Professor Haddleton's group at the University of Warwick to commence her Ph.D studies and was awarded the Jon Weaver Prize for the best PhD thesis

in Polymer Chemistry in the UK and the prize for the best PhD in Chemistry at the University of Warwick.



She then won an Elings Prize Post-doctoral Fellowship and a Global Marie Curie Fellowship at the University of California, Santa Barbara where she worked alongside Professor Craig Hawker. As of January 2019, she is an Assistant Professor at ETH and her group focuses on the development of new methodologies in controlled radical polymerization to synthesize smart polymers and polymeric nanomaterials with ultimate aim to control all properties of polymeric materials including the molecular weight, dispersity, architecture, and functionality as well as their self-assembly into nanostructures with various size, shape, surface, and core properties. In May 2019, she was awarded the element curium on the IUPAC100 Periodic Table of Younger Chemists. She is currently serving on the Editorial Board of Polymer Chemistry and she is a co-author of more than 85 peer-reviewed publications (h-index 38), which have been cited approximately 4000 times.

Changle Chen is a professor for polymers at University of Science and Technology of China. The central theme of the research in Chen group is the development of new catalysts and new strategies for metal catalyzed polymerizations and polymer synthesis, with special focus on polyolefins.



He obtained his B.S. degree from University of Science and Technology of China (USTC, 2005), and PhD from the University of Chicago (2010). After postdoctoral studies at Northwestern University and some time at Celanese Corporation, he started his independent career as a professor at USTC in 2013. He has published more than 120 scientific papers (h-index 46) with over 5500 citations. He is currently associate editor of Science Bulletin and European Polymer Journal, and is member of a number of editorial boards of prominent scientific journals. He has recently been awarded Chinese Chemical Society Award for Outstanding Young Chemist, Society of Polymer Science Japan International Leading Young Scientist, NSFC Excellent Young Scholar Fellowship and Young Talent Award on Polymer Processing and Industrial Development.

<https://iupac.org/hanwha-total-iupac-young-scientist-award-2020/>

Ang Li is the recipient of the 2020 Thieme-IUPAC Prize

Professor Ang Li is the recipient of the 2020 Thieme-IUPAC Prize and becomes the 15th recipient of the prize, joining a distinguished group of scientists under the age of 40 whose research has had a major impact on the field of synthetic organic chemistry. The prize is awarded every two years and includes an award of €5000.



Ang Li completed his undergraduate studies at Peking University, Beijing, and then obtained a PhD from the Scripps Institute, CA, where he worked under the supervision of Professor K. C. Nicolaou. He then spent time as a Research Fellow at the Institute of Chemical and Engineering Sciences, Singapore, before joining the faculty of the State Key Laboratory of Bioorganic and Natural Products Chemistry at the Shanghai Institute of Organic Chemistry, China, in 2010, where he is currently a professor.

Li's research is focused on the total synthesis of structurally and biologically interesting natural products. To this end, he has developed powerful strategies for the construction of complex molecular architectures, which have enabled his group to complete the synthesis of more than 90 natural products (from over 15 classes) in his independent career to date, several of them for the first time. In particular, he has developed and demonstrated the power of 6π electrocyclizations and the Prins reaction as useful tools for the efficient construction of key structural motifs.

Ang Li is one of the best young practitioners of the art and science of total synthesis in the world today, and his work has contributed to the field of synthetic organic chemistry in major and innovative ways through his numerous and imaginative total syntheses and new synthetic methods.

The Thieme-IUPAC Prize is awarded based on scientific merit for independent research dealing with synthesis in the broadest context of organic chemistry, including organometallic chemistry, medicinal and biological chemistry, designed molecules, and materials.

<https://www.thieme.de/en/thieme-chemistry/thieme-iupac-prize-55182.htm>

Winners of the 2020 IUPAC-Solvay International Award for Young Chemists

On 31 March 2020, IUPAC and Solvay announced the winners of the 2020 IUPAC-Solvay International Award for Young Chemists, presented for the best Ph.D. theses in the chemical sciences:

The five winners are:

- **Muhammad Jbara (Israel), Ph.D.**, Technion Israel Institute of Technology
- **Hung VanThanh Nguyen (Vietnam), Ph.D.**, Massachusetts Institute of Technology
- **Ron Shah (Canada), Ph.D.**, University of Ottawa
- **Namrata Singh (India), Ph.D.**, Indian Institute of Science
- **Qi Zhang (China), Ph.D.**, East China University of Science and Technology

The winners will each receive a cash prize of USD 1000 and travel expenses to the 48th IUPAC World Chemistry Congress, 13-20 August 2021, in Montréal, Canada. Each winner will also be invited to present a poster at the IUPAC Congress describing his/her award-winning work and to submit a short critical review on aspects of his/her research topic, to be published in *Pure and Applied Chemistry*. The awards will be presented to the winners of the 2020 and 2021 competitions during the Opening Ceremony of the Congress. The titles of the winners' theses are:

- Muhammad Jbara: "Chemical Protein Synthesis of Modified Histone Proteins for Biochemical Studies"
- Hung VanThanh Nguyen: "Bottlebrush and Related Polymer Architectures for Biomedical Applications"
- Ron Shah: "Autoxidation and Its Inhibition In Both Industrial and Biological Contexts: New Molecules, Methods & Mechanisms"
- Namrata Singh: "Development of Nanomaterials as Antioxidant Enzyme Mimetics for Cellular Redox Homeostasis"
- Qi Zhang: "Controlled Self-Assembly of Nanoparticles Enabled by Macrocyclic Host-Guest Chemistry and Their Functional Exploitation"

There were 50 applications from individuals receiving their Ph.D. degrees from institutions in 18 countries. The award selection committee, chaired by Professor Qi-Feng Zhou, IUPAC Past President, comprised members of the IUPAC Bureau and a senior science advisor

from Solvay, all of whom have a wide range of experience in chemistry.

In view of the many high-quality applications, the Committee also decided to award three Honorable Mentions to:

- **Aisha N. Bismillah (UK), Ph.D.**, University of Durham, UK
- **Zhen Liu (China), Ph.D.**, The Scripps Research Institute, USA
- **Federica Rossi (Italy), Ph.D.**, Università degli Studi di Torino, Italy

The call for applications for the 2021 IUPAC-Solvay International Award for Young Chemists will open soon. Eligible candidates must have received a Ph.D. or equivalent degree in any of the countries that have National Adhering Organizations or Associate National Adhering Organizations in IUPAC during the year 2020.

2020 IUPAC-ThalesNano Prize In Flow Chemistry and Microfluidics—Call For Nominations

The IUPAC-ThalesNano Prize in Flow Chemistry and Microfluidics is to be awarded to an internationally recognized scientist, whose activities or published accounts have made an outstanding contribution in the field of flow chemistry, microfluidics, micro fabrication, and micro systems engineering in academia or industry.

The IUPAC-ThalesNano Prize was established in 2011. C. Oliver Kappe, the 2018 recipient, is Professor of Chemistry at the University of Graz (Austria). The 2020 Prize will be presented during the Flow Chemistry Congress Conference in 2021 in Boston and where the recipient will also give a lecture on the subject of his/her research.

The Prize, of USD 7500, has been established by a generous gift from the Hungarian Technology company ThalesNano Inc. to acknowledge the key role that flow chemistry plays towards the improvement of chemical processes.

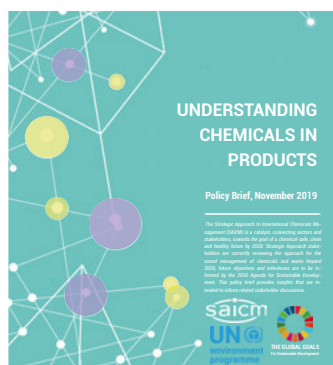
Applications should be received by nomination only, with just one person acting as the nominator, with a total of five (5) individuals as referees overall. The package must be submitted electronically and should contain a complete resume, a professional autobiography of not more than two pages, and a one-page

summary of what the individual considers to be his/her activities, accomplishments and/or publications that have had the most significant impact upon the field of Flow Chemistry. **Extended Deadline: 31 July 2020**

<https://iupac.org/2020-iupac-thalesnano-prize-in-flow-chemistry-and-microfluidics-call-for-nominations/>

Understanding Chemicals in Products

The Strategic Approach to International Chemicals Management (SAICM) has published a policy brief that addresses chemicals of concern in products such as textiles, toys, building materials, and electronics, and efforts to minimize their adverse effects on human health and the environment. The policy brief titled, "Understanding Chemicals in Products," is a contribution from the Global Environment Facility (GEF)-funded project on "Global Best Practices on Emerging Chemical Policy Issues of Concern under SAICM."



"Life cycle management of chemicals present in products" is one of the main components of the project, developing new tools and guidance to reduce the use of chemicals of concern in the building materials, electronics and toys sectors. The project also provides training and support for government and value chain actors to trial and adopt new guidance and tools.

http://www.saicm.org/Portals/12/Documents/EPI/CiP_policy_brief_Nov2019.pdf

The Beijing Declaration on Research Data

CODATA, the Committee on Data of the International Science Council (ISC), wrote The Beijing Declaration on Research Data after discussions regarding current data policy issues during their yearly conference, held in China in September 2019.

The declaration mentions the *FAIR Principles* and global *Open Science* as requirements for supporting the understanding of environmental, health and sustainability challenges we face in science and society. "Scientific discovery must not be impeded unnecessarily by fragmented and closed systems, and the stewardship of research data should avoid defaulting to the traditional, proprietary approach of scholarly publishing. Therefore, the adoption of new policies and principles, coordinated and implemented globally, is necessary for research data and the associated infrastructures, tools, services, and practices. The time to act on the basis of solid policies for research data is now."

The Beijing Declaration is intended as a timely statement of core principles to encourage global cooperation, especially for public research data. It builds on and acknowledges the many national and international efforts that have been undertaken in the policy and technical spheres on a worldwide basis. These major contributions are listed in the Appendix."

For more information, check out the CODATA website or go directly to the Beijing Declaration on Research Data:

<https://codata.org/the-beijing-declaration-on-research-data/>
<https://doi.org/10.5281/zenodo.3552330>

Announcement of the 2020 L'Oréal Women in Science awardees

During the International Day of Women and Girls in Science on February 11, the Fondation L'Oréal and UNESCO revealed the laureates of the 22nd international awards for women in science.



Convinced that the world needs science and that science needs women, the Fondation L'Oréal and UNESCO are committed to promoting women in science. Their aim is to give women scientists greater visibility, to make their talent more widely known, and to inspire women and girls to engage with science. Since 1998, 112 laureates have been rewarded and more than 3,300 talented young women scientists, Ph.D students and post-doctorate graduates have been supported and recognized in 118 countries, thanks to the Women in Science program.

Since 1998, L'Oréal Foundation and UNESCO have held the For Women in Science Awards, which recognize five outstanding women scientists from different regions of the world for the excellence of their work in life sciences. Each laureate will receive €100,000. In 2020, the International L'Oréal-UNESCO Award for Women in Science has gone to researchers whose work is particularly remarkable in the field of life sciences: biotechnology, ecology, epigenetics, epidemiology and infectious diseases.

The 2020 For Women in Science laureates are: **Africa and the Arab States: Professor Abba Mehio Sibai:** Medicine and Health sciences, Professor of Epidemiology, Faculty of Health Sciences, American University of Beirut, Lebanon, for her pioneering research and advocacy to improve healthy aging in low- and middle-income countries and their impact on health and social policy programs.

Asia-Pacific: Doctor Firdausi Qadri: Biological sciences, Senior Scientist, Head Mucosal Immunology and Vaccinology Unit, Infectious Diseases Division, International Centre for Diarrhoeal Disease and Research, Dhaka, Bangladesh, for her outstanding work to understand and prevent infectious diseases affecting children in developing countries, and promote early diagnosis and vaccination with global health impact.

Europe: Professor Edith Heard: Biological sciences, Director General of the European Molecular Biology Laboratory, Chair of Epigenetics and Cellular Memory at the Collège de France, Paris, and former Director of the Genetics and Developmental Biology Unit at the Institut Curie, Fellow of the Royal Society (UK), for her fundamental discoveries concerning the mechanisms governing epigenetic processes, which allow mammals to regulate proper gene expression and are essential for life.

Latin America: Professor Esperanza Martínez-Romero: Ecology and Environmental sciences, Professor of Environmental Science at the Genomic

Science Center of the National Autonomous University of Mexico, Mexico City, for her pioneering work on the use of environmentally friendly bacteria to support plant growth for increased agricultural productivity and reduced use of chemical fertilizers.

North America: Professor Kristi Anseth: Biological sciences, Distinguished Professor, Tisone Professor and Associate Professor of Surgery at the University of Colorado, Boulder, United States of America, for her outstanding contribution in converging engineering and biology to develop innovative biomaterials that help tissue regeneration and drug delivery.

<https://www.loreal.com/media/news/2020/march/fwis-laureates>

IUPAC Periodic Table Challenge 2.0

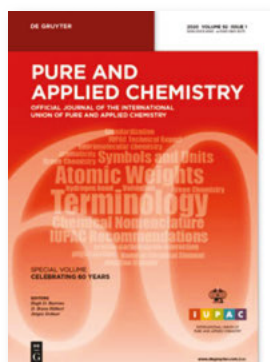
The Periodic Table Challenge is re-opening. After a successful period during the International Year of the Periodic Table with participants from over 130 countries,



IUPAC has decided to make the Periodic Challenge a permanent feature of IUPAC website, linked to information about the Periodic Table.

The challenge has new exciting questions. In order to obtain a certificate one will need to answer 6 out of 10 questions correctly. For schools and classes groups, there is also an opportunity to win a Periodic Table signed by a Nobel Laureate.

<https://iupac.org/periodic-table-challenge>



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In Memoriam

Maurice (Mo) Williams, 1933 - 2020

Mo Williams passed away peacefully on 17 April 2020, aged 87 years. Beloved husband of Patricia, a much-loved father and grandfather.



For three decades, Mo was known as Mr. IUPAC. Mo was the first professional IUPAC Executive Secretary, establishing the Secretariat in Oxford, UK, in April 1968 and retiring in 1997.

Mo was born and raised in Birmingham, UK. He graduated BSc in chemistry at Birmingham University in 1953, and went on to earn a PhD in Ron Belcher's eminent School of Analytical Chemistry under the joint supervision of Belcher and (then) Tom West. Leaving Birmingham University in 1956, he spent two years in ICI Metals Division's Research and Development Department, which was much concerned at that time with the analysis of new metals like titanium, zirconium, and beryllium, and their alloys. In 1959 he moved to become lecturer in analytical chemistry at Birmingham College of Advanced Technology, which is now the University of Aston. While there, he became Editor-in-chief of Robert Maxwell's international analytical chemistry journal *Talanta*. His qualities were recognized by Maxwell, who offered him the post of managing editor of learned journals at Oxford, which he accepted from the start of 1966. When he was offered the opportunity to become the first professional IUPAC Executive Secretary in April 1968, he accepted provided that the office could be in Oxford.

Mo Williams was undoubtedly "the right person at the right time" to organize the IUPAC Secretariat and handle all details with meticulous care over 29 years. Following his retirement, during the 39th Council meeting at Geneva (29–30 August 1997), IUPAC's President, Albert Fischli, presented to Mo a silver salver with the signatures of all the 15 Presidents of IUPAC under whom he served. In his reply,

Mo said that, despite the inevitable ups and downs, overall the 29 years had been an exciting time and a privilege to serve as the Union's Executive Secretary. In addition to working under 15 Presidents, there had been six Secretaries General and five Treasurers, and he had made countless friends throughout the world. The growth in work for the Secretariat was reflected in the fact that only two Commission reports were published in *Pure and Applied Chemistry* during 1968, but there would be over 50 in 1997. Fortunately, he had been supported throughout by excellent colleagues: besides the three secretaries present at Geneva, two others had remained at Oxford, and there had been exceptional backing from Ann Troughton (Assistant Executive Secretary) for 20 years and from Mike Freemantle (Information Officer/Affiliate Affairs Secretary) for nine years. Williams offered his best wishes to John W. Jost for the wider development of electronic services at the new Secretariat in Research Triangle Park, North Carolina.

Twenty years has passed since Mo retired, but his marks are still present as evoked in these spontaneous echoes received at the announcement of his passing:

"Mo was actually the soul and the stability of IUPAC during his time in office. It was really a pleasure and a privilege to work with him."

"It is with great regret that I learned about the sad news of Mo Williams passing away. I knew Mo Williams since the General Assembly, held in Munich (1973); he was such a kind and highly professional person. In fact, Mo and Anne Troughton made an excellent team at the IUPAC Secretariat in Oxford. I also have fond memories of the Bureau meetings, held at Hawkwell House, Oxford. Mo Williams was a keen golf-player. He always spoke fondly of the golf he played at the Pretoria Country Club during his visit to South Africa, Mo Williams was a great gentleman and a true friend."

"Mo Williams was a gentleman. I met him many years ago, I cannot remember when. At the same time, he was the "housekeeper" of IUPAC, the spirit of IUPAC, and somehow the soul of IUPAC. A true memory for all like me who stayed only for a short period of time at the head of the Union...I shall remember a very nice man."

"I knew Mo well when IUPAC was based in Oxford. He was a lovely man and did a super job for IUPAC. I would like his family to know that I am so sorry to learn of his leaving us, and that he will be remembered fondly." 🕯️

Guidelines on developing robust biocatalysts for biorefinery

Global consumption of crude oil was doubled within the past half century, hitting 4.5 billion tons in 2018 compared to 2.4 billion tons in 1971 (www.iea.org), which has raised concerns not only on its reliable supply, but also on environmental impact associated with the over-consumption of petroleum-derived products. Lignocellulosic biomass is abundant, renewable, and environmentally friendly. Within the past decade, unprecedented progress has been made in omics analysis for life science and biotechnology innovations on metabolic engineering and synthetic biology for developing robust biocatalysts, either enzymes or microbial cell factories to perform bioconversion more efficiently than ever before. However, guidelines for scientists and engineers with different backgrounds to work efficiently, as well as for graduates to learn and start their research quickly on how to engineer and develop robust biocatalysts, are lacking. Many of them are inundated with references that need to be assessed for merits. Therefore, it is imperative to edit guidelines for scientists, engineers, and graduates to work more efficiently to support the biorefinery industry, and through them stakeholders, ventures, and policy makers can be convinced to make use of historical opportunities with biorefinery for sustainable development.

Group members for this project are mainly from IUPAC and the European Federation of Biotechnology (EFB). While IUPAC is fostering chemistry and biochemistry internationally, EFB is a voice for biotechnology in Europe. The organizations are fulfilling the objectives of this project through interdisciplinary and international cooperation.

For more information and comments, contact Task Group Chair Fengwi Bai <fwbai@sjtu.edu.cn> <https://iupac.org/project/2019-046-3-300>

Development of a Standard for FAIR Data Management of Spectroscopic Data

As a key data class for characterizing chemical substances, spectroscopic data are increasingly required for reporting. To facilitate accurate dissemination and analysis of these data in the online environment, it is necessary to develop interoperable representations that are readable by both humans and machines. In 2016, guidelines were proposed that establish FAIR principles for research data management ensuring that data are findable, accessible, interoperable, and reusable in the digital environment [<https://www.go-fair.org/fair-principles/>].

This project will consider metadata elements that are critical for the FAIR management of spectroscopic data, including those that are general to all experimental techniques (such as ORCID and InChI) as well as specialized elements for specific fields, such as NMR spectroscopy. A minimum implementation will be proposed based on already established metadata efforts, including those of the Allotrope Data Framework and nmrML to encourage adoption and facilitate widespread use. These elements have been partially reviewed in IUPAC CPCDS sponsored workshops (Amsterdam, 2018 and Orlando, 2019) and in conference calls during early 2019.

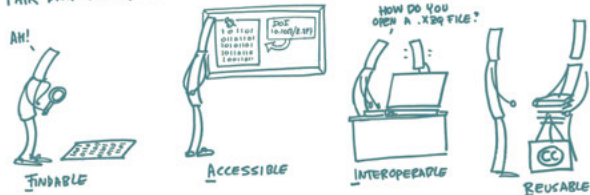
The tasks of this project include:

- a. development of clear recommendations for meta-data that allow the registering of spectroscopic data with a registering agency such as DataCite or CrossRef;
- b. specification of a standard format for the meta-data that will be associated with the actual data, whatever that data's actual form (JCAMP-DX files, vendor-specific raw data formats, etc.); and
- c. validation criteria to check files for readable and interoperable representation of data and metadata based on the standard; for example, the CheckCIF model used in managing crystallography data.

This project will be carried out in coordination with other efforts in this area, including:

1. IUPAC Project 2016-023-2-300, with their interest in the *de facto* JCAMP-DX 6.0 specification and possible changes that we might propose to that which would add metadata-related values such as ORCID persistent identifiers and InChI compound identifiers.

FAIR DATA PRINCIPLES



The FAIR data principles. Image: <https://book.fosteropenscience.eu/>

2. data publishing pilots involving chemistry journal publishers proposed at the recent FAIR Chemical Data workshop in Orlando, who will be developing workflow methods around our proposed standards.
3. DOI registering agencies such as DataCite and CrossRef, to effectively integrate the metadata we propose into these schema and ensure they are discoverable via these platforms and those that leverage this metadata
4. broad engagement of the stakeholder community in testing the recommendations and other efforts underway internationally.

We expect this work to provide the general basis for other areas of spectroscopy, not just NMR, that future projects can use as a starting point to also create standards for FAIR data management in those areas as well.

For more information and comments, contact Task Group Chair Robert M. Hanson <hansonr@stolaf.edu> | <https://iupac.org/project/2019-031-1-024>

Development of a Machine Accessible Kinetic Databank for Radical Polymerizations

Machine learning is a young discipline in the chemical sciences that has nonetheless led to significant changes in research approaches in a relatively short time span. Any machine-assisted research approach requires training sets and machine-readable databases to retrieve information from. A standardization of notations allows for data exchange between computer systems and softwares. As an example, the recently introduced BigSmiles (simplified molecular-input line-entry system) notation (Lin *et al.* *ACS Cent. Sci.* 2019, 5, 9, 1523-1531; <https://doi.org/10.1021/acscentsci.9b00476>) allows to exchange structural data for polymer across computer systems.

The IUPAC working party on Modelling of

Polymerization Kinetics and Processes has collated significant kinetic data on free radical polymerization in recent years, and published a series of benchmark papers on the topic. While generally available, still many researchers do not make full use of these data sets. A central database will increase awareness and foster better use of the data. More importantly, a machine-readable database will allow for direct and automated exchange of data. For example, kinetic models can always retrieve the latest and most updated kinetic data for specific monomers. In machine-learning approaches, algorithms can make use the data for deep learning and interconnection with other data such as molecular characteristics, physical properties or further kinetic data. This can range from prediction of materials properties to automated process control in synthesis.

The kinetic database will consist of all IUPAC benchmarked kinetic data for free radical polymerization. A further selection of reliable kinetic data will be made to also include monomers that have not yet been critically assessed. For these monomers, the database can serve as a future starting point for data collection. While not part of this project, the same database could later be extended by other parameters, such as overall time conversion relations, molecular weights, and physical properties of the resulting polymers from polymerization. The database will be designed in a fashion to allow facile extension to either direction. First versions of the database will be hosted via Monash University. Source codes will be published open access and long-term migration of the database to central servers is envisaged.

For more information and comments, contact Task Group Chair Tanja Junkers <Tanja.Junkers@monash.edu> | <https://iupac.org/project/2019-045-1-400>

A review of current status of analytical chemistry education

There is plenty of anecdotal evidence for the erosion of analytical chemistry as a discipline. This is impacted by faculty appointments, funding structures and perception of the field as being a service function. Additionally, as instruments become easier to use there is a mistaken belief in some industrial organisations that there is a reduced need for highly trained analytical specialists. There have been warning signs that the current, university chemistry curriculum, often with a does not address the needs of chemistry graduates and future employers and does not enable analytical

Project Place



practitioners to maximise the value of their work. The project will reflect on the interdisciplinary curriculum development efforts which has been the trend in many universities worldwide. This is a significant economic cost, considering that in many economies the most used practical skills of graduates is actually related to chemical analysis. A deep and fundamental understanding of analytical chemistry is required to foster the next generation of analytical scientists who have the insight and capacity to contribute to fundamental new developments in this field as well as the generation of new disruptive technologies.

The project will document the status quo in various regions of the world regarding the health of the discipline, proportion of professorships, funding and quality

of analytical chemistry education. It will examine current attempts to address these shortcomings and offer some ways forward. The findings will be published in the form of white paper to support future curriculum development, funding and hiring decision.

For more information and comments, contact Task Group Chair Zoltán Mester <Zoltan.mester@nrc.ca> | <https://iupac.org/project/2019-039-3-500>

What is the NPU Terminology, and how is it used?

The NPU terminology is a coding system and terminology for identification and communication, storage, and presentation of examination results from clinical laboratories in the health area. The NPU Terminology is implemented in nearly all electronic systems in laboratory departments at the hospitals, in the private labs, suppliers of laboratory systems and EHRs in Health Care Systems in the three Scandinavian Countries, and the Terminology has proved useful in Health Informatics and in Health Care for more than 15 years, and is today a national standard in Denmark, Sweden and Norway. The problem is that the NPU Terminology is poorly known outside the Scandinavian Countries.

Seeking to increase the general knowledge of the NPU Terminology, create interest, and demonstrate the use and the value of terminology, this project delivered a video and a flyer, both available online at <https://iupac.org/project/2019-009-1-700>.

The background of the NPU Terminology

The form and content of the NPU terminology is based on international recommendations and Standards from:

- The Bureau International des Poids et Mesures (BIPM)
- The International Organization for Standardization (ISO)
- The European Committee for Standardisation (CEN)
- IUPAC Compendium of Chemical Terminology - The Gold Book
- International vocabulary of metrology - Basic and general concepts and associated terms (VIM)
- Vocabulary on nominal property, examination, and related concepts for clinical laboratory sciences (IFCC-IUPAC Recommendations 2017) (VIN)
- Compendium of Terminology and Nomenclature of Properties in Clinical Laboratory Sciences -The Silver Book
- Recommendations and Technical Reports from IUPAC-IFCC, published since 1966

A joint IFCC-IUPAC Committee-Subcommittee on Nomenclature for Properties and Units (C-SC-NPU) has been an active participant in much of this work, describing and harmonizing the NPU terminology of the various subject fields. Maintaining and adding entries to the terminology is done in a continuous process according to the advice of the C-SC-NPU.



For more information: www.npu-terminology.org

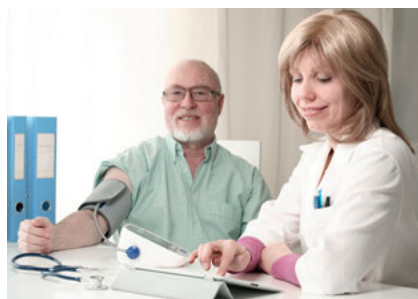
Contact: Helle Møller Johannessen hmj@sundhedsdata.dk

June 2019



NPU Terminology

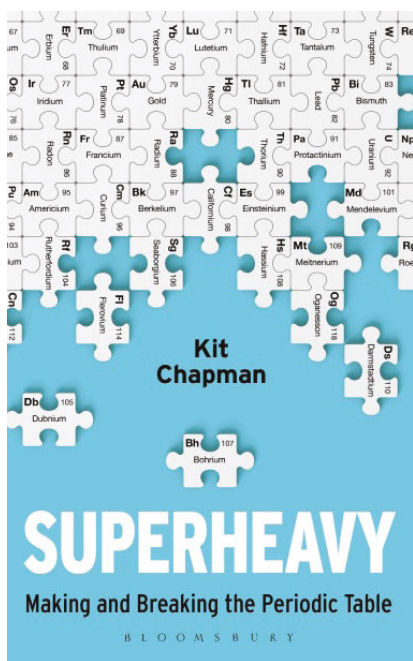
An IUPAC-IFCC succes in Health Care



The NPU Terminology (NPU: Nomenclature for Properties and Units) is a patient centered clinical laboratory terminology for use in the clinical laboratory sciences.

The terminology is in use today in Denmark, Norway and Sweden, where standardized reporting of laboratory results in health care is communicated on a national basis.





Superheavy

Kit Chapman
Bloomsbury Sigma,
2019

Reviewed by Juris
Meija, Chair, IUPAC
CIAAW

As the world celebrates the 150th anniversary of the Periodic Table in 2019, this book offers a most unique inside view into the makings of one of the greatest icons of humanity. Many books have told the stories of classical chemical elements, yet little is available

to cover the contemporary discoveries of all those elements way past the uranium which, to be frank, most chemists have never heard of. This book is a masterful science travelogue as Chapman has met most key players involved in expanding the Periodic Table.

The book opens with a vivid account of the first isolation of plutonium in the Gilman Hall attic at Berkeley. While the official accounts place this event on 23 Feb 1941 and during a storm, Chapman has poured over the meteorological records to contradict this historical date. While seemingly innocuous, this detail illustrates the rigor and effort it has taken to craft this book. Indeed, much of science revolves around gathering information from diverse sources and on how we go about resolving any discrepancies as they emerge. This charming vignette exemplifies scientific journalism at its best.

So what does it take to make an element? Chapman shows that besides hard-work it may also take circumstance (as with Seaborg), resourcefulness (Segré), or perseverance (Morita). Chapman also does not shy from exposing the more shameful cultural practices that have denied early access or recognition to talented scientists for simply not being male. In doing so, Chapman provides a counterpoint to the male-dominated role models with many strong female element hunters: champions such as Darleane Hoffman, Nancy Stoyer, Clarice Phelps, or Dawn Shaughnessy. More importantly, Chapman shows that in 2019 our search for science role models does not have to stop with Mendeleev and

his deeply flawed character—we can do much better.

Science needs, in fact demands, books detailing deeply engaging contemporary endeavors of its heroes. People do not become enchanted with science by reading Wikipedia entries; it is personal stories like Levi's *The Periodic Table* or Curie's *Madame Curie* that spark the interest of next generation scientists. Told through countless first-account interviews, Chapman's well-researched *Superheavy* is such a book. Do a service to science—give this book to your nephews and nieces.

Biomass Burning in Sub-Saharan Africa: Chemical Issues and Action Outreach

Liliana Mammino, editor

Springer, ISBN 978-94-007-0808-2, Feb 2020

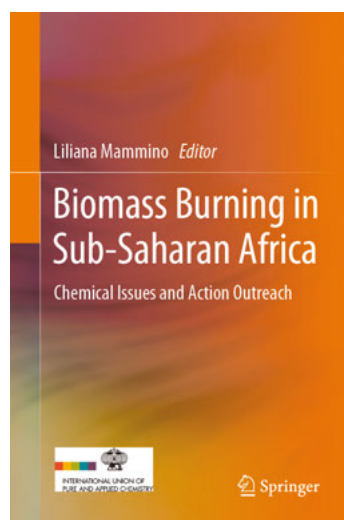
This book offers a comprehensive overview of the various aspects involved in biomass burning, highlighting the complexity of the phenomenon and the ensuing challenges for the design of approaches aimed at reducing fires in the open air.

Chemical issues are discussed in the first 7 chapters, providing the core of the scientific and technical information. In the following chapters, experts in the human sciences provide information on people's attitudes and perceptions. Both types of expertise are needed in the design of interventions that can motivate people and communities to opt for sustainable practices.

In closing, this book underscores the importance of pursuing an interdisciplinary approach in order to tackle the problem effectively. It offers a valuable resource for undergraduates, graduates, and policymakers working in the fields of chemistry, environmental science, science education and sustainability.

This book was conceived as part of IUPAC project 2007-025-1-300, <https://iupac.org/project/2007-025-1-300>.

The content is available on the publisher's website at <https://www.springer.com/gp/book/9789400708075>



Successful Drug Discovery

by János Fischer

The IUPAC Subcommittee on Drug Discovery and Development is a section of the Chemistry and Human Health Division (Div VII) of IUPAC. Additional subcommittees are the Subcommittee on Toxicology and that on Clinical Chemistry. I received an invitation to join the drug discovery subcommittee in 1998 from Camille Wermuth, who was a famous professor of medicinal chemistry in Strasbourg. His books are very useful for researchers of medicinal chemistry. "The Practice of Medicinal Chemistry" was published in 1996 by Academic Press, and "The Handbook of Pharmaceutical Salts," co-edited with Heinrich Stahl, was published in 2002 by Wiley-VCH.

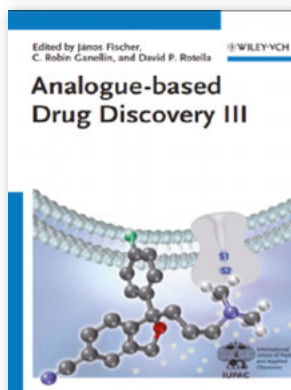
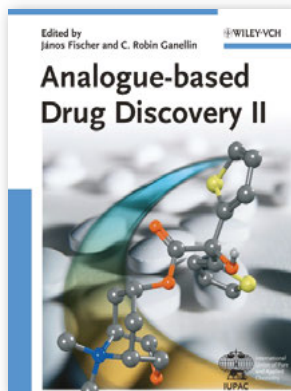
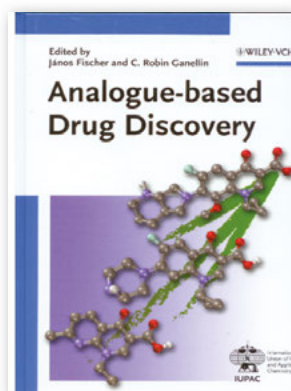
The Drug Discovery Subcommittee had several well-known participants from various countries and different companies and academic institutions. Robin Ganellin, professor of medicinal chemistry in London, having founded the Subcommittee, played the most important role both as member and later as leader of this group. He was one of the inventors of cimetidine, the first blockbuster in the history of drug discoveries. It is used for the treatment of heartburn, dyspepsia and hyperacidity. Its commercial use started in 1977 in Europe, and in 1979 in the United States. Robin Ganellin also participated in the discovery of pitolisant, which was approved in Europe in 2016 for the treatment of narcolepsy (it is the subject of Chapter 13 in Volume 3 of "Successful Drug Discovery" —see below). Robin initiated several projects as the leader of the Drug Discovery subcommittee. I was lucky to have had the opportunity to work with him as co-editor on the book series "Analogue-based Drug Discovery" between 2006–2013.



Left, Professor Wermuth speaks at a drug discovery meeting in Modena in 2005. At right, Robin Ganellin in 2009, when he presented a lecture in Budapest at the Richter Company.

Three volumes of "Analogue-based Drug Discovery" were published in 2006, 2010, and 2013, and each volume represented a IUPAC project. The first volume included 19 chapters set in three parts. In the first part, Part I, the topic of analogue-based drug discovery was discussed from different viewpoints: Camille Wermuth gave an overview on the analogues and the analogue approach in drug research; John Proudfoot studied the role of drug-like properties in analogue-based drug discovery; and Hugo Kubinyi analyzed the term "privileged structure" and reviewed chemogenomics as a strategy in drug research. Part II consisted of drug class studies and case studies: the main goal was to demonstrate how the activity profile of drugs was optimized within different drug classes. Robin Ganellin described the H_2 -receptor histamine antagonists. My task was to write chapters on the HMG-CoA reductase inhibitors, the ACE inhibitors and the angiotensin-II receptor blockers. Several case studies were prepared by key inventors who were also members of the IUPAC subcommittee on drug discovery: Gioavanni Gaviraghi described the story of lacidipine, a calcium antagonist. Joerg Senn-Bilfinger wrote a chapter on the discovery of pantoprazole, a proton-pump inhibitor. Rudolf Wiechert summarized the discovery of drospirenone. Part III was a table of analogue classes with the structures and important data of the drugs. (See ref. 1 for a review published in C/)

These books were part of an effort to counteract the derogatory use by some commentators of the term "Me-too" drugs. This was part of the approach to



The cover designs of the first three editions of *Analogue-based Drug Discovery*.

slander the drug industry for just making easy copies of medicines to boost their profits. The point is that successful analogue drugs were not simply copies but always had some clinical advantage. Indeed this is actually the way that drug action is optimised to give the best available medical use.

The project-based model of IUPAC facilitated our work. Projects usually last for two years and provide modest financing that covers travel costs to project and subcommittee meetings.

Last but not least, a good working relationship with the publisher Wiley-VCH has contributed to our work. Frank Weinreich, the contact person at the publisher, was an excellent partner to the editors.

For the third volume David Rotella joined the editorial board and it was he who suggested starting a new series entitled “**Successful Drug Discovery**” that would cover all drug discoveries, not only the analogue-based ones.

The new book series “Successful Drug Discovery” has a broad scope encompassing both small-molecule drugs and biologics and the books focus on recently approved drugs. The first volume was edited by David Rotella and myself and we co-authored a introductory chapter on the role of serendipity in target-based drug discoveries. Nowadays drug research is based on molecular biological targets; nevertheless, one should not forget that the serendipity often plays an important role in those target-based drug discoveries as well. Serendipitous target-based drug discoveries have been realized in development of several marketed drugs, including drosiprenone, escitalopram, ezetimib, lamotrigine and omeprazole. Our contribution was reviewed by key inventors. The second part of the book was an excellent overview of insulin analogues, written by John M. Beals from the Eli Lilly company. This chapter about an analogue-based project would have fit equally well in the previous series “Analogue-based Drug Discovery” since insulin analogues have taken on a dominant role in the treatment of Type 1 of diabetes. In the third part of this book eight case studies were provided by their key inventors. As an example I would like to mention William N. Washburn’s chapter on dapagliflozin (Bristol-Myers Squibb), a pioneer drug, which acts as SGLT2 inhibitor. Dapagliflozin plays an important role in the treatment of Type 2 of diabetes. Another example is pemetrexed, a drug that resulted from an excellent long-term collaboration between academia and industry. It is a drug for the treatment of non-small lung cancer. The author of the chapter on pemetrexed was Edward C. Taylor from Princeton

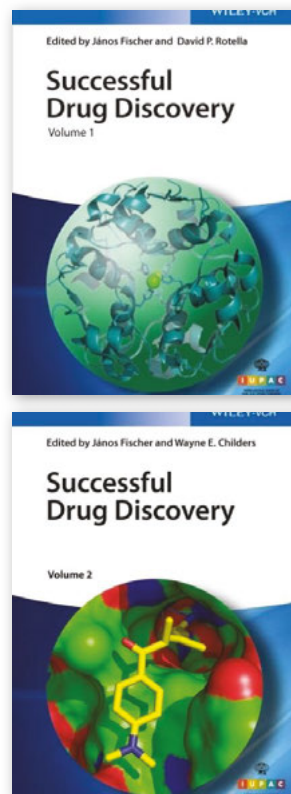
University. The book also included an example of a biologic drug in the case study of trastuzumab emtansine, an antibody-drug conjugate for the treatment of HER-2-positive cancer.

The cover design of the first volume derived from a figure of insulin, in which an insulin hexamer is stabilized by two zinc ions. This spherical motif was subsequently maintained for the covers of all the following volumes of this book series.

The first volume resonated well with the scientific community and, in agreement with the Publisher, we continued our work. Co-editors János Fischer and Wayne E. Childers (Temple University, Philadelphia) collected eleven case studies of new drugs from different therapeutic fields. It is not an easy task to organize such a book series, which is based on the invitations of the editors. First, enough interesting topics to support 10-12 chapters

must be identified. The number of the FDA-approved drugs between 2015-2018 amounts to 172. That means that only a restricted part of new drugs can appear in the book. To insure that the subject matter is timely, each volume should mirror the most important trends of modern drug research. Secondly, the key inventor or expert for each chapter must be identified, which is again not an easy task because drug discovery and development is a team effort involving several experts. When the editors are lucky to get a positive response to the invitation, then a third question arises: whether a given company is willing to approve such a publication. Beside these three questions there are several individual issues, which the editors must also solve.

In the second volume the case history of sofosbuvir was an excellent contribution from Michael Sofia (Arbutus Biopharma). This drug has played an important role in the treatment of hepatitis C. A separate part of this volume was a section covering the HDAC-inhibitor anticancer drugs. The section editor of this part was Professor Ganesan (Norwich University, UK), a



member of the IUPAC drug discovery subcommittee. The schematic model of belinostat served as a motif for the cover design. This volume contained case studies from six different therapeutic fields and was published in 2017.

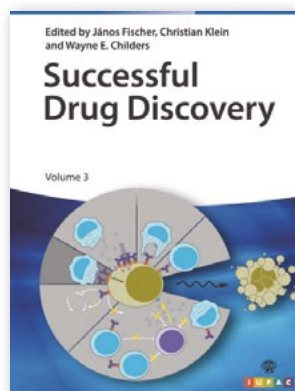
Today, every third drug is a biopharmaceutical product and we were fortunate that Christian Klein (Roche, Zurich) joined the editorial board as an expert of biologics. The third volume contained 15 chapters and appeared in 2018. In this volume we introduced a book structure consisting of three parts, as follows:

- Part I. General Aspects
- Part II. Drug Class Studies and
- Part III. Case Studies.

In the first part, Gerd Schorrenberg, the Chair of the IUPAC Subcommittee of Drug Discovery and Development, gave an overview on new trends in drug research. He wrote in his chapter that the differences between New Chemical Entity (NCE) and the New Biological Entity (NBE) discoveries are beginning to blur and that scientists from both areas need to learn from each other. This observation supports and confirms our decision to publish the achievements of both small and large molecule drug research in the same book series. Out of the drug class studies the overview on kinase inhibitors should be mentioned, which was written by Peter Wu (Harvard Medical School). This volume was also rich in case studies; all together 11 case studies appeared in this volume, 8 case studies of small molecule drugs and 3 case studies of biopharmaceutical products. The cover design of the book derived from a figure of daratumumab. The chapter on this monoclonal antibody was provided by Maarten L. Janmaat (Genmab) in cooperation with Johnson and Johnson. Daratumumab is approved for the treatment of multiple myeloma.

The book series focuses on interesting drug discovery stories, so the commercial success of a drug does not influence its selection as a topic. Nevertheless,

I would like to mention that in the case of the third volume, two drugs achieved blockbuster status (i.e. sales are higher than \$ 1 billion/year). One of the blockbuster drugs from Volume 3 (daratumumab) has already been mentioned. The other is osimertinib, a small molecule EGFR inhibitor for the treatment of non-small cell lung cancer. The author of



2015 : 45 drugs approved by FDA

Darzalex	(daratumumab)	SDD-Vol-3	case study
Farydak	(panobinostat)	SDD-Vol-2	case study
Lenvima	(lenvatinib)	SDD-Vol-4	case study
Lonsurf	(trifluridine/tipiracil)	SDD-Vol-3	case study
Rexulti	(brexpiprazole)	SDD-Vol-4	drug class study
Tresiba	(insulin degludec)	SDD-Vol-1	drug class study
Vraylar	(cariprazine)	SDD-Vol-4	drug class study

16 % appeared in SDD-books

2016 : 22 drugs approved by FDA

Spinraza	(nusinersen)	SDD-Vol-5	drug class study
Ocaliva	(obeticholic acid)	SDD-Vol-3	case study
Rubraca	(rucaparib)	SDD-Vol-4	case study
Venclexta	(venetoclax)	SDD-Vol-4	case study

18 % appeared in SDD-books

2017 : 46 drugs approved by FDA

Kymriak	(tisagenlecleucel)	SDD-Vol-5	drug class study
Yescarta	(axicaptogene ciloleucel)	SDD-Vol-5	drug class study
Kisquali	(ribociclib)	SDD-Vol-5	case study
Hemlibra	(emicizumab)	SDD-Vol-5	case study
Parsabiv	(etelcalcetide)	SDD-Vol-4	case study
Ocrevus	(ocrelisumab)	SDD-Vol-4	case study
Xadago	(safinamide)	SDD-Vol-3	case study
Ozempic	(semaglutide)	SDD-Vol-5	drug class study

17 % appeared in SDD-books

2018 : 59 drugs approved by FDA

Ajovy	(fremanezumab)	SDD-Vol-5	drug class study
Emgality	(galcezezumab)	SDD-Vol-5	drug class study
Aimovig	(erenumab)	SDD-Vol-5	drug class study
Tegsedi	(inotersen)	SDD-Vol-5	drug class study
Tibsovo	(ivosidenib)	SDD-Vol-5	case study
Onpattro	(patisiran)	SDD-Vol-5	drug class study

12 % will appear in SDD-Vol-5

Table: Drugs appeared in SDD series out of the FDA approvals.

the osimertinib chapter was Michael Waring (Newcastle University, UK).

One interesting analysis of the "Successful Drug Discovery" series to date is the ratio of FDA-approved drugs to the drugs which have been published as case studies or drug class studies in the books to date. In 2015 the number of FDA-approved drugs amounted to 45. Seven of these drugs were discussed in the books (i.e. 16 %). In 2016, the FDA approved 22 drugs and 4 of these approved drugs appearing in the books (18 %). In 2017 the number of FDA approvals was 46 and 8 of those drugs were the subjects of a case study or a drug class study in the books (17 %). Finally in 2018 a very high number of drugs was approved by the FDA (59) and 6 of those approved drugs were published in the books (11 %). One should emphasize that these numbers are constantly changing, since subsequent volumes may increase these ratios. (see Table)

The books within the series "Successful Drug Discovery," which is supported by IUPAC projects, are useful for three reasons. First of all they afford reference books for drug researchers. These books are useful as tools to teach medicinal chemistry and biological drug research scientists. Last but not least, these books represent a publication forum of successful drug research to herald the achievements of scientists who have devoted their lives to making the world a better, healthier place to live.

Volume 4 and 5 are under preparation; see <https://iupac.org/project/2019-021-1-700>.

János Fischer <j.fischer@richter.hu> is working at Richter Plc. in Budapest, Hungary and a member of the Chemistry and Human Health Division of IUPAC. <https://iupac.org/member/janos-fischer/>

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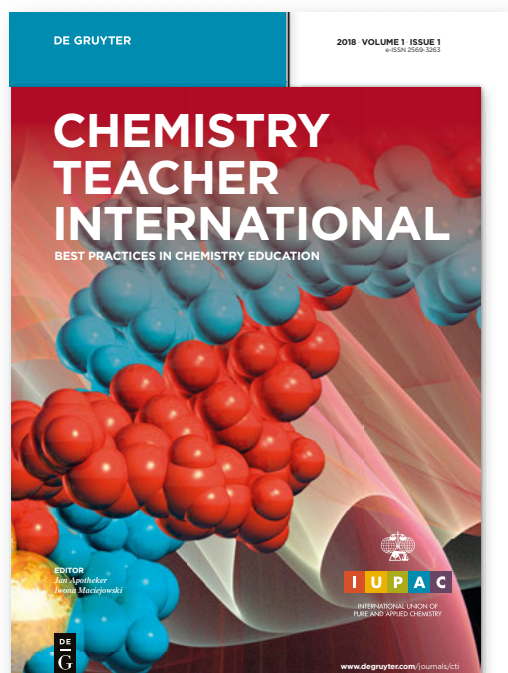
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"Analogue-based Drug Discovery" afforded three books published by Wiley-VCH in 2006 (IUPAC project 2002-051-1-700), 2010 (project 2008-013-1-700) and 2013 (project 2011-011-1-700).

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Successful Drug Discovery, Volume 2, Janos Fischer (Editor), Wayne E. Childers (Editor), ISBN: 978-3-527-34115-3, June 2017 WILEY-VCH Verlag, Print ISBN:9783527341153 | DOI:10.1002/9783527800315

Successful Drug Discovery, Volume 3, János Fischer, Christian Klein, and Wayne E. Childers (eds.), April 2018, Wiley-VCH Verlag, Print ISBN: 9783527343034 | DOI:10.1002/9783527808694



Chemistry Teacher International (CTI) is a peer-reviewed Open Access journal from the Committee on Chemistry Education of IUPAC. The journal aims to be a platform for teachers of all levels, focusing on researchers in chemistry education. The objectives of the journal are:

- Bridging the gap between research and education
- Creating a platform for all IUPAC activities in the field of education
- Building an international journal not linked to a specific area or nation

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Conference Call

The World Chemistry Leaders meet the century-old IUPAC

by Christopher Ober

The 2019 World Chemistry Leadership Meeting (WCLM) was a special and rare opportunity to bring together leaders of industry to IUPAC's 50th General Assembly during its 100th anniversary and the 150th anniversary of the periodic table. This meeting enabled leaders of chemical industry to provide their view of the future of the chemical industry in the context of challenges facing society and the UN sustainable development goals. IUPAC was founded in part because of the strong interest by the chemical industry of 100 years ago in having a common language of chemistry to facilitate trade between countries. That effort to develop this important language has largely succeeded and today IUPAC, while continuing that original mission in the cyber connected world, is a societal educator and provides an important forum for open discussions of the role of chemistry in society.

Our panelists included the following CEO's: Martin Brudermüller (BASF SE), Andrey Grigoryevich Guryev (PhosAgro), Ilham Kadri (Solvay), and Thierry Le Hénaff (Arkema). Solvay, it should be noted, was one



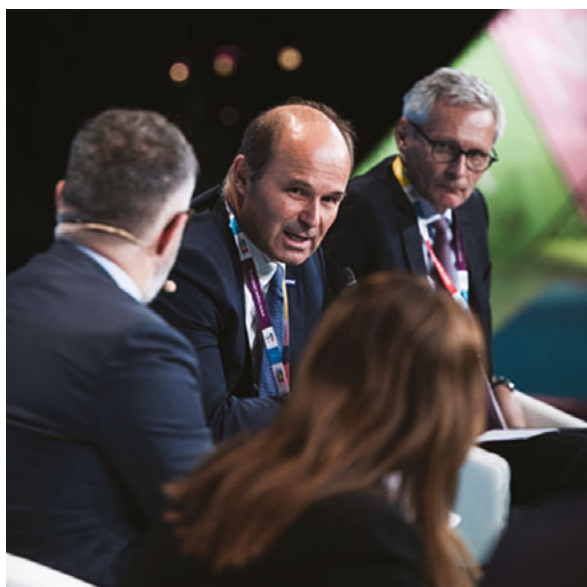
The WCLM featured a discussion with several CEOs. From left: Andrey Grigoryevich Guryev (PhosAgro), Ilham Kadri (Solvay), Paul de Brem (scientist journalist/moderator), Martin Brudermüller (BASF SE), and Thierry Le Hénaff (Arkema).

of the founding companies of IUPAC so it was appropriate to hear from them and other chemical companies on the occasion of IUPAC's centenary.

The meeting was introduced by Christopher Ober and Frances Separovic who asked our panelists to discuss the chemical industry in the context of the United Nations Sustainable Development Goals (SDGs). The SDGs were adopted by world leaders in September 2015 at an historic United Nations summit and were the subject of a prior WCLM held in Busan, South Korea in 2015. A report of that meeting is described in a previous article published in *Chemistry International* [1]. At this prior meeting leading academics including a Nobel prize winner discussed the UNSDGs and Young Observers in attendance drafted project proposals aimed at sustainable chemistry. In Paris, the 2019 WCLM gave the GA and conference attendees a chance to hear from industry on this topic.

Separovic briefly summarized the 17 Goals of the 2030 Agenda for Sustainable Development for the audience and the panelists. The SDGs represent a blueprint to achieve a better and more sustainable future for all. Briefly, these goals are:

1. End Poverty;
2. Zero Hunger;
3. Good Health & Well-Being;
4. Quality Education;
5. Gender Equality;
6. Clean Water & Sanitation;
7. Affordable & Clean Energy;
8. Decent Work & Economic Growth;
9. Industry, Innovation & Infrastructure;
10. Reduced Inequalities;
11. Sustainable Cities & Communities;
12. Responsible Consumption & Production;
13. Climate Action;
14. Life Below Water;
15. Life on Land;
16. Peace, Justice & Strong Institutions;
17. Partnerships for the Goals.



Martin Brudermüller speaks about the future of chemistry.

The SDGs are a call to action to promote prosperity while at the same time protecting the planet. They recognize that ending poverty must go hand-in-hand with strategies that build economic growth and address the global challenges we face, including those related to poverty, education, health, social protection, and job opportunities, while tackling climate change and environmental protection.

A successful sustainable development agenda will require partnerships between governments, the private sector and the chemistry community, and diverse partnerships will be essential at all levels (global, regional, national and local) to bring about better solutions. Given the importance of both the fundamental and the applied aspects of IUPAC to finding such solutions it was invaluable to have this dialog.

During the panel discussion these corporate leaders made the point that the chemical industry subscribes to and supports the SDGs and considers it a roadmap that provides clear structure and priorities. They noted that stable goals by governments are essential for long term planning and action. And they pointed out that today the chemical industry aligns its projects and activities with the SDGs as key providers of sustainable solutions to society, e.g., growing food more efficiently, improved renewable energy, or reducing poverty.

Our panelists described a global industry, that like IUPAC, believes in the value of education—educating the consumer, educating users of chemical products such as farmers, and educating people about the value of chemistry to providing future solutions. For example, industry trains farmers in new agriculture technology that both raises incomes and helps to feed developing countries.

Industry is addressing climate change by reducing CO₂ emissions, making lighter vehicles to reduce fuel use and providing better energy storage materials. Executives told the audience assembled at this plenary event that decisions must be good for people, the planet, yet still provide a profit.

Diversity is also an important element of the SDGs and industry is working hard on this aspect. There was extensive discussion on this topic leading up to the presentation of the IUPAC Distinguished Women in Chemistry awards for 2019. Inclusion and Diversity are extremely important. Emphasis should be according to the panelists on an inclusive culture (support, advocacy, ensuring everyone is part of a team). Companies with diverse leadership teams have a statistical and sustained improvement in financial performance.

In a closing talk Bruder Müller (BASF) gave an impressive presentation that summarized these points

and also discussed ways for industry to engage with the public on sustainability through the alliance for ending plastic waste. It will take industry working with consumers to solve this problem and consumers will have to support sustainable solutions and change some of their habits while industry rethinks some of its approaches.

The chemical industry finds that setting tough targets on sustainability requires innovation and in that way attracts the best talent to its community. Bruder Müller concluded that innovation needs diversity and openness.

It is clear that both industry and IUPAC want the United National Sustainability Goals to succeed. IUPAC supports the UN SDGs and is working to convey to the public the importance of chemistry in providing societal solutions. There are numerous opportunities for IUPAC to work with industry and it is our hope that WCLM held during this year of the IUPAC centenary will lead to greater and long term interactions working towards these common goals of serving society.

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Noncovalent Interactions

By Kamran T. Mahmudov and Armando J.L. Pombeiro,
Conference Chairs
1st ICNI (2019)

Intermolecular interactions were first taken into consideration by van der Waals in 1873 in adapting the ideal gas equation of state for real gases [1]. The energetics and structures of molecules as well as the reactivity and selectivity of their reactions are strongly dependent on the type of noncovalent interactions, such as hydrogen, noble gases, halogen, chalcogen, pnictogen, tetrel, triel and pancake bonds, cation- π , anion- π , lone pair- π , π - π stacking, agostic, pseudo-agostic, anagostic, metal-metal, dispersion-driven, lipophilic interactions, etc., which can play a crucial role in synthetic transformations, catalysis, crystal engineering, drug design, materials, molecular biology, molecular recognition, etc.

The past thirty years have seen remarkable advances in this field,



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for example, several books in major publishers [2-6], a special issue namely “Aromatic Interactions” in *Accounts of Chemical Research* in 2013 (Edited by Prof. Marcey L. Waters) [7] and thematic issues on noncovalent interactions in *Chemical Reviews* in 1988, 1994, 2000 and 2016 (Edited by Prof. Pavel Hobza) have been published [8]. Moreover, the hydrogen, halogen, and chalcogen bonds have already been defined by IUPAC (Recommendations 2011, 2013 and 2019, respectively) [9], and the definitions for pnictogen and tetrel bonds are under progress [10]. International Conferences have also been held, namely “Horizons in Hydrogen Bond Research” (established by Lucjan Sobczyk in Poland in 1977), the International Symposium on Halogen Bonding (established by Pierangelo Metrangolo and Giuseppe Resnati in Porto Cesareo (Lecce, Italy) in 2014), the first and second Humboldt Conferences on Noncovalent Interactions (chaired by Snežana Zarić in Serbia in 2007 and 2009, respectively), the Workshop “Aromatic Interactions in Chemistry and Biology” (organized by Ken Houk and Marcey L. Waters in Mesilla, New Mexico in 2011), the 54th Symposium on Theoretical Chemistry (the topic of the conference was “Noncovalent Interactions”, chaired by Daniel Sebastiani) in Germany in 2018, etc.

In order to discuss all sorts of noncovalent interactions, contributing towards a scientific systematization of the field, and share ideas, the **1st International Conferences on Noncovalent Interactions (ICNI)** was held from 2-6 September 2019 in Lisbon, Portugal, being chaired by the authors [11,12]. Further editions within this series will be followed every two years, in odd number years (2021, 2023, etc.).

The International Advisory Board members of ICNI are well-recognized scientists (including 9 women) in this field [11,12], representing Europe, Asia, Africa and America. ICNI has already been recognized by IUPAC for endorsement, although without financial support [13]

The logo of the 1st ICNI edition is based on a form



A special coin was created to commemorate the conference



Opening ceremony. Prof. Dario Braga, Prof. Armando J.L. Pombeiro, Dr. Kamran T. Mahmudov and Prof. Djamaladdin G. Musaev (from left to right).

of representation of interactions, and it can be easily adapted to the subsequent editions. A conference celebratory medal was also coined, with its logo. The reverse of the medal was inspired on the types of noncovalent interactions.

We have also established “**The van der Waals Prize**” at the 1st ICNI 2019. This distinction was awarded for the first time on the occasion of this Conference to Pavel Hobza as a recognition of his outstanding achievements in this field.

The Conference was broadly international, with approximately 250 participants representing 36 countries. After Portugal, the Russian Federation and Japan were dominant (27-25 attendees for each). They were followed, in number of delegates, by China, Spain, Poland, and the USA. Then came the Czech Republic, France, and the UK. The Conference aimed to highlight the role of Noncovalent Interactions in synthesis (23 contributions), catalysis (32 contributions), crystal engineering (55 contributions), molecular recognition (30 contributions), medicinal chemistry (11 contributions), biology (5 contributions), materials science (32 contributions), electrochemical immobilization (2 contributions), and theoretical aspects (56 contributions). All approaches were considered, from fundamental to applied ones, including discussion of new types of noncovalent interactions (halogen, chalcogen, pnictogen, tetrel and triel bonds) and multidisciplinary studies.

The Conference Program included 18 plenary lectures (45 minutes each), 22 keynote lectures (30 minutes each), 60 invited lectures (20 minutes each), 43 oral communications (15 minutes each), 7 flash presentations (5 minutes each) and 102 posters. Moreover, there were 5 poster prizes (Presented by Ms. Amelia Newman, Editor at RSC): Chemical Science (Anh Tuan Pham, University of Geneva, Switzerland), Dalton Transactions (Sara R.G. Fernandes, University

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of Lisbon, Portugal), RSC Advances (Errui Li, Zhejiang University, China), Inorganics (Elena Tupikina, Saint Petersburg State University, Russia) and Pharmaceuticals (Claudia C. Gatto, University of Brasília, Brasil).

In order to highlight a particular type of noncovalent interaction in this ICNI first edition we selected π -interactions for one conference day. Thus, there were 3 plenary (Tutorial), 2 keynote and 6 invited lecturers on π -interactions. This approach can be continued in the next editions of ICNI by highlighting other types of noncovalent interactions.

Due to the broad/multidisciplinary character of noncovalent interactions we established a themed collection (named "1st International Conference on Noncovalent Interactions") published in various RSC journals, such as *Chem. Comm.*, *Chem. Sci.*, *J. Mat. Chem. A*, *Dalton Trans.*, *RSC Adv*, *New J. Chem.*, *CrystEngComm.*, *Phys. Chem. Chem. Phys.* [11,14]. The selected topics

reflect the current trends in weak bonding chemistry. Each article was peer-reviewed as in the usual submissions. Their themed collection gathers 181 papers which can inspire researchers, students, and newcomers in the fields of noncovalent chemistry and related interdisciplinary subjects.

The 1st ICNI International Advisory Board (IAB) meeting was held on 4 September 2019 at the Conference venue, and the following points were agreed: *i*) the next ICNI editions will be in 2021, 2023, 2025, *etc.*; *ii*) the ICNI 2021 and the ICNI 2023 will be held in Strasbourg (Chairman: Jean-Pierre Djukic) [15] and in Moscow (Chair persons: Elena Shubina and Oleg Fillipov), respectively; *iii*) further collaboration of ICNI and RSC should be reached; *iv*) the IAB formally agreed on a proposal, from the Chairs of the Conference, for the establishment of the award named "The van der Waals Prize," to distinguish scientists of high scientific

International Advisory Board

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F. Dean Toste	University of California, USA
Leyong Wang	Nanjing University, China
Andrew S. Weller	University of Oxford, UK
Steven E. Wheeler	University of Georgia, USA
Snežana D. Zarić	University of Belgrade, Serbia

merit who have contributed in an outstanding way to the development of the field of Noncovalent Interactions in Science; in addition, it was further agreed that this prize should distinguish a senior and a young (not older than 45 years) scientist in *alternating years*; v) if an IAB member misses two consecutive editions of ICNI, he/she should automatically be released from the IAB list; vi) Dr. Kamran T. Mahmudov was nominated the Secretary of ICNI; vii) the minutes of the meeting should be circulated to all the IAB members and their feedback would be collected and incorporated.

We warmly thank the IAB and Local Organization Committee members and participants for their support and valuable contributions. Mike Andrews and Amelia Newman of the Royal Society of Chemistry are much appreciated for their kind assistance to organize the themed collection at the RSC.

As mentioned above, the 2nd edition of this conference, ICNI 2021 (<http://icni2021.unistra.fr/>), will be held in Strasbourg, France, 19-23 July 2021, chaired by Prof. Jean-Pierre Djukic.

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IUPAC For Africa

IUPAC Postgraduate Summer School on Green Chemistry 12-19 May 2019 - Dar es Salaam (Tanzania)

The IUPAC Postgraduate Summer School on Green Chemistry took place in Dar es Salaam, Tanzania from 12-19 May 2019. Dar es Salaam is the commercial center of Tanzania and one of the biggest cities in East Africa, nestled along a natural harbour on the Indian Ocean.

The present edition of the Summer School was the first IUPAC Summer School on Green Chemistry to be held in Africa managed by **IUPAC Interdivisional Committee on Green Chemistry for Sustainable Development (ICGCSD)**.

The event was proposed by its Chairman, Pietro Tundo from Ca' Foscari University of Venice, Member of the IUPAC Bureau and Chair of ICGCSD, in collaboration

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with the late Egid Mubofu of Tanzania. The event was therefore, initially managed under the organization of the late Mubofu as the chairperson of the Organizing Committee in Tanzania and later on the chairmanship was given to Charles Kihampa after the death of Mubofu. Kihampa managed the event with a team composed of Esther H. J. Lugwisha, Kessy F. Kilulya, Clarence A. Mgina, Joan J. E. Munissi from the University of Dar es Salaam, Rehema Nyamoga from the Tanzania Bureau of Standards (TBS) and Mr. Elias Mlima from the Government Chemist Laboratory Authority in Tanzania. The event was endorsed by the Tanzanian Ministry of Education, Science, and Technology.

The School was Hosted by the Chemistry Department of the University of Dar es Salaam in collaboration with the Tanzania Chemical Society (TCS), TBS, the University of Dodoma (UDOM) and the Government Chemist Laboratory Authority (GCLA), and sponsored by IUPAC, PhosAgro, the Organization for the Prohibition of the Chemical Weapons (OPCW), UNEP, IUCEA, ISC3 and NEMC.

Main topics of the Summer School were:

- Exploitation of Natural Resources,
- Green Methodologies Chemistry,
- Green Analysis,
- Green Synthesis of materials,
- Green Technologies and
- Recycling

The choice of Tanzania as the host country for the first IUPAC Postgraduate Summer School in Africa has offered the opportunity to more collaboration for African chemists, chemical institutions, universities and chemical societies.

85 Selected post-graduated attendees and 16 resource persons coming from 22 different countries participated in the Summer School in Dar es Salaam. In total, 143 applications were received, and 51 paying students were considered eligible to attend the school after a thorough selection by the Organizing Committee based on their CVs and list of publications. 53 Scholarship applications were received by 28 February 2019 from students coming from developing countries. A Scientific Committee composed of 8 IUPAC members selected a first list of 36 applications on merit bases out of the 53 received scholarship applications. The first 34 students of the list were awarded with a scholarship to attend the school from IUPAC, UNEP, PhosAgro and IUCEA.



Group Picture after the opening ceremony of the IUPAC Summer School on Green Chemistry: Monday 13 May 2019, Dar es Salaam Tanzania.

The Organizing Committee expectations were completely met for the quality of resource persons, student,s and the diversity of participants in terms of their geographical origin and also on their professional affiliations. During the event all of the young academicians could contribute their thoughts and ideas on relevant issues of green chemistry and sustainability. All students had an opportunity to have a flash presentation of their posters at a session which provided them the chance to exchange their scientific knowledge and establish important links with other participants and professors for fruitful joint projects and research activities. This was a real success for this summer school.

2019 PROGRAMME

DAY 1

Arrival of participants

DAY 2

Opening Ceremony

The opening ceremony started with welcoming remarks from Charles Kihampa, Chairman of the Organizing Committee.

Followed by Qi-Feng Zhou, IUPAC President, then Pietro Tundo, Chairman ICGCSD, W. Anangisye, VC UDSM. Guest of Honor: Edwin Mhede; Deputy Permanent Secretary on behalf of the Minister for Industries, Trade and Investments and lastly was the vote of thanks delivered by Charles Kihampa, Chairperson of TCS.

Session I Chair: C.A. Mgina

The First Session after opening ceremony had three presentations;

- a. Q.A. Mgani: *Tribute to Egid Mubofu*—this was a special session to commemorate the late Mubofu who was the first chairman of the summer school local organizing committee in Tanzania.

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- b. Siroj Loikov, Deputy Director General for International Projects, PhosAgro: *Promotion of green and sustainable chemistry by PhosAgro*
- c. Peter Licence: *Ionic Liquids in vacuo—Suck it and see!*

The first session continued after the lunch break with two presentations:

- Pietro Tundo: *What is green chemistry— Principles*
- Christopher Brett: *Green Materials and Electro-chemistry*

Poster Session

The first session continued after tea break where students had the opportunity to display their posters.

DAY 3

SESSION II: Chair: Prof. Obuzor

- Neil Coville: *Carbon nanomaterials from propylene waste*
- Darkwa: *Catalysis driven conversion of substrates in chemical production: selected examples.*
- Kasozi: *Environmental sustainability utilizing renewable feed-stock, chemical waste and recycling*

Poster Short Presentations

After lunch students were given five minutes to give brief descriptions of their posters. The poster session then continued with visiting posters after the afternoon tea break.

DAY 4: Excursion

This was an excursion day where participants had opportunities to visit the Zanzibar Island, the old city the ancient city of Bagamoyo, and the Dar es Salaam city itself.

DAY 5

Session III Chair: Kasozi

The session started with one presentation until tea break.

- Nannake-Abasi Offiong: *Exploitation of Natural Resources: "Surfactants for Groundwater Remediation from Green and Renewable Feedstocks"*

The rest of the day was for lectures from UNEP officials about the 17 UN Sustainable Development Goals followed by Poster short presentations and visits.

DAY 6

Session IV Chair: Prof. Coville

The session started with short poster presentations followed by lectures

- Tundo: *The Chemistry of Dimethyl Carbonate*
- Mammino: *The design of environmentally-Benign substances: Interfaces between green chemistry and computational chemistry*
- Urassa: *Global Networking for Professional Training and Development in the Chemical Sciences: ACS Model*
- John Ryan: *Green Chemistry and Pyrolysis*

At the end of the session the name of the five best posters were announced.

DAY 7

Session V: Chair: Dr. Kasozi

The session had two lectures and was followed by oral presentations from the best five posters before the closing ceremony

Lectures

- Xuefeng Jiang: *Green Organosulfur Chemistry*
- Gloria Obuzor: *Nature the Chemists' Untapped Warehouse*

Best Posters Presentations

- Florence Masese, University of Nairobi, Kenya: *Photocatalytic Activity of Coupled Semiconductor Oxide, TiO₂-WO₃ Nanocomposite Material under Visible Light Irradiation*
- Camila Renson, University of Dar es Salaam: *Application of Entomopathogenic Fungi as Bio-Pesticide against Tuta absoluta*
- Emmanuel C. Ohaekenyem, Nnamdi Azikiwe University, Nigeria: *Tetraaza Macrocycles: Reaction Mechanism, Synthesis and Elucidation of Cobalt (IV) Complex of Novel Ethano and Dihydroxy Ethano Bridged 1,10-Phenanthroline Based Macrocyclic Ligands*
- Jemilugba Olufunto Tolulope, University of Johannesburg, South Africa: *Antimicrobial Activities of Silver Nanoparticles synthesized using Combretum erythrophyllum's Extracts, Endophytes and Secondary Metabolites*
- Catherine Peake, University of Nottingham, United Kingdom: *High Energy Density Electrolytes for Symmetric Redox Flow Batteries.*

Closing Ceremony

The guest of honor during the closing ceremony was Yusuph Ngenya, the Director General of TBS. In the ceremony the five best poster presenters were given certificates by the guest of honour and books by Tundo, the chairman of the ICGCSD.

Chemistry and its Applications

1 to 31 August 2020, ONLINE

A Virtual Conference on Chemistry and its Applications (VCCA-2020) will be held from 1 to 31 August 2020. VCCA-2020 is endorsed by IUPAC.

The Organising Committee has adopted the theme ***“Research and Innovations in Chemical Sciences: Paving the Way Forward”*** for this virtual event.

This virtual conference will provide an online platform for participants to present, share and discuss recent findings of their research covering topics related to Chemistry and interdisciplinary Sciences.

VCCA-2020 will also provide the opportunity for scientists to interact in the current situation the World is facing due COVID-19 and travel restrictions.

It is not required to be always online for VCCA-2020 and there will not be live presentations. VCCA-2020 will also feature Nobel Prize presentations and Keynote speakers.

We look forward to welcoming you, academicians and researchers, to participate in VCCA-2020.



For more information about the conference, registration, and submission of abstract, please visit: <https://sites.uom.ac.mu/vcca2020/>

Prof Ponnadurai Ramasami, <vccamru@uom.ac.mu> **Chairman of VCCA-2020**



4 JULY 2020 - 10 JULY 2020

ONLINE – POSTGRADUATE SUMMER SCHOOL ON GREEN CHEMISTRY



DATE & TIME

4 July 2020 - 10 July 2020

Event Tags:
green chemistry, ICGCSD

VENUE
Palazzo Ducale
Venice, Italy
[+ Google Map](#)

WEBSITE
<https://www.unive.it/ssgc>

EVENT CATEGORY
Summer School

log in now!

Note:

The 2020 calendar of conferences has been disrupted by the COVID-19 pandemic. Most events originally planned are been cancelled, postponed, and in a few instances reframed as virtual events.

All IUPAC-endorsed events originally scheduled in 2020 and that are postponed will retain their endorsement. We invite you to review regularly the calendar of IUPAC endorsed events at <https://iupac.org/events/>

2020 – see online for updates

2021

19-20 January 2021 • Metrology, Quality and Chemometrics • Tel Aviv, Israel

Correlation of Test Results and Mass Balance Influence on Conformity Assessment

Ilya Kuselman, Independent Consultant on Metrology, Israel, e-mail: ilya.kuselman@gmail.com,
iupac.org/project/2019-012-1-500

25-29 January 2021 • POLY-CHAR 2021 • Auckland, New Zealand

World Forum on Advanced Materials and “Short Course on Polymer Characterization”

Jianyong Jin, e-mail: j.jin@auckland.ac.nz, www.polychar2021.org

26-30 January 2021 • Chemistry Education • Cape Town, South Africa

26th IUPAC International Conference on Chemistry Education (ICCE 2020)

Contact/chair of the local organizing committee: Bette Davidowitz <Bette.Davidowitz@uct.ac.za>, Chemistry Department, University of Cape Town, Rondebosch, South Africa, www.icce2021.org.za

9 June - 12 May 2021 • Biotechnology • Maastricht, Netherlands

19th International Biotechnology Symposium, joint with the Congress of European Federation of Biotechnology and NBC-20, the annual Netherlands Biotechnology Conference

Richard van Kranenburg, Corbion and Aldrik Velders, Wageningen University, Program Committee co-chairs, E-mail: ecb2020@tfi-group.com, www.ecb2020.com

16-20 May 2021 • MACRO2020+ • Jeju Island, Korea

48th World Polymer Congress

Chair: Doo Sung Lee, ex-President, PSK; program chair: Jun Young Lee; secretary general: Dong June Ahn <ahn@korea.ac.kr>; E-mail: secretariat@macro2020.org; www.macro2020.org

17-19 May 2021 • New Trends in Polymer Science • Turin, Italy

Polymers 2020: New Trends in Polymer Science: Health of the Planet, Health of the People, 2nd PDFa, Polymers: Design, Function and Application

Francesco Trotta, Pierangiola Bracco, Marco Zanetti, Co-chairs of Program Committee, E-mail: _polymers2020@mdpi.com, polymers2021.sciforum.net

9-11 June 2021 • CLEAR • London, United Kingdom

5th International Conference on Contaminated Land, Ecological Assessment and Remediation—CLEAR 2020

Yong Sik Ok, Chair of Program Committee, and Diane Purchase, Chair of Local Organizing Committee, E-mail: clear2020@mdx.ac.uk, clear2020.mdx.ac.uk

27 June - 2 July 2021 • Coordination Chemistry • Rimini, Italy

The_44th_International_Conference_on_Coordination_Chemistry—ICCC2020

Maurizio Peruzzini <maurizio.peruzzini@iccom.cnr.it>, Chairman and Giuliano Giambastiani <giuliano.giambastiani@iccom.cnr.it>, Scientific Secretary <iccc2020@iccom.cnr.it>, www.iccc2020.com

18-22 July 2021 • Polymer Colloids • Prague, Czech Republic

84th Prague Meeting on Macromolecules – Frontiers of Polymer Colloids

Daniel Horák, Program Committee Chair, E-mail: horak@imc.cas.cz, Conference Office: Ms. Daniela Illnerová, E-mail: sympo@imc.cas.cz, www.imc.cas.cz/sympo/84pmm

Chair: Russell J. Boyd, Dalhousie University, E-mail russell.boyd@dal.ca; contact Chemical Institute of Canada (CIC), 222 Queen St, Suite 400, Ottawa, Ontario, Canada, toll free: 1-888-542-2242, watoc2020.ca



IUPAC | CCCE
Montréal
2021
August 13-20

51st IUPAC GENERAL ASSEMBLY AND
48th WORLD CHEMISTRY CONGRESS
104th **CCCE** CANADIAN CHEMISTRY CONFERENCE
AND EXHIBITION

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Integrated Awards Ceremony
August 19, 2021

Abstract Submission Opens	December 2020
Abstract Submission Closes	February 2021
Registration Opens	February 2021
Early Bird Registration Deadline	April 2021
IUPAC General Assembly	August 13-20, 2021
World Chemistry Congress CCCE	August 15-20, 2021

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