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Working in the Field of Metrology ►

Transcending Borders for Chemistry, ►
Sustainability, and Education



Chemistry International

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Cover: Cover image and poem below generated by ChatGPT 3.5, a language model developed by OpenAI, in response to the queries by Ilya Kuselman, April 2024.

The World Metrology Day is the annual celebration of the signature of the Metre Convention on 20 May 1875 by representatives of seventeen nations. The Convention set the framework for global collaboration in the science of measurement and in its industrial, commercial and societal applications. The original aim of the Metre Convention -the world-wide uniformity of measurement- remains as important today as it was in 1875. This year, the theme for World Metrology Day was Sustainability. The annual event of May 20 is also now recognized by UNESCO as an official International Day. This designation opens new avenues to promote metrology, aligning with UNESCO's mission to construct a better world through science and education. To celebrate the occasion, Ilya Kuselman queried ChatGPT.

See also "IUPAC working in the field of metrology", p. 29

Metrology by ChatGPT

Metrology, the science of measure,
A dance of precision, a tale to treasure,
From length and time to weight and force,
It guides our lives on a steady course.

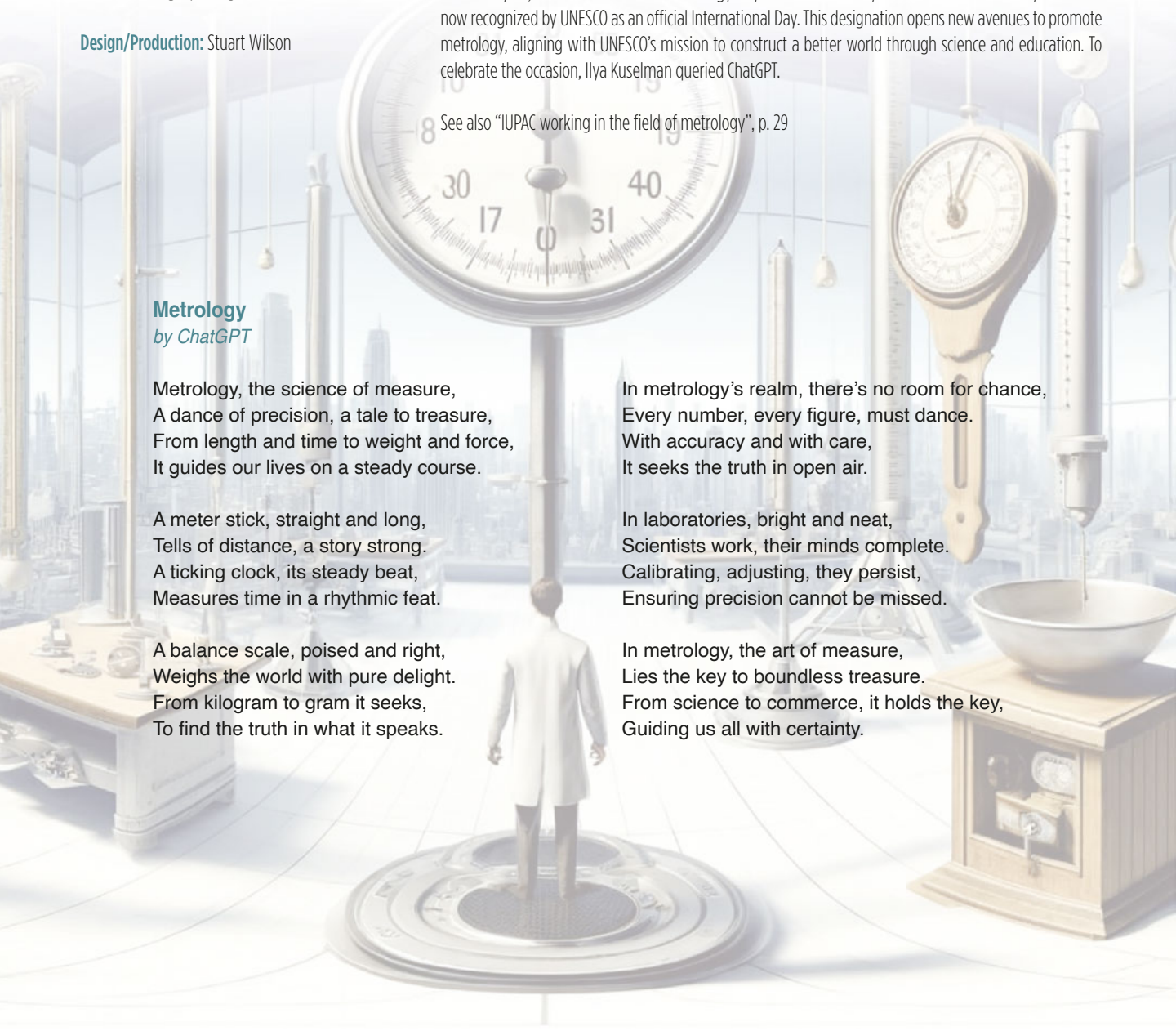
A meter stick, straight and long,
Tells of distance, a story strong.
A ticking clock, its steady beat,
Measures time in a rhythmic feat.

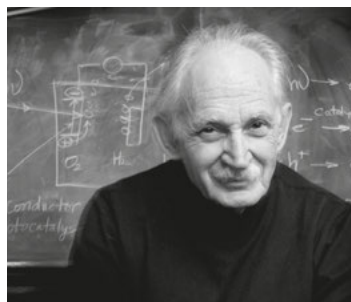
A balance scale, poised and right,
Weighs the world with pure delight.
From kilogram to gram it seeks,
To find the truth in what it speaks.

In metrology's realm, there's no room for chance,
Every number, every figure, must dance.
With accuracy and with care,
It seeks the truth in open air.

In laboratories, bright and neat,
Scientists work, their minds complete.
Calibrating, adjusting, they persist,
Ensuring precision cannot be missed.

In metrology, the art of measure,
Lies the key to boundless treasure.
From science to commerce, it holds the key,
Guiding us all with certainty.





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Managing the affairs of the Union, a brief history of the IUPAC Secretariat

by Zoltan Mester

Ensuring the efficient functioning of the Union has been the challenge of the Secretaries General for more than a century. The journey of administering the Union began at 49 Rue des Mathurins, in the 8th arrondissement of Paris where the headquarters of the *Société de Chimie Industrielle* and the French NAO were located. The first Secretary General of the Union, Jean Gérard, also served as Secretary General of these host organizations, and as such the arrangement provided the newly formed Union with stable administrative support and a physical address.

During the interwar period (1920-1940), this arrangement served the Union exceptionally well, essentially leveraging the corporate infrastructure of the French host to support IUPAC's budding operation. Following the retirement of Gérard, Raymond Delaby was appointed Secretary General in 1945 and served until 1955. Recognizing the importance of timely communication and an informed and engaged membership, Delaby initiated the *Circulaire d'information*, a newsletter designed to keep members informed. This later evolved into an English-language newsletter and then into today's *Chemistry International*, our corporate magazine. During the Delaby years, the Union's headquarters remained at the *Maison de la Chimie* in Paris. Managing the growing organization was a major challenge, as Delaby worked with a single secretary!

The next Secretary General (from 1955) was Rudolf Morf, an industrial engineer from Basel, Switzerland. Like his predecessor, he served not only as Honorary

Secretary General, but also as Executive Secretary, managing the day-to-day operations of the Union. He was better supported than Delaby thanks to the generosity of the Swiss pharmaceutical industry (Sandoz, Hofmann-La Roche, Ciba, Geigy), which underwrote much of the secretariat's expenses for a number of years, giving the Union a significantly improved corporate posture. For half a century, the Union was a volunteer organization, and any administrative support for the Secretary General was provided by other organizations that employed staff and "seconded" them to Union duties. This arrangement allowed for a much leaner organization that did not have to bear all the responsibilities of an employer. However, in 1964, for the first time, an assistant to the General Secretary was hired who was directly employed by the Union, a significant departure from previous practice.

The 1967 Executive Committee minutes noted that the growing Union required more administrative support, which could probably best be provided by hiring staff dedicated to these tasks. (see excerpt Fig. 1) This paved the way for the employment of a full-time Executive Secretary to support the work of the Secretary General and the establishment of a permanent Secretariat for the Union.

In 1968 the Union hired Maurice (Mo) Williams as Executive Secretary and at his request, the Secretariat was established in Oxford, UK with offices in the Cowley Centre (now called Templars Square). Interestingly, the opening of the new offices and the appointment of an Executive Secretary and support staff did not result in the immediate closure of the Secretary General's office in Switzerland, which was apparently budgeted for a few more years.

The separation of the operational activities managed by the Executive Secretary, from the board level with oversight role of the Secretary General, along with having two offices, was a source of confusion for a few years. (see Fig 2) Still, it soon became apparent that there were significant advantages to having a stable, dedicated core support function in the Union to assist the ever-changing elected leadership of the organization. As the Executive Secretary, Williams has served 15 Presidents, 6 Secretaries General and 5 Treasurers! He has seen it all!

This procedure, dictated by the special circumstances, is no longer tolerable. IUPAC must also be aware that a necessary increase in the size and the activity of the Secretariat cannot be carried by the Basle Companies, but that it must move towards accepting the full financial support of the Secretariat. A detailed discussion was held and it was

Fig. 1 Minutes of the 59th meeting of the Executive Committee, Prague, 1967. Highlights added.

APPENDIX A

RELATIONS BETWEEN THE EXECUTIVE COMMITTEE, OFFICERS AND THE EXECUTIVE SECRETARY.

STATEMENT OF RESPONSIBILITIES AND AUTHORIZATIONS

1. The statutory position is that the Executive Secretary is responsible to the President and Executive Committee (Bureau/Council) through the Honorary Secretary General and the Honorary Treasurer.

The purpose of the creation of an executive secretariat is to separate the executive and policy functions, which are the responsibility of the Officers and Executive Committee (Bureau/Council), and the administrative and implementation functions, which are the responsibility of the Executive Secretary and the IUPAC Secretariat.

2. The IUPAC Secretariat, which is presently located at Cowley Centre, Oxford, shall have staff, facilities and authorizations adequate for its independent operation without detailed supervision by the Secretary General and Treasurer.
3. The Executive Secretary shall report to the Secretary General on all matters except those which, according to the By-Laws, fall within the Treasurer's responsibility. Other Officers will have access to the Executive Secretary. The President, who is the statutory administrative head of the Union, is ultimately responsible to the Executive Committee (Bureau/Council) for the orderly and proper operation of the IUPAC Secretariat.

4. Correspondence

The official address of IUPAC for correspondence is:

2/3, Pound Way,
Cowley Centre,
Oxford, U.K.

All correspondence, including that of a formal nature addressed to the Secretary General, should go to the IUPAC Secretariat. The Executive Secretary will deal with this correspondence in accordance with relevant decisions on agreed procedures on his own judgement, sending copies to the Secretary General and Treasurer and, as necessary, to the President and Vice-President.

When direct correspondence between the Secretary General, Treasurer or other Officers and other Officials of IUPAC and other organizations is necessary on major or general issues (e.g. policy), copies of such correspondence should normally be transmitted to the Executive Secretary.

Fig 2 Executive Committee Minutes, Monte Carlo, 1968
Highlights added

In the 1990s, the Union became synonymous with Oxford and the long-serving Secretariat staff. There was even talk of investing in a permanent home for the Union in the UK. In the second half of the 1990s, after three decades of service, Williams and the senior Secretariat staff were preparing for retirement, creating an opportunity for the Union to reconsider the location of its offices. Several options were considered, and in 1996 the Union decided to establish offices in the United States, in Research Triangle Park (RTP), North Carolina. Paris and Frankfurt were also considered, as well as the option of remaining in Oxford. As is often the case, financial considerations were paramount, but significant non-financial considerations went into this decision, along with the intention to review the location of the Secretariat periodically to reflect the global nature of the Union.

Part of IUPAC's records did not move to the new offices, but were transferred to the Science History Institute in Philadelphia (then the Chemistry Heritage Foundation) to be archived, preserved, and made available for research.

The new offices were staffed and John W. Jost was hired to head the Secretariat. (Interestingly, the 1997 Geneva Council approved changes to the statutes and by-laws and restyled the Executive Secretary to Executive Director. It was probably felt at the time that the role would be better understood with the new title, especially in the North American context).

The Secretariat was housed in RTP, rent-free for ten years in a small structure, affectionately called "the trailer," that provided about 50% more space than the Oxford offices. The move to the US also resulted in savings of over 30% in secretariat costs and improved

In addition to consideration of costs factors for the future Secretariat, Prof. Jortner stressed the need to avoid any criticism of dominance of a member country in IUPAC affairs, to ensure vital stability in the Secretariat activity for the Union (bearing in mind the relatively quick turnover of its Officers), and to avoid isolation of the Secretariat intellectually and regarding accessibility.

The views of Dr. Eaton and of Profs. Brown and Steyn were noted, especially the importance of appointing an appropriate successor to Dr. M. Williams as Executive Secretary.

In summarizing the discussions, the President pointed out that, apart from Prof. Ward, there was a consensus in favour of moving the Secretariat during 1997 to North Carolina for at least the next ten years, and then to review the location every ten years. This would confirm IUPAC as a globally active, international organization. Prof. Fischli would convey the outcome of the discussions to the authorities in Frankfurt, North Carolina, and Paris.

Fig. 3 (Excerpt from the Minutes of the 123rd Executive Committee Meeting, Oxford, 1996) Highlights added.

service to our volunteers and member organizations.

The 2000s saw the digital transformation of the Secretariat's workflows and communications, creating significant efficiencies and improved services. (The transition from paper to electronic records has been a challenge, not just for IUPAC, in developing new systems for the safekeeping and archiving of our significantly increased number of records.)

In 2015, after 17 years, the Secretariat was on the move again, moving from the "trailer" to more appropriate office space in the Research Triangle Park.

The advent of teleconferencing and further digitization of office workflows has resulted in 50% of our staff now working outside of North Carolina at the time of this writing, which has significantly reduced the pressure on office space.

Also, given that our current office lease commitment will be fulfilled in the coming years, this is an opportune time to reopen the discussion within the Union about the practical arrangements for our Secretariat operations.

In this spirit, I will be reaching out to our member and affiliate organizations to solicit proposals for hosting our Secretariat and to assist in reimagining the operation of this key support function to serve the Union for decades to come.

I have outlined several key parameters to guide the selection and ensure a comprehensive evaluation process. I envision an open, collaborative, and iterative process in developing these proposals with the host organizations. I will work with the proposing organizations and the Executive Board to ensure that the proposals are consistent with the values and needs of the Union.

We request that your proposal provide the following information

1. Financial System:

- Outline measures, and legislations in place in

your country to ensure the security of financial assets.

- Confirm the availability of international financial transactions.
- Confirm the ability to host accounts preferably in major currencies such as USD, EUR, or CHF.

2. Office Space:

- Detail the office space that will be provided for the Secretariat, including size, location, and facilities.
- Specify the availability of board rooms for meetings of up to 20 people.

3. Staffing:

- Describe the number and roles of staff members that will be provided to support the Secretariat (key functions: IT, finance, communication, members relations, and general administration).

4. Operational Support:

- Describe Human Resources, Finance, and IT infrastructure available to support Secretariat operation.
- Detail any additional support that you consider offering to the Secretariat.

5. Support in Establishing Legal and Operational Presence:

- Provide details on the assistance available for establishing IUPAC, including legal, tax, and regulatory support within your jurisdiction.

6. Other Relevant Information:

- Please provide any additional information that would support your proposal and demonstrate your institution's capability to effectively host the Secretariat.

In addition, we will be seeking a commitment of at least ten years for these arrangements to ensure stability and continuity in our operations.



Like most of IUPAC volunteers, the Secretariat staff regularly meets virtually: from top left, Greta Heydenrych, Fabienne Meyers, Tammy Bridges, and Enid Weatherwax.

Proposals will be evaluated based on the criteria listed above, as well as the overall feasibility and potential for a successful partnership. Our goal is to select a host organization that meets the logistical and operational needs of the Secretariat and aligns with our vision and values.

We appreciate your interest in this important opportunity and look forward to receiving your proposal. Should you have any questions or require further information, please do not hesitate to contact me at zmester@iupac.org. Thank you for your continued support and commitment to the Union. 🏛️

See Request for Proposals <https://iupac.org/hosting-the-iupac-secretariat/>

Notes

As a chemist with a penchant for dabbling in our Union's history, I have relied on the following resources:

1. Roger Fennell: History of IUPAC 1919-1987, Blackwell Science, 1994
2. Stanley S Brown: History of IUPAC 1988-1999, IUPAC, 2001.
3. Danielle M. E. Fauque: Jean Gérard, Secretary General and Driving Force of the International Chemical Conferences between the Wars, International Workshop on the History of Chemistry 2015 Tokyo
4. The IUPAC100 Special issue of CI, Chemistry International Volume 41, Issue 3, July 2019
5. IUPAC Executive Board June 2024 meeting minutes
6. Hundred years' worth of digitally accessible records of Council, Bureau and Executive Committee meeting minutes; see iupac.org

Zoltan Mester <zmester@iupac.org> works at the National Research Council (NRC) in Ottawa, Canada, and also serving as an adjunct professor at Queen's and Ottawa Universities contributing to the training of the

next generation of analytical chemists. Since joining IUPAC in 2003, has served in numerous leadership roles including two terms as the President of Analytical Chemistry Division (2018-2019, 2020-2021) and also as an Elected member of the last Bureau of the Union (2022-2023). For more than a decade he represented Canada at the Consultative Committee for Amount of Substance (CCQM), the "chemistry arm" of the Metre Convention. He started as Secretary General of the Union in January 2024.

IUPAC administrative offices over the years

France (1919 -1955)

1919-1934

49 Rue des Mathurins 75008 Paris

1934-1955

Maison de la Chimie

28 Rue Saint-Dominique, 75007 Paris

Switzerland (1955-1967)

Postbox 165, CH-8058 Zürich-Airport

United Kingdom (1968-1997)

Bank Court Chambers, 2-3 Pound Way, Cowley Centre, Oxford OX4 3YF

United States (since 1997)

1997 to 2014,

104 T.W. Alexander Drive, Building 19, Research Triangle Park, North Carolina 27709

Since 2014

79 T.W. Alexander Drive, Research Commons Building 4201, Suite 260, Research Triangle Park, NC 27709

The PARTY Approach: How Friendship Transcended Borders for Science

by Yvonne S. L. Choo, Fun Man Fung, and Juliana L. Vidal

Just as organic reactions necessitate the interaction of different molecules, groundbreaking discoveries in chemistry burgeon from a diverse mix of minds working in close collaboration. While the COVID-19 pandemic presented unforeseen challenges by restricting physical interaction and international research, technology stepped in as a game-changer. Digital connections transcended geographical borders, fostered friendships and ignited a spirit of cooperation like never before. This article delves into the PARTY Approach, where (P)assion, (A)spiration, (R)elationship, (T)eamwork and (Y)outh come into play. Here, we explore the stories behind a remarkable trio brought together by their shared passion for chemistry, sustainability and education. Through their conversation, we will discover how friendships blossomed across borders, fuelled by a collective drive to make a positive impact on the world.

The PARTY Approach is a coined abbreviation for (P)assion, (A)spiration, (R)elationship, (T)eamwork and (Y)outh. In this narrative interview piece, we delve into a meaningful conversation with three unique individuals who embody these principles:

Yvonne Choo (YC) is an Assistant Professor based in the School of Energy and Chemical Engineering, Xiamen University Malaysia.

Fun Man Fung (FM) is an Instructor at the Department of Chemistry, Faculty of Science, National University of Singapore, and Academic Affiliate at the NUS Centre for Teaching, Learning and Technology.

Juliana Vidal (JV) is a Program Manager, Higher Education at Beyond Benign.

Tell us a little bit more about yourself and what you do on a day-to-day basis?

YC: I am an organic/polymer chemist by training. My research revolves around the design and development of new shape-memory polymers a.k.a. 'Smart Materials' for use in, but not limited to, 4D-Printing and energy applications. In addition to making polymers 'smart', I strive to put my creativity and passion for chemistry to good use—in education. I like to help students learn and better visualise complex chemistry/biochemistry



concepts through the use of toys, like LEGO [1]! On working days, I juggle the responsibilities of a full time academic—I teach, do research, handle administrative duties, supervise postgraduate students, *etc.*

FM: At the National University of Singapore (NUS), I work on educating future-ready chemists via evidence-based mentoring and research. My current research interest lies at the intersection of learning sciences and technology focusing on chemical education. My work explores the development of digital technology to enhance learning experiences [2], supporting students in overcoming appropriate obstacles in their learning and strengthening continuous learning for professionals. My research is informed by my classroom and laboratory teachings. In short, I think about how to help learners learn better daily.

JV: At Beyond Benign, we work to support and empower the chemistry community to achieve sustainability at the molecular level through green chemistry. My main focus is on the Green Chemistry Commitment program [3], which aims to promote the inclusion of green chemistry in the curriculum of higher education institutions. I work with a lot of inspiring people every day, and I'm so thankful for that! Previously, my Ph.D. and then post-doctoral research was based on renewable materials and greener processes to reduce our impact on human health and the environment.

What was the backstory behind your acquaintance with each other?

YC: I believe it was during the COVID-19 pandemic that I read a news article on X (then Twitter) about the release of the 2020 CAS Future Leaders [4]. JV and FM

were from the same cohort. Did the both of you meet in person back in 2020?

FM: Unfortunately, 2020 was not meant to be. The 2020 CAS Future Leaders was supposed to be an in-person week-long program but it was unfortunately being conducted online with regular training and a revised schedule. We met online but in the absence of a full cohort due to different time zones. It wasn't until three years later, at ACS Spring Meeting 2023 at Indianapolis, that I met JV in person!

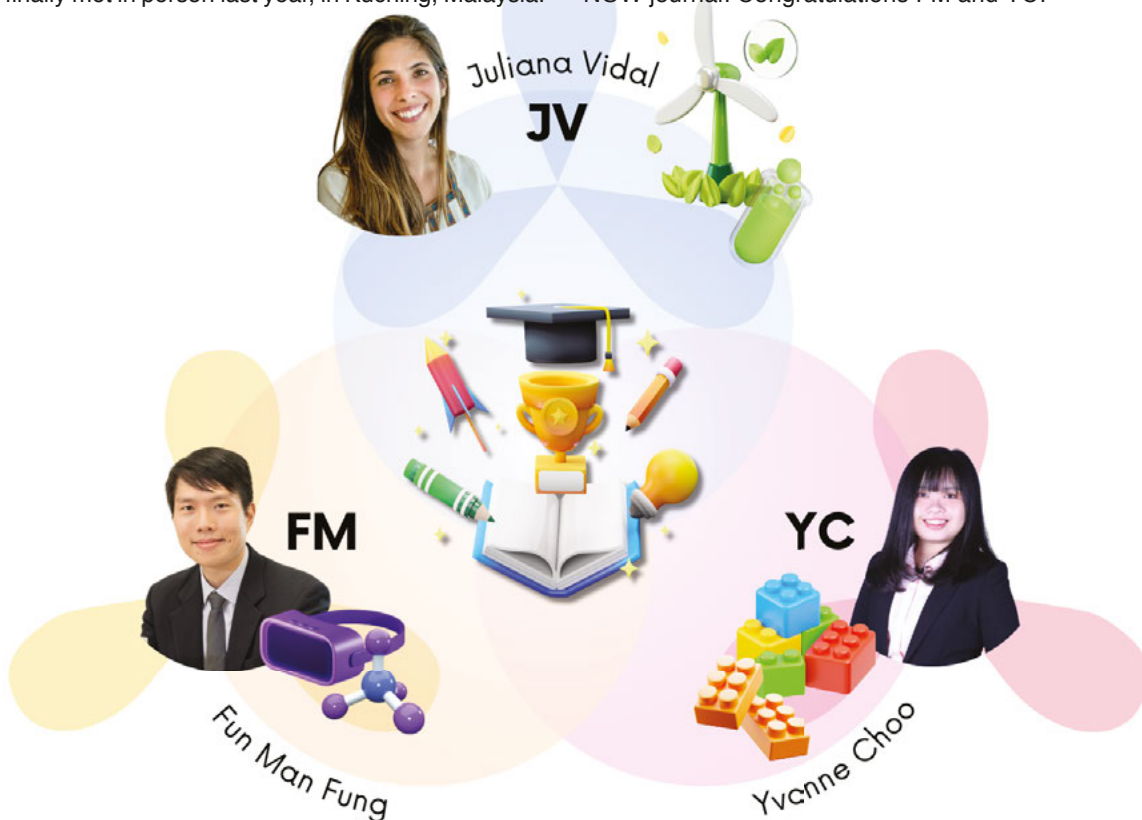
YC: Yes, it was definitely a challenging period for us all, but I am so glad that X kept us connected somehow [5,6]. I followed you (FM) on X at the start of the pandemic, where teaching and learning were forced to be conducted online. It was refreshing to find someone so passionate about chemistry education amidst the situation. We were also involved in the International Younger Chemists Network (IYCN) [7], so we met on several of the online meetings, as well as ones involving the International Union of Pure and Applied Chemistry (IUPAC)'s Committee on Chemistry Education (CCE). We finally met in person last year, in Kuching, Malaysia.

FM: We did! It was for the 9th Network of Inter-Asian Chemistry Educators (9NICE) Conference 2023 [8]. JV and YC, the both of you worked on an IUPAC-IYCN project together. How did the both of you meet?

JV: No, we have not met in person! We have worked together since 2022 in the Global Conversation on Sustainability (GCS) project (IUPAC project 2021-034-2-041) [9]. This project was co-created by IUPAC and IYCN to disseminate the adoption and practices of more sustainable discussions and actions. This year, both of us serve on the Committee on Chemistry Research Applied to World Needs (CHEMRAWN) of IUPAC [10].

YC: I remember we were also connected on X way back then, JV. It's interesting as I can figuratively see our 'orbitals' overlap in terms of our friendships, shared interests and involvements.

JV: And now the two of you are Thieme Chemistry Journals Award recipients [11] where I am working as an Associate Editor for the Sustainability & Circularity NOW journal! Congratulations FM and YC!



Yvonne Choo (YC), Fun Man Fung (FM) and Juliana Vidal (JV), showcasing their individual areas of interest and overlapping regions.

The PARTY Approach:

What were the unique journeys that led each of you to engage with IUPAC?

YC: My journey started back in 2011, sometime in August. That year, IUPAC celebrated the International Year of Chemistry. I participated and won first place in the IUPAC Polymer Video and Essay Competition on the topic of “A World without Polymers?” and was then given the chance to attend the 43rd IUPAC World Chemistry Congress in San Juan, Puerto Rico. I talked about what inspired the creation of my video and held a screening to those in attendance [12].

FM: For me, it was in 2013 that I attended my first International Chemistry Olympiad (ICHO) in Moscow, Russia Federation [13,14] where I became aware that IUPAC provided sponsorship to this global competition for the youths. In 2017 when the 49th ICHO was held in Nakthon Pathom, Thailand, then, as an elected Steering Committee member, I met and hosted Jung-Il Jin, then IUPAC President, where we had a long conversation and I learned about IUPAC CCE helmed by Jan Apotheker. At the time, Singapore was not part of

the IUPAC family yet, but in 2019, when Singapore made an application to join IUPAC, I was in Paris, France, as a volunteer mentor guide for the IChO, upon invitation from the Inspector General of French Ministry of Education and Youth, and President of the 51st IChO organizing Committee, so I was invited to join the centennial celebration [15]! When IUPAC Council and country delegations voted Singapore in, I was nominated to be the National Representative of Singapore National Institute of Chemistry (SNIC) to serve on CCE. I was just lucky to be at the right place at the right time!

YC: It's amazing how the stars aligned! In 2019, IUPAC also celebrated the International Year of Periodic Table, and both of us were awarded an element each in the Periodic Table of Younger Chemists [16]! I was Bohrium, and you, FM, were...Fluorine?

FM: Yes, I represented Fluorine. Altogether, 118 younger chemists from diverse backgrounds around the world who embodied the mission and core values of IUPAC were showcased.



YC, FM and JV's IUPAC journeys represented on a timeline (2011 – 2025).

How Friendship Transcended Borders for Science

YC: How special! You got to witness the meaningful celebration first-hand! Although I was not physically present in Paris, the bidding slides I prepared for IUPAC 2025 were presented by delegates from the Malaysian Institute of Chemistry (IKM) there at IUPAC 2019. Malaysia won the bid! It wasn't until exactly 10 years after my first IUPAC congress in 2011 that I got to attend another IUPAC congress in 2021, virtually, thanks to the pandemic [17]. For me, what made it even more memorable is that I was nominated by IKM to serve IUPAC as a National Representative of CHEMRAWN, a young observer in the Polymer Division and a Malaysian Delegate in the IYCN. My IUPAC journey came full circle! What about you, JV?

JV: My first encounter with IUPAC was in 2019, helping to co-organize the Global Women's Breakfast (GWB) in the institution where I was getting my Ph.D., Memorial University of Newfoundland (MUN), in Canada. My Ph.D. supervisor, Francesca Kerton, was already super involved with IUPAC then and her support was fundamental to the event's success. I was involved with the GWB organization until I completed my Ph.D. in 2021. In 2024, I was thrilled to support the organization of a GWB at Beyond Benign, in collaboration with The U.S. National Committee for the International Union for Pure and Applied Chemistry (USNC/IUPAC) [18-20]. I became directly involved with IUPAC in 2022, and we (YC and JV) worked together on the GCS project mentioned earlier. This year we serve CHEMRAWN together, too! I am a National Representative, while you (YC), are the Associate Member. I remember you were physically there at The Hague, Netherlands last year when that was announced? [21]

YC: Oh yes! I remember seeing you on screen, attending our hybrid CHEMRAWN meeting online, during IUPAC 2023. Hopefully, in 2025, we can all reunite, and I can finally meet you (JV) in person at IUPAC 2025, to be held in Kuala Lumpur, Malaysia! [22] Looking forward to welcoming the both of you!

JV: We look forward to being there too! Since we are on the topic of IUPAC, there is the Thieme-IUPAC Prize coming up this year by the Thieme Group in collaboration with IUPAC and the Editors of SYNTHESIS, SYNLETT, SYNFACTS, and Science of Synthesis. The award of €5,000 is presented every two years on the occasion of the IUPAC–International Conference on Organic Synthesis (IUPAC–ICOS) [23].

FM: That is certainly a wonderful opportunity!

Can you shed more light on projects related to chemistry, sustainability, or education with global reach that you've been involved in, either individually or in partnership with others?

JV: Since my undergraduate studies, I have been interested in the communication aspect of science. This is how I ended up as the Director of Marketing and Communications of the Network of Early-Career Sustainable Scientists and Engineers (NESSE), which led to my initial work at Beyond Benign as their Communications Intern. At Beyond Benign, I now work full-time to empower the community to achieve a more sustainable future through green chemistry education. I currently manage the Green Chemistry Commitment (GCC) program, focused on the higher education space. I have also been in the Governance Task Force of the Chemical Institute of Canada (CIC) and was involved with the IYCN helping to translate chemistry experiments from English to Portuguese used in outreach [24]. Currently, besides the GCS and CHEMRAWN, I am also involved with the Chemicals & Waste Youth Platform of the Major Group for Children and Youth at UNEP. Regarding my impact on the community, I just trust the process and try to make meaningful connections along the way of disseminating green chemistry at any chance I get! In this regard, I see education as a catalyst for the sustainable future we need and want—and I feel inspired by people like you, YC and FM, every day!

FM: I do my best to support whenever people feel that I can be helpful. If there's an endeavour people reached out to me that aligns with my values, I am always open to considering it. For instance, I recently participated in the event DiscovHER 2024, organized by the Science Centre Singapore [25]. This event promotes STEM for Societal Change, where attendees engaged in various immersive experiences, understanding sustainability via life cycle assessment, and getting their hands on crafting decorative pottery from recycled polymers. The Science Centre Singapore is an amazing place to learn how science is integrated into our daily lives. I enjoy collaborating with the people there as they are passionate about how science can transform lives and the future of Singapore. I find that via experiential learning, it sticks more! What it means is, education that activates more senses of the learner lasts longer [26]. I vividly remember during the pandemic, I was involved as a Task Group Member of the IUPAC Young Ambassadors for Chemistry in Cape Town (IUPAC project 2021-031-2-050). We supported organizing a science festival in

The PARTY Approach:

the form of an Open Day for the general public. The main objective is to initiate a lasting project at the Cape Town Science Centre on the relevance of chemistry to the grand challenges of sustainability [27,28].

YC: I am a science communication enthusiast and have been actively involved in various public engagement and outreach events since 2010. Back in my undergraduate days, I was invited to speak at several Malaysian Chemistry Carnival (K2M) aimed to promote public awareness and appreciation of Chemistry. I got more involved in scientific dissemination during my Ph.D. through events like Soapbox Science [29]—I literally stood on a soapbox in the middle of Grey Street, Newcastle, to have an informal chat about polymers and my research, with anyone who would come by my soapbox. The Big Ideas Event where I was given the chance to share my ‘Big Ideas’ to 10-11 year-olds with the help of a children’s book and STEM for BRITAIN is where I got to talk to policymakers at the Houses of Parliament about my Ph.D. research on membranes for artificial photosynthesis [30]. After my Ph.D., I started to engage myself more actively with learned societies which have broadened my reach and network, allowing me to contribute to different projects involving the wider international community. That’s how our ‘orbitals’ began overlapping!

What are some of the impediments you have encountered in the process, and what key takeaways have you garnered from them?

YC: Every journey has its set of challenges; especially when you are embarking on new or less travelled paths, you are bound to be faced with disbelievers and naysayers. I could still remember bystanders telling me I was wasting my precious research time and energy on outreach activities during my Ph.D. No doubt, outreach activities do take up a portion of my time that could have been used for research; however, outreach activities bring me joy and a sense of satisfaction as I am able to share my passion for chemistry and education in the hope of inspiring them. Had I let their thoughts and perceptions deter me from doing what I find value in, I would not have reached where I am today. We all have different journeys and life goals, trust your instincts and try not to be swayed unnecessarily. Most importantly, surround yourself with like-minded people who resonate well with you. Have them in your support system—in your circle of close friends or even collaborators! So glad I have both FM and JV in mine!

JV: I agree with you—also, resistance to change is another challenge that we see at Beyond Benign

through our Green Chemistry Commitment program, since higher education institutions can be resistant to including green chemistry in the chemistry curriculum and adapting to the change that is so desperately needed on our planet right now. This can be translated into different projects and aspects of our lives.

FM: This resonates so much with me. It is sometimes challenging to convince others that our group’s intentions and approaches are in line with the broad strokes. I learned to realize that individuals have different interests, and sometimes, these interests change with situations, which can divert the project in either way. In addition to having the right team and the right timing, I find that great projects eventually succeed because the stars are aligned, which is incredibly fortunate. There are many moving blocks, and we may not be able to control all these variables.

What advice would you give to people looking to get involved more actively (e.g. volunteering/learned societies, etc.)?

JV: I am thankful for being able to work with so many people who inspire me, and I found my heroes by going outside of my very small bubble. By volunteering yourself to do things outside your comfort zone, you can grow a different set of skills and get to know different people, with whom you can collaborate on diverse projects associated (or not) with your primary field/research. I have problems saying ‘no’ to things, which can be something very overwhelming (and I totally do not recommend it), but it is something that also took me into different projects that I had no idea I could take part in, in which I learned a lot (personally and professionally) and made new friends!

FM: My journey was off the beaten path. I have been a volunteer for a long time, even at sporting events. If volunteering is in your DNA, I would suggest having some level of self-awareness—knowing your strengths and lesser strengths. In some groups, your strengths might not be needed at that point as there are already people who can contribute better. If you are a versatile person with various skills, good on you! Then you can offer a hand based on your expertise. Do the right thing in the right way.

YC: You got to be willing to try because very often, it is when we put ourselves forward and take that first step that we will realize whether a certain activity or involvement is suitable for us. In the process, you will

How Friendship Transcended Borders for Science

gain exposure, pick up different skill sets, expand your network and learn new things! The term ‘active involvement’ can be very subjective as the level of activeness varies between individuals; find a pace and a level of involvement that best suits your current journey. Lend a helping hand whenever possible.

Conclusions

Through the PARTY Approach, the stories shared by these individuals reflected how their shared (P)assions, mutual (A)spirations, meaningful (R)elationships, collaborative (T)eamwork and the fresh perspectives gained from working with (Y)ouths can make a difference and most certainly pave the way for innovative solutions to solve some of the world’s most pressing challenges in the field of Chemistry, Sustainability and Education!

We hereby invite you to use this approach or create your own to promote systemic change regardless of the field you are in. So, let’s PARTY! 

Disclaimer: The views and opinions expressed in this article are solely those of the authors and do not represent the views of this journal and the organizations they work in.

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References

1. Choo, Y. S. L. *ChemRxiv* **2024**, preprint; DOI: 10.26434/chemrxiv-2024-nmrcx.
2. Han, J. Y.; Fung, F. M. In Digital Learning and Teaching in Chemistry; *The Royal Society of Chemistry* **2023**, 205.
3. Cannon, A. S.; Warner, J. C.; Vidal, J. L.; O’Neil, N. J.; Nyansa, M. M. S.; Obhi, N. K.; Moir, J. W. *Green Chem.* **2024**, Advance Article; DOI:10.1039/d4gc0057.
4. Wang, L. CAS names its 2020 Future Leaders, <https://cen.acs.org/acs-news/programs/CAS-names-2020-Future-Leaders/98/web/2020/03>, (accessed April 14, 2024).
5. Fung, F. M.; Jilani, S. Z.; Ohnsorg, M. L.; Pinals, R. L.; Saraf, M.; Tropp, J.; Carlton, P. *ACS Cent. Sci.* **2022**, 8, 294.
6. Hickman, D. Younger chemists thriving during the global COVID-19 pandemic, https://www.chemistryviews.org/details/ezone/11297391/Younger_Chemists_Thriving_during_the_Global_COVID-19_Pandemic/, (accessed April 14, 2024).
7. Pournara, D. T.; Tormet-González, G. D.; Weber, S.; Borges, J.; Menche, M.; Milić, J. V. *ChemView* **2020**; DOI:10.1002/chemv.202000020.
8. Kueh, S. T.; Zakaria, Z.; Lann, Y. C. S. *Chem. Int.* **2024**, 46(1), 44.
9. Vidal, J. L.; Borges, J. *Chem. Int.* **2023**, 45(2), 10.
10. Kerton, F. M. *Pure Appl. Chem.* **2021**, 93, 407.
11. Ito, H.; James, M. J. 2024 awardees - Thieme chemistry - Georg Thieme Verlag, <https://www.thieme.de/en/thieme-chemistry/thieme-chemistry-journals-awardees-107362.htm>, (accessed April 14, 2024).
12. A word without Polymers, *Chem. Int.* **2011**, 33(6), 24.
13. Fung, F. M.; Putala, M.; Holzhauser, P.; Somsook, E.; Hernandez, C.; Chang, I.-J. *J. Chem. Educ.* **2018**, 95, 193.
14. Chang, I.-J.; Fung, F. M. In *10 things you must know about the international chemistry Olympiad (IChO): A guide to the IChO Competition Revised edition*, World Scientific, **2023**.
15. Sotério, C.; Borges, J.; Martínez, J. G. *Chem. Int.* **2022**, 44(2), 39.
16. Ferrins, L.; Dunne, C.; Borges, J.; Fung, F. M. *Chem. Int.* **2020**, 42(3), 3.
17. Lann, Y. C. S. *Chem. Int.* **2022**, 44(2), 2.
18. Garson, M.; McConnell, L. *Chem. Int.* **2020**, 42(1), 22.
19. Garson, M. J.; McConnell, L. L.; Soby, L. M. *Chem. Int.* **2021**, 43(3), 8.
20. Kerton, F. M. *Chem. Int.* **2022**, 44(4), 18.
21. Kon, M. W. R.; Teo, J.; Fung, F. M.; Potgieter, M. *Chem. Int.* **2024**, 46(2), 22.
22. <https://iupac.org/event/iupac-world-chemistry-congress-2025/> (accessed April 26, 2024)
23. Thieme-IUPAC prize - Thieme chemistry - Georg Thieme Verlag, <https://www.thieme.de/en/thieme-chemistry/thieme-iupac-prize-55182.htm>, (accessed April 14, 2024).
24. Walshe, A. A. *ChemView* **2019**; DOI:10.1002/chemv.201900088.
25. Events in Science Centre Singapore, <https://www.science.edu.sg/whats-on/workshops-activities/discoverh>, (accessed April 14, 2024).
26. Fung, F. M.; Gehring, T. Turn on the music and use sounds when learning!, <https://network.febs.org/posts/turn-on-the-music-and-use-sounds-when-learning>, (accessed April 14, 2024).
27. Davidowitz, B. *Chem. Int.* **2023**, 45(1), 31.
28. García Martínez, J. *ChemView* **2022**; DOI:10.1002/chemv.202200065.
29. Iliyah, Closing the gender gap in science, <https://www.scientia.global/closing-the-gender-gap-in-science/>, (accessed April 16, 2024).
30. Where politics meets science, <https://www.rsc.org/news-events/articles/2017/mar/stem-for-britain-2017/>, (accessed April 16, 2024).

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Blockchain Technology and its Use Along the Scientific Research Workflow

A IUPAC White Paper Coming Soon

by Bonnie Lawlor, Stuart Chalk, Jeremy Frey, Kazuhiro Hayashi, David Kochalko, Richard Shute, and Mirek Sopek

At the Council meeting held during the 2019 World Chemistry Congress in Paris, a representative from one of IUPAC's National Adhering Organizations raised the question "What is Blockchain Technology?" They went on to say that both "Blockchain" and "Artificial Intelligence" were prominent buzzwords and asked if IUPAC could provide information on how these technologies were impacting science in general and chemistry in particular. Coincidentally, at that same Congress, the technology had been the subject of a presentation by Richard Shute [1], one of the authors of this paper, and the technology had already captured the interest of Bonnie Lawlor, another of the authors of this paper, to the extent that she published an article in *Chemistry International (CI)* on the topic the following year [2]. As a result of the question raised at the Council meeting, Javier García-Martínez, IUPAC President 2022-2023, suggested that a white paper on Blockchain be developed (Note: Artificial Intelligence was made the focus of the global, virtual 2021 World Chemistry Leadership Meeting (WCLM) and a brief article on that special event was published in the July 2022 issue of *CI* [3]).

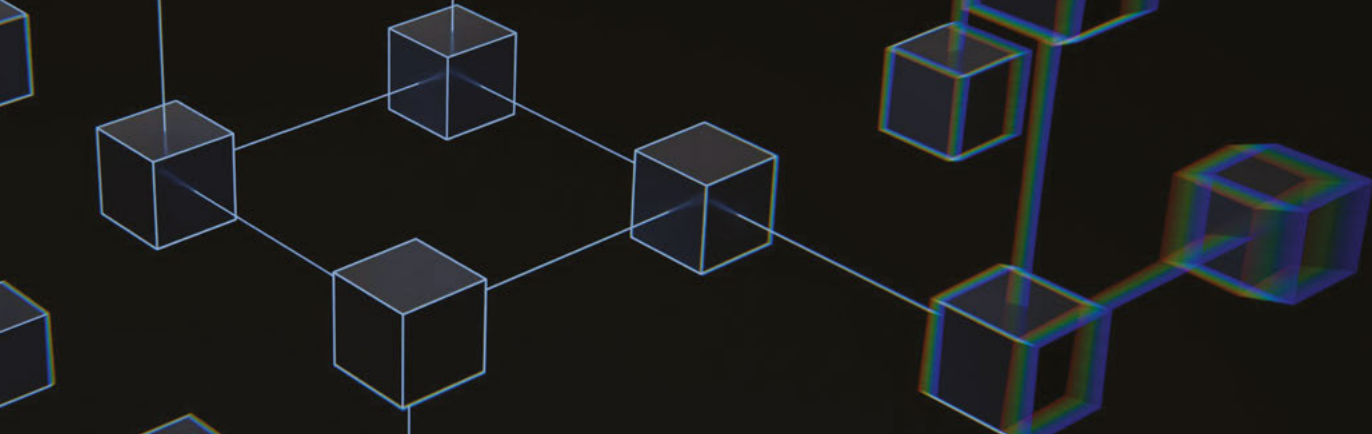
While not a technologist herself, Lawlor agreed to organize a team of experts to develop a white paper on the technology, and in 2020 the group began interviewing experts around the world and researching how the technology is being applied along the scientific research workflow. Over the next few pages, we want to provide a high-level overview of what you can expect when the paper is published in *Pure and Applied Chemistry* in the coming months. The paper will drill down in much more detail, plus provide a wealth of reading material for those interested in learning more.

What is Blockchain?

In its current iteration, what is commonly referred to as "the blockchain" is a platform that can be used to support many diverse applications. While this new technology gained popularity because of its use by a community of those interested in cryptocurrencies, specifically Bitcoin [4], the technology is simply the engine "under the hood" of Bitcoin—an engine that can be used for other purposes as well. Indeed, "Blockchain is to Bitcoin, what the Internet is to email. A big electronic system, on top of which you can build applications. Currency is just one." [5] In fact, blockchain technology actually predates Bitcoin by almost twenty years. It was co-invented in 1991 by Stuart Haber and W. Scott Stornetta who both worked at Bell Communications Research (Bellcore) and who were attempting to ensure the integrity of digital records via time stamping. They believed that the ability to certify when a document was created or last modified would be essential to the resolution of conflicts over such things as intellectual property rights.

Their initial efforts involved working on a cryptographically-secured chain of blocks such that no one could tamper with the timestamps of documents. Within a year they upgraded the efficiency of their system by incorporating Merkle trees [6], enabling the collection of more documents on a single block [7]. The Merkle trees created a series of data records, each connected to the one before it. The newest record in the chain would contain the history of the entire chain, making it more efficient by allowing several documents to be collected into one block [8]. Hence the name "Blockchain." (Note: the technology is also referred to as distributed ledger technology (DLT) due to its similarity to the double-entry book-keeping [9] method that dates to the fourteenth century).

The blocks record and confirm the time and sequence of transactions and each block contains a digital fingerprint or unique identifier (a "hash"), time-stamped batches of recent valid transactions, and the hash of the previous block. The hash of the previous block links the blocks together and prevents any block from being altered or a block being inserted between two existing blocks. Each subsequent block strengthens the verification of the previous block and hence the



entire blockchain. The method renders the blockchain tamper-evident, lending to the key attribute of immutability [10]. Time stamping even today remains one of the more common applications of the technology and the technology is becoming widely-used by researchers to protect their work and provide proof-of-concept and intellectual property ownership (data provenance).

Haber and Stornetta left Bellcore in 1994 to co-found a spin-off company, Surety, which provided time-stamping services based upon their algorithms and it was the first company to provide commercial blockchain-based services [11]. Things remained quiet on the blockchain front until 2008 when Satoshi Nakamoto released a white paper entitled, “Bitcoin: a peer-to-peer electronic cash system,” which proposed a system of electronic transactions that did not require a reliance upon trust—the middleman (*e.g.* a bank) was removed [12]. Haber and Stornetta’s seminal paper, “How to Time-Stamp a Digital Document,” [13] is referenced in the Bitcoin white paper. To this day no one knows anything about Nakamoto—whether it is a single person or a research group, and he/she/they left the Bitcoin community in about 2010, leaving blockchain technology development in the hands of those passionate about the technology—computer scientists, cryptographers, and mathematicians around the world [14].

The Importance of Blockchain Technology to Science

Over the years since Nakamoto built upon Haber and Stornetta’s work there have been a series of enhancements to blockchain technology, primarily driven by the realization that the technology did *not* need to be tethered to Bitcoin—it could be used for all sorts of cooperative efforts between organizations—including scientific research.

According to a 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 (fraudulently) once published.” [15]

In addition, a recent report from the European Chemical Industry Council, “Artificial Intelligence and Blockchain: Insights and Actions for the Chemical Industry,” [16] states that blockchain technology holds the potential for disruption across the chemical enterprise—both along a company’s internal scientific research and development workflow and externally along a company’s manufacturing supply chain to end-user consumption. The technology is important for many reasons, but the primary reason is that it provides incontrovertible proof-of-creation of an idea, research data, *etc.* Once linked to a blockchain and time-stamped, the data can be changed, but such changes are captured and time-stamped, making fraudulent tampering visible. This makes digital goods immutable, transparent, externally-provable, decentralized, and distributed. Consequently, blockchain technology could do much to mitigate the inability to duplicate research results.

According to Sönke Bartling (Mannheim University), all parts of the research cycle could take place within a blockchain system [17]. Attribution, data, data post-processing, publication, research evaluation, incentivization, and research fund distribution could thereby become comprehensible, open (at will), and provable to the external world. It would make more of the research cycle open to audited scientific correction and eliminate duplicative research. Bartling believes that it can potentially open the way to true collaborative, real-time research, thus expediting the advancement of science. A secondary reason for the importance of blockchain is that it allows the attachment of formal terms of agreement with digital goods, *e.g.*, licenses, usage limitations, smart contracts, *etc.* In addition, it also holds the potential for creating totally new business models, for reducing administrative and labor costs, and for providing rewards for work performed, such as for peer review in scholarly communication.

While use of blockchain technology beyond its original association with bitcoin is still in its early stages, there has been increased experimentation and adoption of the technology during the last six years. Those closely monitoring its adoption and the emergence of new use cases predicted that the rate of adoption would increase once Ethereum 2.0 (one of the major

blockchain technologies) was released. As expected, the new release is mitigating several obstacles to blockchain adoption— speed, cost, and scalability [18]. Indeed, Universities are beginning to focus on the technology to foster innovative research. Two examples in the USA are Stanford University's Stanford Center for Blockchain Research and the Walton College Blockchain Center for Excellence at the University of Arkansas. A European example is the Open University in the UK who is a member of the Bloxberg Consortium and who uses their blockchain for several blockchain-related research projects.

To quote the aforementioned report from the European Chemical Industry Council, "Blockchain is still an emerging technology and its use in the chemical industry is limited. But early proof-of-concept applications in other industries have already illustrated its benefits and are now moving to market adoption... blockchain is moving ahead quickly, but adoption will take time and effort. Chemical companies should start now to understand the benefits and develop a plan to incorporate it into their organization (where appropriate)."

Current Applications

As noted earlier, the objective of the white paper is to demonstrate how blockchain technology is being used along the scientific research workflow which has been defined as having the following five steps:

- Step #1: Develop Hypothesis/Define an idea;
- Step #2: Seek Funding (if needed);
- Step #3: Perform the Experiment/make observations;
- Step #4: Perform analysis/make insights;
- Step #5: Publish/share results.

The authors of this paper have held about a dozen in-depth interviews with major global players across diverse disciplines who are successfully using blockchain technology for a variety of purposes in the scientific workflow and the white paper will provide details on these uses. A sampling of the applications includes the following use cases:

- Time-stamping of data, ideas, etc. to provide proof-of-concept and intellectual property ownership (data provenance)
- Data sharing within closed networks/communities
- Near real-time research tracking (e.g., Covid-19 tracking is done via blockchain by the U.S. Department of Health and Human Services; the same can be applied to any research having global priorities)
- Authentication of data at the source for auditing,

compliance, and regulatory purposes

- Equipment management (maintenance records, training, usage history, ownership history, etc.)—can even ensure compliance with the Good Manufacturing Practices required by regulatory agencies
- Supply-chain tracking for both tangible/physical and digital/data assets
- Decentralized publishing/peer review
- Research Funding/tracking
- Crowd-sourcing/collaborative research (both public and within companies) where blockchain helps to confirm who owns what because it can demonstrate who did what
- Degree and qualification certification
- Identity certification of people and objects
- Research data re-use (including sales of such data)
- Retrieval of chemicals/pharmaceuticals at the end of their life cycles or during their life cycle for re-purposing
- Digital asset ownership using non-fungible tokens (NFTs).

Some of this activity is commercial (for-profit) and other applications are in the academic/non-profit market sector as well as in government sectors. A few examples of organizations using the technology are as follows:

ARTiFACTS: Established in 2018, this is a for-profit organization that uses the Bloxberg Consortium blockchain to ensure provenance of research along the scientific workflow, from time stamping of ideas/research, data sharing, through to publishing (see: <https://artifacts.ai>). More recently, ARTiFACTS has partnered with Marya Lieberman and the Distributed Pharmaceutical Analysis Lab (DPAL) at the University of Notre Dame to develop a prototype solution for tracking pharmaceutical chain-of-custody information in real-time using distributed ledger technology. Working with ARTiFACTS, DPAL records all physical handling and research metadata starting from the point-of-purchase of prescription drugs and sustained throughout the testing, analysis, and reporting requirements.

Bloxberg Consortium (out of the Max Planck Digital Library (MPDL)): Formally established in February 2019, MPDL has created a non-profit global network for the use of blockchain technology. Members of this network operate the nodes of a blockchain ledger for the development and deployment of diverse services and use cases in support of research. The number

of members has grown from the original eleven to more than fifty and will likely increase as the pandemic winds down and in-person meeting return. This consortium is being perceived as the blockchain for science and is used across diverse scientific disciplines, including chemistry (see: <https://bloxberg.org>). It should be noted that at the fourth Bloxberg Summit meeting held 4-5 May 2022 more than twenty-five research organizations decided on several proposals regarding the future development of the Bloxberg network. They made a groundbreaking decision, introducing a significant and forward-looking change for the future of the network: the “Bloxberg Association for the Advancement of Blockchain in Science” which was founded under German legislation that same year [19].

Open Science Chain (OSC): Launched in 2018, this is a consortium blockchain (like Bloxberg) that is funded by the U.S National Science Foundation (Award: 1840218 [20]) and is based at the San Diego Supercomputer Center at the University of California San Diego. Its main objective is to support data sharing to enable independent verification of scientific data and to foster reuse for the advancement of science (see: <https://opensciencechain.org>). They provide for the time stamping of datasets along with data ownership; promote the transparency and traceability of research data by tracking and storing all changes made to the data on the blockchain; and allow for independent verification of the authenticity of scientific data using information stored in the OSC blockchain. The project has been successful and, in the summer of 2021, received an additional half million dollars from the NSF for expansion [21]. The service is free to members of the academic and research communities. For more information about the OSC mission see its seminal paper [22].

U.S. Health and Human Services (HHS): Uses blockchain technology to reduce the time required to find the best deal for purchases of equipment, clinical tools, etc. This regularly could take four to five months and their new service, Accelerate, allows people to find what they needed in real time. After the success of Accelerate, HHS almost immediately initiated a pilot, the Grant-recipient Digital Dossier (GDD), to manage their grant program more efficiently. As of July 2021, GDD has reduced the time required to complete grant assessment tasks from four-plus-hours to a fifteen-minute process [23].

The white paper will include other examples, including those in areas such as education and identity management.

Other Areas Covered

The white paper also includes a section on legal and regulatory issues related to blockchain technology. What this section attempts to offer is some background on legislation and regulation as it currently applies to blockchain technology for organizations who actually want to “use” the technology—basically what you need to learn more about before venturing in. There is also a section on the current developments to improve the technology as well as what readers can expect in the not-too-distant future along with an extensive reading list.

A clear conclusion is that the use of the technology is not for everyone, and is not the solution to every problem. The white paper also provides examples of where the technology has failed, and why. The authors concur with the following statement from the NIST report mentioned earlier: “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...To avoid missed opportunities, organizations should start investigating whether or not a blockchain can help them.” [24] What we learned from our interviews is that usage of the technology is growing in general and is accelerating in the life and health sciences. We found that Sönke Bartling is right - all parts of the research cycle *can* take place within a blockchain system. We expect new developments to emerge, and we plan to update the white paper at regular intervals as the technology is enhanced and new use cases and new players emerge. In fact, a recent report from the Davos 2023 World Economic Forum states that “blockchain technology offers more promises than problems and that as a technology it will continue to grow exponentially, and its use cases expand. The real-world applications of blockchain, many already in use by organizations focused on international development, offer greater utility and cost savings.” [25]

In closing we believe that the future of blockchain technology looks bright. While the scope of its impact is hard to predict as it is in the early stages of broad adoption, according to Gartner, Inc., a market research company that follows the rise (and fall) of technologies, “The evolution of blockchain cannot be ignored...The impact of the technology will be significant.” [26] (*Note*: Blockchain Technology was selected as one of the Top Ten Emerging Technologies in Chemistry in 2021. An article on those technologies appears in the October 2021 issue of *Chemistry International*. [27]) 

Notes and References

- (all accessed 1 May 2024)
- Shute, R. E., "Blockchain and Distributed Ledger Technology: Enhancing Trust in Science," 2019; see the slides at: <https://www.slideshare.net/RichardShute1/blockchain-and-distributed-ledger-technology-enhancing-trust-in-science>
 - Lawlor, B., "Blockchain Technology: Uses in Research and Communication" *Chem. Int.* 2020, 42(3), 8-11; <https://doi.org/10.1515/ci-2020-0304>
 - Frey, J., Lawlor, B., McEwen, L., Ober, C., Williams, A., "A Global Conversation on the Use of Artificial Intelligence in Chemistry," *Chem. Int.* 2022, 44(3), 8-11; <https://doi.org/10.1515/ci-2022-0303>
 - See "What is Bitcoin": <https://www.bitcoin.com/get-started/what-is-bitcoin/>
 - Davies, S., "How Bitcoin and its Blockchain Works," *Financial Times*, video, February 3, 2015, see: <https://www.ft.com/video/2be94381-66dc-3320-a292-6a1cde0a3d5f>
 - Merkle tree, Wikipedia, https://en.wikipedia.org/wiki/merkle_tree
 - Iredale, G., "History of Blockchain Technology: A Detailed Guide," 3 Nov 2020, see: <https://101blockchains.com/history-of-blockchain-timeline>
 - Lytovchenko, A., The History of Blockchain: From Establishment to Broad Adoption, *eleks*, 8 May 2020, updated 5 March 2021, see <https://eleks.com/blog/the-history-of-blockchain/>
 - Double Entry Bookkeeping, Wikipedia, https://en.wikipedia.org/wiki/double_entry_bookkeeping
 - Gupta, M., Blockchain for Dummies," IBM, 3rd edition released 2020, p. 13, see: <https://www.ibm.com/topics/what-is-blockchain>
 - See: <https://www.worldcryptoindex.com/creators/w-scott-stornetta/>
 - Nakamoto, S., "Bitcoin: a peer-to-peer electronic cash system," 2009, see: <https://www.bitcoin.com/bitcoin.pdf>
 - Haber, S., Stornetta, W. S., "How to Time-Stamp a Digital Document," *The Journal of Cryptology* 1991, 3(2), 99-111, 1991; <https://doi.org/10.1007/BF00196791>
 - Redman, J., "Bitcoin's Creator Satoshi Nakamoto is Now a Member of the Top 20 World's Richest People," Bitcoin.com, 12 April 2021, see: <https://news.bitcoin.com/bitcoins-creator-satoshi-nakamoto-now-a-member-top-20-worlds-richest-people/>
 - Yaga, D., Mell, P., Roby, N., Scarfone, K., *NISTIR 8202 Blockchain Technology Overview*, National Institute of Standards and Technology, U. S. Department of Commerce, January 2018, <https://arxiv.org/abs/1906.11078>
 - See: AI and Blockchain in the Chemical Industry, Accenture, June 2019; <https://www.accenture.com/us-en/insights/chemicals/ai-blockchain-chemical-industry>
 - Bartling, S., Fecher, B., "Blockchain for science and knowledge creation," 2016, <https://doi.org/10.5281/zenodo.60223>
 - See: [cryptocurrency/what-is-ethereum-2-merge/](https://www.forbes.com/advisor/in/investing/cryptocurrency/what-is-ethereum-2-merge/)
 - See press release at: <https://www.mpg.de/ueber/presse/812-fourth-bloxxberg-summit-2022.html>
 - See: https://www.nsf.gov/awardsearch/showAward?AWD_ID=1840218
 - Bruch, K. M., SDSC's Open Science Chain Awarded \$500,000 NSF Grant, 3 Aug 2021; see: https://www.sdsc.edu/News%20Items/PR20210803_opensciencechain.html
 - Sivagnanam, S., Nandigam, V., Lin, K., "Introducing the Open Science Chain: Protecting Integrity and Provenance of Research Data," Proceedings of the Practice and Experience in Advanced Research Computing on Rise of the Machines (learning), Association for Computing Machinery (ACM), p. 18, July 2019.
 - Harris, M., "How Blockchain is Transforming Grants Management," Government CIO Media and Research, 27 July 2021; see: <https://governmentciomedia.com/how-blockchain-transforming-federal-grants-management>
 - Yaga, D., Mell, P., Roby, N., Scarfone, K., *NISTIR 8202 Blockchain Technology Overview*, National Institute of Standards and Technology, U. S. Department of Commerce, Jan 2018.
 - A. Nath, In Davos, Blockchain Yields More Promises Than Problems, <https://www.coindesk.com/consensus-magazine/2023/01/18/in-davos-blockchain-yields-more-promises-than-problems/>
 - Furlonger, D., Uzureau, C., *The Real Business of Blockchain: How Leaders can Create Value in a New Digital Age*, Gartner, Inc., Harvard Review Press, Boston, Massachusetts, USA, 2019, ISBN: 9781633698048.
 - Gomollón-Bel, Fernando. "IUPAC Top Ten Emerging Technologies in Chemistry 2021: Breakthroughs for a circular, climate-neutral future" *Chem. Int.* 2021, 43(4), 13-20; <https://doi.org/10.1515/ci-2021-0404>

The White Paper in *Pure and Applied Chemistry* is scheduled to be released ahead of print in the coming weeks; check <https://www.degruyter.com/pac>
See also <https://iupac.org/project/2023-009-1-024/> for details.

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IUPAC2025



KUALA LUMPUR, MALAYSIA

50th World Chemistry Congress (50WCC)
13 - 18th July 2025

53rd IUPAC General Assembly (53GA)
11 - 15th July 2025



We welcome you to enchanting Malaysia!



IUPAC and Wikipedia: A Story with Upsides, Downsides, Lessons & Rewards

by Stuart J. Chalk, Guido Raos, Paul D. Topham, and Martin A. Walker

A random person on the street may have never heard of IUPAC, but it is very likely that they have some familiarity with Wikipedia. This is extraordinary, as a sign how much the world has changed over the last twenty years, but it is not surprising.

Since its inception in 2001, Wikipedia has grown enormously in size, popularity and importance. For most people around the world, “the free encyclopedia that anyone can edit” is the first and foremost source of independent information on science, technology, arts, history, sports, entertainment, and much more. For several years, it has been consistently within the 7-8 most visited sites on the internet, after giants such as Google, YouTube, and Facebook [1]. An internet search for a technical term is also very likely to return the link to a Wikipedia article, as one of the first two or three options.

As emphasized by its logo (Figure 1), Wikipedia is a decentralized, international, multi-lingual endeavor. In fact, there are more than 300 Wikipedias in different languages [2]. The most populated and visited Wikipedia is that in English (almost seven million articles at the time of writing this article), but there are currently another 17 Wikipedias with more than one million articles. The Wikipedia foundation has also launched and supports several “sister projects”, such as Wikimedia Commons, Wikidata, Wikiquote, Wiktionary, etc.. The international nature of this wide-ranging project and the aim of spreading and sharing knowledge have a clear affinity with IUPAC’s mission and history.

Since 2015, recognizing the importance of Wikipedia as a vehicle for scientific information and dissemination, the Polymer Division of IUPAC (Division IV) has sponsored two projects related to embracing Wikipedia to disseminate knowledge:

- Synchronizing Wikipedia: Polymer Definitions and Terminology (<https://iupac.org/project/2015-032-2-400/>).
- Hands-on training on Wikipedia and Wikidata for application of IUPAC terms across Wikipedia (<https://iupac.org/project/2018-038-1-400/>).

The first project is the follow-up to a previous one by the Subcommittee for Polymer Terminology (SPT), that was covered 10 years ago in another article in *Chemistry International* [3]. The aim was to check polymer-related articles on Wikipedia—there are hundreds of



Figure 1: The Wikipedia logo

them—for accuracy, especially with respect to the use of polymer terminology, and if necessary correct or improve them. Relevant IUPAC definitions were also inserted in text boxes, with links to the original publications. The presence of the formal definition of a concept next to more extended explanations within an article allows the readers to better appreciate both of them. The boxes also increased the visibility of IUPAC’s work on terminology.

Shortly before the breakout of the COVID-19 pandemic in 2020, the project came to a standstill when some Wikipedia administrators [4] flagged the text boxes with the IUPAC definitions for plagiarism and possible copyright violations. The reason is that definitions had been copied *verbatim*—as one should do, for an official definition—from old technical documents with copyright restrictions. A few years ago, IUPAC and its publisher (De Gruyter) reached an agreement to publish new documents with an open access policy [5], but even in this case there were some restrictions on the re-use of the material that is not compatible with Wikipedia policies (the CC-BY-NC-ND license forbids commercial and derivative work) [6].

Call for Wikipedia editors

If you are interested in contributing to the dissemination of IUPAC definitions while becoming a Wikipedia editor, please reach out to Guido Raos. The next editing course at the Politecnico di Milano will take place the week of 8-12 July; online attendance is also possible.

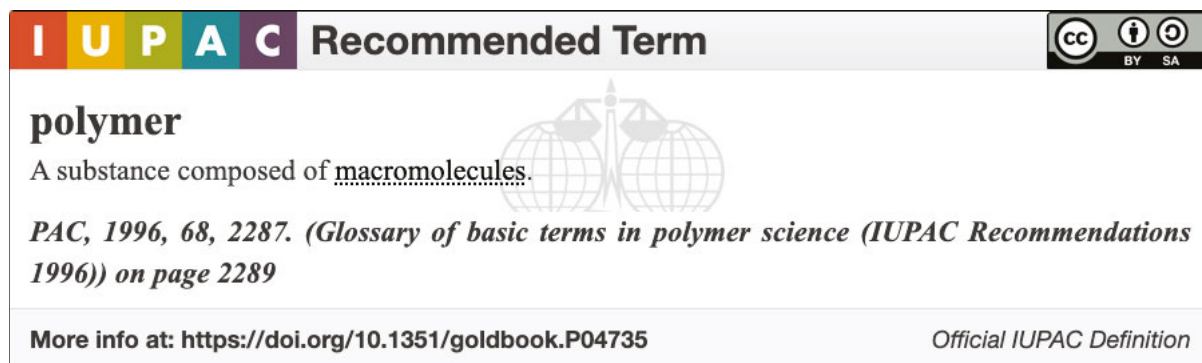


Figure 2: Image of a definition extracted from the IUPAC Gold Book for use in Wikipedia.

A possible solution to this problem came after a couple of years, when after consultation with the Committee on Publications and Cheminformatics Data Standards (CPCDS), IUPAC decided that images containing definitions from the Gold Book could be released with a Creative Commons license that is fully compatible with Wikipedia (CC-BY-SA) [7]. Figure 2 contains an example of such an image. Following this decision, about 70 images were generated, uploaded on Wikimedia Commons, and subsequently (early in 2024) inserted within a comparable number of relevant Wikipedia articles. Compared to the text boxes, the images also have a certain aesthetic appeal. Unfortunately, even this solution generated some negative reactions by some Wikipedia editors, to the point that some of the images were deleted from the articles. Among the reasons for the complaints, was the size of the images (the images could take up too much space within the articles, especially when consulted from a mobile device) and poor accessibility to the definitions by blind readers. At first, these negative reactions generated some understandable disappointment, as some of us believed that we had reached a dead end of the project. However, this was recently revived by IUPAC's decision that the Gold Book (including the text of the definitions, not just the images derived from them) could be released with the CC-BY-SA license [8]. This re-opens the possibility of going back to the text boxes, with an updated format.

The second project is sponsored by the Subcommittee for Polymer Education (SPeD), also from the Polymer Division (Div IV). It is a spin-off of a Wikipedia-editing course, that one of us has co-organized yearly at the Politecnico di Milano since 2016. Nearly 300 graduate students from the Politecnico have taken the course, whereby over the course of a week, they learn about Wikipedia and how to contribute to it, writing new articles, or improving and expanding existing ones (e.g., those classified as "stubs"). The topics

of the articles extend across all disciplines taught at the Politecnico: science, engineering, design and architecture. The rationale of the course is that it increases the technical writing abilities of the students and it renders them better, more critical users of Wikipedia's contents. Editing Wikipedia also allows us to give back to society and reach out to many more people, compared to a scientific publication.

The IUPAC project has allowed eight visitors to attend the course in Milano, learn the basic rules and contribute with articles on polymer-related topics. Some of the articles are rather general, such as "Polymer" [9], whereas others can be much more technical and specific (e.g., "Chain transfer" [10]). At the time of writing, the Polymer page still contains the image with the definition in Figure 2, while the Chain transfer page features an old-fashioned text box. The impact of the editing work can be appreciated from the statistics on page visits. Over the last month, the Polymer article has been getting over 1200 visits per day, the Chain transfer one a respectable 30 visits per day.

In conclusion, the collaboration of IUPAC and Wikipedia has been at times difficult. There are undoubtedly some cultural and technical barriers, some of which were not expected but can nonetheless be overcome by patient work and discussion. The rewards are already tangible, in terms of visibility for IUPAC and for our scientific work.

References and Notes

1. See e.g. <https://www.similarweb.com/top-websites/> (accessed on 25 March 2024).
2. See <https://www.wikipedia.org> (accessed on 25 March 2024).
3. "Synchronizing Polymer Definitions and Terminology with Wikipedia" *Chem. Int.* 2014, 36(2), 19; <https://doi.org/10.1515/ci.2014.36.2.19>
4. A Wikipedia administrator is a user with special editing

continued on page 31



Franziska Schoenebeck is the Thieme-IUPAC Prize Winner 2024

We are delighted to announce that the 2024 Thieme-IUPAC Prize has been awarded to Franziska Schoenebeck of RWTH Aachen University. Professor Schoenebeck becomes the 16th recipient of the prize and joins a distinguished group of scientists whose research has had a major impact on the field of synthetic organic chemistry. The prize, which is awarded every two years and includes an award of € 5000, will be presented to Schoenebeck at the ICOS-24 conference before her Thieme-IUPAC lecture.

Following undergraduate studies in Berlin and Glasgow, Franziska Schoenebeck obtained a PhD from the University of Strathclyde under the supervision of John A. Murphy. She then spent time as a Research Fellow in the group of K. N. Houk at UCLA, before joining the faculty of the ETH, Zurich, as an Assistant Professor in 2010. In 2013 she moved to her current institution, RWTH Aachen University, achieving promotion to full Professor in 2016.

Franziska Schoenebeck is leading an internationally recognized research program at the interface of organic synthesis, homogeneous catalysis, and physical organic chemistry and uniquely combines a cutting-edge synthetic organic chemistry program with state-of-the-art computational and mechanistic studies. Her group has made pioneering contributions in diverse areas such as the use of organogermanes in synthesis

and catalysis, the development of efficient methods for the trifluoromethylation of nitrogen groups, and the application of machine learning in the study and development of dinuclear metal complex catalysts.

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. It is presented every two years to a scientist within the first 15 years of their independent career whose research has had a major impact in synthetic organic chemistry.

<https://iupac.org/franziska-schoenebeck-is-the-thieme-iupac-prize-winner-2024/>

Christine Luscombe is the recipient of the 2024 Stepto Lecture Award

The Stepto Lecture award was established in 2016 to honour the memory of Bob Stepto, who passed in 2015, at the age of 78. Professor Stepto served IUPAC for 28 years, including his tenure as Chair of the Commission on Macromolecular Nomenclature (now known as the Subcommittee on Polymer Terminology) from 1991 to 2000, followed by his presidency of the Polymer Division from 2002 to 2005. An essential aspect of this award is that the recipient should not only be an exceptional polymer scientist acknowledged as a global leader in their research area but, in the true spirit of Bob, should also have made a lasting contribution to the polymer science community beyond their research, whether through IUPAC or other avenues. The recipient is chosen by the Polymer Division based on nominations received during the year of the biennial World Polymer Congress (MACRO Meeting).

In 2024, Professor Christine Luscombe from the Okinawa Institute of



Science and Technology will receive the award, joining the esteemed ranks of polymer scientists recognised for their exceptional contributions to both research and service to the broader community. The award acknowledges her groundbreaking work in precision polymerization, particularly in conjugated polymers for a wide range of optoelectronic applications. Additionally, it recognizes her significant service to IUPAC, having served as Secretary of the IUPAC Polymer Terminology Subcommittee (2014-2015) and as Vice President and subsequently President of IUPAC's Polymer Division (2016-2019, 2020-2023). Christine serves as an invaluable ambassador and role model for women in STEM. Beyond her contributions to Polymer Science, Christine also balances her responsibilities as a mother to a young family, exemplifying excellence both in her professional career and her role as a parent. Christine will deliver the Bob Stepto plenary award lecture at the upcoming 50th World Polymer Congress (MACRO 2024), scheduled for early July in Warwick, UK.

<https://iupac.org/christine-luscombe-is-the-recipient-of-the-2024-stepto-lecture-award/>

Athina Anastasaki is the recipient of the 9th Polymer International-IUPAC Award

The SCI® (Society of Chemical Industry), the Editorial Board of Polymer International and the IUPAC Polymer Division are delighted to announce that Athina Anastasaki, Assistant Professor of Polymeric Materials at ETH Zurich, Switzerland, is the winner of the 9th Polymer International-IUPAC award for Creativity in Applied Polymer Science.

The award celebrates the outstanding contributions that Professor Anastasaki has made to polymer chemistry where she has developed an outstanding, independent, innovative, and highly visible research profile spanning across the broad areas of polymer synthesis, polymer self-assembly and depolymerization leading the next generation of polymer chemists.

In polymer synthesis, she has been able to settle a long-lasting misconception in controlled radical polymerization whereby polymers with high dispersity have been traditionally associated with low livingness and increased termination, thus limiting several applications. Her in-depth knowledge and understanding in polymerization mechanisms led her group to develop a number of ATRP and RAFT polymerization approaches

in which the initiation and deactivation steps were elegantly regulated, unambiguously showing that extremely high end-group fidelity can be maintained regardless of the targeted dispersity.

Anastasaki has also initiated a new research niche by revolutionizing the depolymerization of polymers made by controlled radical polymerization. Before her work, depolymerization was mainly observed as an unwanted reaction during the polymerization of bulky monomers. In a completely new perspective, she developed the first example of near-quantitative depolymerization of RAFT-synthesized non-bulky polymers (such as PMMA) and showed that, under thermodynamically favourable conditions, both the monomer and the original RAFT agent can be recovered.

Recently she showed the first true reversal of controlled radical polymerization with polymer chains uniformly reducing in size during depolymerization, direct inverse of the uniform growth observed in controlled polymerizations. This recent work is expected to receive hundreds of citations from various chemistry fields as it unlocks many additional opportunities.

Anastasaki will give a lecture and receive this award at the 50th World Polymer Congress (MACRO 2024), which will be held in Warwick, UK from 1-4 July, 2024.

<https://iupac.org/9th-polymer-international-iupac-award-goes-to-athina-anastasaki/>



2025 Distinguished Women in Chemistry/Chemical Engineering Award – Call for Nominations

IUPAC announces the call for nominations for the IUPAC 2025 Distinguished Women in Chemistry or Chemical Engineering Awards. The purpose of the awards program, initiated as part of the 2011 International Year of Chemistry celebrations, is to acknowledge and promote the work of women in chemistry/chemical engineering worldwide. In 2011, 23 women were honored during a

ceremony held at the IUPAC Congress in San Juan, Puerto Rico, on 2 August 2011. At each of the subsequent IUPAC Congresses, 12 women received this recognition; in Istanbul in 2013, in Busan, Korea in 2015, in Sao Paulo in 2017, in Paris in 2019, virtually in 2021, and in The Hague in 2023. A similar award ceremony will take place during the 2025 IUPAC Congress in July in Kuala Lumpur, Malaysia.

Awardees will be selected based on excellence in basic or applied research, distinguished accomplishments in teaching or education, or demonstrated leadership or managerial excellence in the chemical sciences. The Awards Committee is particularly interested in nominees with a history of leadership and/or community service during their careers. A list of recipients of the award since its inception in 2011 is available online.

Each nomination requires a primary nominator and two secondary nominators who must each write a letter of recommendation in support of the nomination. A CV of the nominee is required. Self-nominations will not be accepted. Nominations should be received by 1 November 2024.

<https://iupac.org/2025-women-in-chemistry/>

2024 IUPAC-Zhejiang NHU International Award For Advancements In Green Chemistry—Call For Nominations

IUPAC-Zhejiang NHU International Award has been established in 2019 to emphasize the importance of advancements in Green Chemistry and the value of sciences to human progress, and to encourage young and experienced chemists. The award covers all the topics of Green Chemistry, such as Green and Renewable Feedstocks, Green Synthetic Routes, Green Solvents, Green Catalysis, Green products, Green Energy, and as broadly defined by OECD as Sustainable Chemistry.*

The 2024 IUPAC-Zhejiang NHU International Award includes:

- Three prizes to be awarded to three early career chemists, USD \$2000 each, who have received their Ph.D. (or equivalent) degree, or completed all Ph.D. requirements including successful defense of their doctoral thesis within the last 3 years (2022-2024). Qualified Ph.D. chemists will be evaluated based on the quality of their

theses work. Application requires submission of a completed entry form, including an essay submitted by the entrant that describes his or her research work and places it in perspective relative to current research in Sustainable Chemistry. The essay must be written in English by the entrant and may not exceed 1000 words.

- One prize will be awarded to an experienced chemist (USD \$10 000) who should have made significant contribution to green/sustainable chemistry throughout their career.

The Award is presented every two years and the work of the winners in progressing Green Chemistry in their applications will be disseminated to the attention of a wider global audience. All scientists are eligible irrespective of gender and nationality. Winners of this award will be expected to submit a review article for publication in *Pure and Applied Chemistry* in the year following their award. The awards will be presented at the 2025 IUPAC World Chemistry Congress to be held in Kuala Lumpur, Malaysia, 13-18 July 2025.

The Prize is managed by the Interdivisional Committee on Green Chemistry for Sustainable Development (ICGCSD).

About Zhejiang NHU—Founded in 1999, Zhejiang NHU Co., Ltd. has been recognized as one of the national high-tech enterprises in China. The company has total assets of 28.5 billion(CNY) with a sales income of 7.6 billion(CNY) and a corresponding profit of 2.6 billion(CNY) in 2019. Over the years, NHU adheres to the mission of “Exploring chemicals and improving life,” focuses on the fine chemicals, holds on to the concept of “innovation-driven development and growth in market competition.” Now, in the fields of nutrition, flavor and fragrance, APIs, and polymer based materials, it’s providing solutions for customers in more than 100 countries and regions. Today, NHU has established tight connections with outstanding universities, scientific research institutes and leading enterprises in the world. It has become a brand that highly trusted and approved by customers, a world-renowned vitamin supplier, a national large-scale flavor & fragrance manufacturer and one of the top 100 listed companies in China. <<http://www.cnhu.com>>

* See <http://www.oecd.org/chemicalsafety/risk-management/sustainablechemistry.htm> and reference therein, including Proceedings of the 1999 workshop, ENV/JM/MONO(99)19/PART3, p. 204

<https://iupac.org/awardees-of-the-2023-iupac-zhejiang-nhu-international-award-for-advancements-in-green-chemistry/>

IUPAC FAIR Chemistry Cookbook

The IUPAC FAIR Chemistry Cookbook is a new living resource developed to enable the chemical sciences community to move toward sharing and reusing data, code, metadata, etc. that are *Findable, Accessible, Interoperable, and Reusable* or **FAIR**.

Chemistry underlies both living and materials systems and chemical data are at the heart of data driven discovery and innovation across the health and environmental science sectors and in many applied engineering fields. Chemical data and analysis tools are increasingly available online and researchers and practitioners alike are increasingly involved in new ways to analyze, visualize, mine, and integrate data and information.

In a digital work environment, well-prepared researchers need to be comfortable working their way

around digital data formats, code, and online computing platforms. Proficiency in basic digital data handling skills can empower chemists to exploit FAIR and open data resources and handle real-world chemical data scenarios more effectively. As a result, the **Cookbook** content is designed to train, encourage, and enable chemistry researchers and data professionals to help support practices, workflows and data that are more FAIR.

Cookbook highlights

- **Practical Training Materials:** Developed by active members to demonstrate protocols for managing machine-readable chemical data.
- **Scope:** Recipes cover a wide range of tasks and use cases for handling chemical data programmatically.
- **FAIR Principles:** Emphasizes data being Findable, Accessible, Interoperable, and Reusable, aligned with FAIR machine-readable data criteria.




IUPAC

FAIR CHEMISTRY COOKBOOK

A new and living resource for managing digital chemical data effectively

- Openly accessible collaborative resource
- Utilized by diverse chemical data users
- Contains practical tools & tips in the hands of practicing chemists
- Aims to lower barriers for adoption of best practices for sharing and re-using FAIR chemical data



bit.ly/CookFAIR

Not sure how to make your practices, workflow, and data more FAIR?

Navigate



bit.ly/CookFeedback

You have a recipe topic to suggest? or a question?

FAIRChemistry@iupac.org

Comment



bit.ly/CookbookWiki

Do you work regularly with data and would like to contribute in recipe development?

Contribute

- **Educational Focus:** Supports learning for researchers and students on navigating diverse data types, extracting insights programmatically, and applying automated approaches for curation, dissemination, and analysis.
- **Interactive Tutorials:** Provides hands-on experience with digital data sources, tools, and workflows, enhancing understanding through executable code blocks and common cheminformatics functions.
- **Community Repository:** Offers readily accessible online tutorials for users to engage with, exemplifying FAIR principles for data reuse.
- **Online Accessibility:** Easily accessible through existing online infrastructure, facilitating widespread use and adoption.

How to use the Cookbook

This cookbook provides a range of protocols developed by active community members. These recipes target different tasks across a range of possible use cases for working with machine-readable chemical data (*i.e.*, FAIR data). The cookbook presents a collection of annotated code snippets and workflows for specific tasks in manipulating machine-readable chemical data and metadata.

- **Jupyter Notebooks:** Many of the recipes on this site take advantage of Jupyter Notebooks to run Python code in the browser for an interactive (and educational) feel for the user.
- **When is a recipe useful and for what?** Info is available in the collapsable 'header' below the title of the recipe. Header: also includes bullets for skills and learning objectives
- **Ideas to further characterize the applicability of recipes?** Ideas are welcome

Contribute to the Cookbook!

If you regularly work with digital chemical data and have useful approaches that could be demonstrated through a Jupyter Notebook, please consider contributing. Best practices for using standards and tools are emphasized and instructions for how to contribute materials are provided.

Unlock Exclusive Benefits as a Contributor to the Cookbook:

- **Gain Recognition:** Your contributions will be acknowledged on the Cookbook's contributions page.
- **Boost Your Profile:** Your ORCID will be integrated into the metadata of your contributions.
- **Secure Your Work Identity:** Each contribution

receives a unique ID through <http://w3id.org>, ensuring your work is properly attributed and easily accessible to others.

More information is available in Cookbook Wiki <<https://bit.ly/CookbookWiki>>

Contact: FAIRChemistry@iupac.org

<https://iupac.org/iupac-fair-chemistry-cookbook/>

In Memoriam—Allen Joseph Bard (1933–2024)

by Larry R. Faulkner and Christopher M. A. Brett

Professor Allen J. Bard, president of IUPAC during the biennium 1991-93, died in Austin at the age of 90 on February 11, 2024. He was a world-renowned electrochemist, recognized especially for placing the study of electrochemical reactions on a level of sophistication similar to that of homogeneous chemical processes.

In more than 60 years at the University of Texas at Austin, he guided 360 PhD students and post-doctoral associates and published more than 1000 peer-reviewed papers. The large topics on which he concentrated comprise a sizable fraction of electrochemistry in his time, including the mechanisms of electrode reactions, chemiluminescence from electrogenerated species, and photoelectrochemistry at semiconductor electrodes. He co-invented immunoassay by chemiluminescence and was an essential innovator in scanning electrochemical microscopy. Both tools have become commercially available and are widely employed. In his later years, he focused on what is now known as single-molecule electrochemistry, establishing methods that could detect individual electrochemical events. He often provided the first demonstrations. Some of his most striking results involved the formation and observation of individual catalytic centers of one to several atoms.

He is remembered as a superb teacher, able to inspire students through his own excitement with science and his ability to convey the essence of a complex subject with clarity and simplicity.

He also contributed through his influential texts, including three editions of *Electrochemical Methods* (Wiley, 1980, 2001, 2022, the last with L. R. Faulkner and H. S. White). Moreover, he edited three leading series in electrochemistry and was Editor-in-Chief of the *Journal of the American Chemical Society* for 20 years.

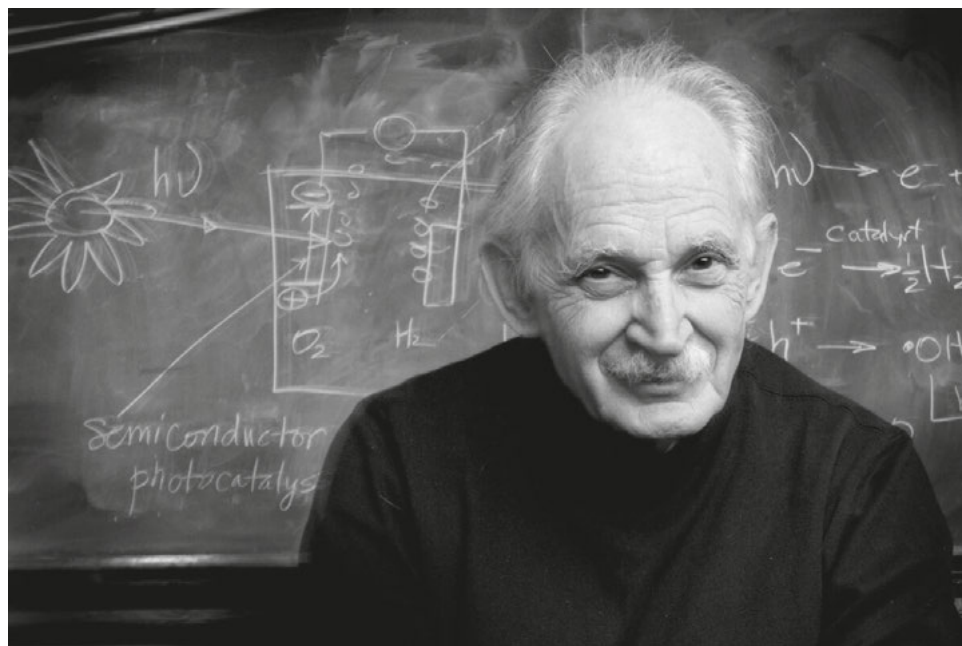


Photo © The University of Texas at Austin.
Photo by Marsha Miller

Allen Bard's activity in the 1980s within IUPAC was very much associated with IUPAC's mission of a common language and the free exchange of information. He was a member of the Commission on Electrochemistry (1975-1983), being Vice-Chairman 1981-1983 and of the Commission on Chemical Kinetics (1983-1987). During this time, the book *Standard Potentials in Aqueous Solution* (A. J. Bard, R. Parsons, and J. Jordan, Eds., Dekker, 1985) was published as an IUPAC-based project. It continues to be an excellent source of data on standard potentials or species of most of the chemical elements.

The future developments predicted in his article "New challenges in electrochemistry and electroanalysis" in the IUPAC journal *Pure and Applied Chemistry* [64 (1992) 185-192; <https://doi.org/10.1351/pac199264020185>, based on his lecture at the 33rd IUPAC Congress, held in Budapest, Hungary, in August 1991] are the challenges felt today, over 30 years later.

In 1989, Bard was elected to be IUPAC Vice President, followed by President in 1991-1993 and Past President 1994-1995. He presented his Vice President's Critical Assessment in the Hamburg General Assembly (1991), which assessed whether work that had been carried out with IUPAC sponsorship was all appropriate and recommending that a move should be made towards a more dynamic structure involving fewer permanent commissions, amalgamation of existing bodies where appropriate, and development of mechanisms for speeding up approval and publication of IUPAC recommendations.

His Critical Assessment commenced discussions that carried into later biennia regarding the IUPAC structure. Only in 2001 was organisational change implemented, with the abolition of most commissions and the creation of a more streamlined division structure in order to respond to the challenges of the 21st century in the chemical and related sciences.

Professor Bard was recognized broadly for his vast contributions. Among the distinctions were the U. S. National Medal of Science, the Priestley Medal, the Enrico Fermi Award, the Wolf Prize, the Welch Award, and the King Faisal International Prize. He was a member of the U. S. National Academy of Sciences.

A tribute to Christo Balarew on the occasion of his 90th birthday

The eminent Bulgarian chemist Christo Balarew was born on June 23, 1934 in Sofia. He received his MSc degree in chemistry from the Sofia University. Balarew devoted many years of his life to the service of Bulgarian chemical science and education. For most of his life he worked at the Institute of General and Inorganic Chemistry of the Bulgarian Academy of Sciences. He was a scientist, teacher, public figure, member of a number of international organizations, editorial boards of scientific journals, organizing and scientific committees of international scientific forums.

The research interests of Christo Balarew are focused on the elucidation of the dependencies between the structure and properties of solutions and those of the phases crystallizing from these solutions. As a result, he has developed a concept for predicting the existence and type of the most probable ionic groups in solutions and the structural patterns in crystalline phases, allowing prediction of the type and composition of crystallizing phases, as well as the kinetics of their crystallization. In this way, the reason for the crystallization of metastable phases is explained as a consequence of similarity between ionic groups in solutions and certain structural patterns in the crystalline phases. Regularities for the preparation of pure salts, double salts, basic salts and mixed crystals are revealed. A theory of isomorphous and isodimorphous co-crystallization has been established, which enables thermodynamic characterization of mixed crystals, calculation of impurity distribution coefficients in crystallization and of free energy in polymorphic phase transitions. Using the results of this fundamental research and the experience gained, several dozen technologies have been developed for the preparation of chemical products of high purity, for the synthesis of new materials, for the hydrometallurgical extraction of useful components from natural raw materials and industrial wastes.

Balarew was an active and devoted member of the IUPAC community: he was National Representative (1979-2004) and Associated Member (1991-1997) of Commission V.8 (Commission on Solubility Data), National Representative (2004-2007), Associate Member (2008-2010) and Titular Member (2010-2015) of the Analytical Chemistry Division. From 1999 to 2021 he was President of the Bulgarian National Committee of IUPAC. In this capacity he took care to



Bulgarian chemist Christo Balarew

consolidate the Bulgarian chemical community and to encourage young researchers at their early-stage careers. He initiated and organized the translation of the IUPAC *Red book* in Bulgarian. Thanks to his personal efforts, the membership of Bulgaria in IUPAC was not interrupted despite some difficulties in the transition years and many Bulgarian scientists were constantly involved in the activities of IUPAC. Balarew is the founder of two awards for young scientists: the *Prof. Christo Balarew Award for Prosperous Young Scientist in Inorganic Chemistry* of the Bulgarian Union of Chemists and the recently established *IUPAC Balarew Award for Outstanding Young Scientist working in the field of critical evaluation of solubility and/or related chemical equilibria*.

For his achievements in the field of science Balarew has been repeatedly awarded with prestigious Bulgarian and foreign awards. The international recognition of Christo Balarew is based not only on the impact of his scientific works published in renowned international journals, but also on his erudition and authority, which have earned him a worthy place among the international chemical community. Having known him for so many years, we also value him as a thoughtful listener and good advisor, someone who always reaches out to you, whether professionally or personally, in a most friendly and considerate manner.

We wish Prof. Balarew many years of good health and enthusiasm to realize new creative ideas!

For details about the recently established IUPAC Balarew Award, see <https://iupac.org/2024-franzosini-prize-and-balarew-award-call-for-nominations/>



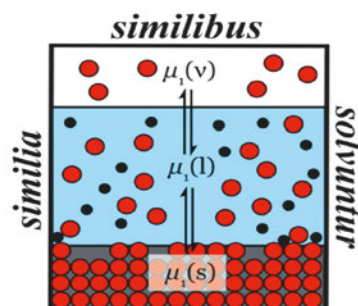
Assessment of Reliability and Uncertainty of Solubility Data

by Simão P. Pinho and Olga Ferreira

Initiated in May 2022, the Project “Assessment of Reliability and Uncertainty of Solubility Data” is supported by the IUPAC Analytical Chemistry Division. The main objectives and expected outcomes are to transfer fundamental and applied knowledge on good practices for phase equilibria measurements (particularly solubility), data analysis, and reporting high-quality data to the whole academic, technical, and scientific communities in the field. The project is largely focused on giving Ph.D. students and young researchers a series of tools to improve the quality of their outputs and their scientific literacy. So far six seminars have been held and recordings are retained online for broader dissemination.

The inaugural session was presented in July 2022 by Brynn Hibbert (University of New South Wales, Australia), entitled “Uncertainties of Solubility Measurements—Dark and Otherwise,” where fundamental questions such as how to evaluate, estimate, and express uncertainties were presented, and discussed. The speaker developed the “dark uncertainty” concept, explaining the DerSimonian-Laird approach and its relevance to consensus solubility values from different laboratories considering unknown between-laboratory systematic effects.

In September 2022, we chaired the 20th edition of the International Symposium on Solubility Phenomena and Related Equilibrium Processes (Bragança, Portugal, online). Well-known and recognized by the researchers working in the field, this conference is associated with the Subcommittee on Solubility and Equilibrium Data and gathered about 110 researchers from 25 countries. One of the significant events at the conference was a workshop organized within this project. First, Ala Bazyleva and Vladimir Diky (National Institute for Standards and



Technology, USA) summarized general methods of building uncertainty budgets and conducting thermodynamic data validation, as well as suggested reference systems for various kinds of solubility measurements. An interesting open discussion with the participants evolved with respect to various types of uncertainty, testing experimental methods and equipment, and evaluating uncertainty for own measurements and evaluations. Then, Johan Jacquemin (Mohammed VI Polytechnic University, Morocco) showed an exhaustive data analysis on gas solubility in materials technical evaluation. Novel materials such as metal-organic frameworks, ionic liquids, or porous liquids were considered, and model systems to test the procedures were proposed, along with a set of requested data to support any scientific paper on the topic.

In 2023, Earle Waghorne (University College Dublin, Ireland) conveyed a rather pedagogical and practical approach using the solubility of dioic acids in different solvents, connecting it with the spirit of the first presentation in the project. Several sets of solubility data were checked for consistency, proposing consensus values, and focusing on the standard uncertainty and systematic errors. Subsequently, involving professionals from the consultancy area, Charles S. Oakes (Insight Geochemistry LLC, USA) brought to attention the truth in science in his presentation entitled “Chemical Thermodynamic Measurements That Are Not What They Are Claimed To Be.” The tangible and intangible costs due to falsified data were discussed. Several examples showing the weaknesses linked to the action required by the scientific and technical communities were highlighted.

In February 2024, Wolfgang Voigt (Technische Universität Bergakademie, Germany) addressed the study of the solubility of salts in water. Three binary aqueous systems containing (CaSO₄, NaCl, or NaNO₃), and the ternary system H₂O + MgSO₄ + MgCl₂ were used to showcase how to deal with uncertainty and evaluation of solubility experimental data in this type of systems. A critical analysis on how statistics contributes more to the robustness than to the accuracy of the data, highlighting the enormous relevance

**21st International Symposium on
Solubility Phenomena and Related
Equilibrium Processes**

9-13 September 2024

University of Novi Sad, Serbia

<https://issp2024.pmf.uns.ac.rs/>

in the knowledge of the solution chemistry as well as in the formation of hydrates, and their stability, was presented. A series of questions to select and screen data from different sources was given and developed, as well as the difficulty of thermodynamic models to produce accurate solubility values of salts in water, under conditions not experimentally studied. In a well contemporary approach, perhaps with more significant impact on younger researchers, it was underlined how AI will not participate in obtaining better data.

Six seminars have been completed, and the videos uploaded to the IUPAC webpage dedicated to the project (<https://iupac.org/project/2022-002-2-500>). Besides the knowledge produced and shared, all these activities underlined the project's impact. On average, fifty participants from Australia to the USA attended the online presentations, always keen to join the discussions and share their expertise vividly. Still, during 2024, new activities will take place in the framework of the project. In September, a workshop will be organized within the scope of the 21st International Symposium on Solubility Phenomena (Novi Sad, Serbia), and a special issue in the *Journal of Solution Chemistry* is to be co-edited by Magdalena Bendová (University of Chemistry and Technology, Czechia) and Earle Waghorne.

For more information and comment, contact Task Group Chair Simão P. Pinho <spinho@ipb.pt> | <https://iupac.org/project/2022-002-2-500>

Human Drug Metabolism Database (hDMdb)

The IUPAC's Drug Discovery and Development Subcommittee (D3SC) has long been considering the assembly of a human drug metabolism database (hDMdb) that, in particular, might be a useful tool for interdisciplinary scientists engaged in small molecule drug discovery or toxicology. Ideally, it would be mounted on the Internet and available at no (or minimal) cost similar to the Protein Data Bank. Prominent applications would be to have an established compilation of human data from which each user could confidentially:

- (i) Predict the biological disposition of new (e.g. proprietary) compounds relative to metabolic possibilities and, more importantly, relative to statistically-derived and ranked metabolic probabilities;
- (ii) Assess the value of preclinical in vitro and in vivo models for predicting human drug metabolism, drug-drug interactions, and off-target toxicity when preceded by one or more competing bioactivation versus detoxification events;

- (iii) Develop general and/or proprietary methods to account for 3D chemical structures and derive structure-metabolism/transporter relationships for specific metabophores or structurally-related families of compounds; and,
- (iv) Explore machine learning (AI and 'facial recognition' at the molecular level) relative to drug metabolism in both humans and in preclinical in vitro and in vivo models of human drug metabolism.

The accompanying paper describes what we were initially thinking in more technical detail (*J. Current Drug Metabolism*, **2003**, 4, 411-422). Current interest in exploiting AI within the context of drug discovery suggests that the concept outlined in this article may be even more relevant today than when it was first being contemplated several years ago (e.g. see *Drug Metabolism – Databases and High-Throughput Testing During Drug Design and Development* published for IUPAC by Blackwell Sciences Ltd. **1999**; ISBN 0-632-05342-9).

For various reasons we made limited progress past the early testing points noted in this initial paper. Alternatively, we feel that databases and the field of predicting/assessing drug metabolism have, in general, moved forward considerably in several directions over the last twenty years. Thus, we now envision writing a white paper update (pros and cons) about today's status of this topic and where it may be heading in the future. For that we are seeking your assistance in whatever way you may want to help, and specifically toward answering three questions. Depending upon which you prefer, your input can be cited in: (a) A non-identifying, confidential manner for you and your organization; (b) An acknowledgement of you and/or your organization; or (c) As a specifically cited reference including as much detail as you may want. Either way, we are not requesting any proprietary information or details for unpublished methods. The three questions are:

1. Is there still a need for a hDMdb like the one described above or for some other version; and can you please elaborate what resources are available for you to currently use in this regard and indicate any missing features that would add value if they could be incorporated?
2. What other types of resources are available or are you trying to develop internally, for you to address items (i) to (iv) above, especially with regard to the cutting-edge machine learning (AI) arena as it might be applied to the field of small molecule drug metabolism?
3. Given today's interest in small molecule

bio-conjugates such as ADCs, and the deployment of immune-related biomolecules as therapeutics, would it be useful to have: (a) A glossary and/or tutorial pertaining to the biological disposition/metabolism of medium and/or large molecule therapeutics, perhaps something like our recently published document pertaining to small molecule therapeutics (Pure Appl. Chem., 2021, 93, 273-403 and then republished in the ACS series Medicinal Chemistry Reviews, 2021, 56, 463-659); and/or (b) A hDMdb something like the one described above but instead dedicated to (focused upon) metabolism data collected only from medium/large molecule (biomolecule) therapeutics?

Any other comments you may want to contribute toward this topic, beyond the questions noted above, are most certainly, additionally welcome. They may also become important for adding to the intended white paper. Please note the level of recognition that you would like to have for whatever additional information you choose to share.

We respectfully request any assistance you can provide for this non-profit undertaking which we hope will be of specific value to the drug metabolism, drug discovery-development, and toxicology fields, as well as to the global pharmaceutical corporate-academic-public enterprise in general. **Please send your response via email attachment to paul.erhardt@utoledo.edu by no later than September 30**, so that a summary white paper can be issued in early 2025. For more information and comment, contact Task Group Chair Paul Erhardt <paul.erhardt@utoledo.edu> | <https://iupac.org/project/2000-010-1-700/>

JCGM Guides in Metrology—IUPAC working in the field of metrology with others broadly-based international organizations

by Stephen L R Ellison

The Joint Committee for Guides in Metrology (JCGM) is a partnership between eight member organisations, all concerned with measurement and the standardisation of measurement.* The Committee maintains guidance on measurement uncertainty, based around the “Guide to the Expression of Uncertainty in Measurement” (known as the GUM) [1] and guidance on terminology for metrology applications, via the “International Vocabulary of Metrology” (known as the VIM) [2]. The JCGM operates through two working groups:

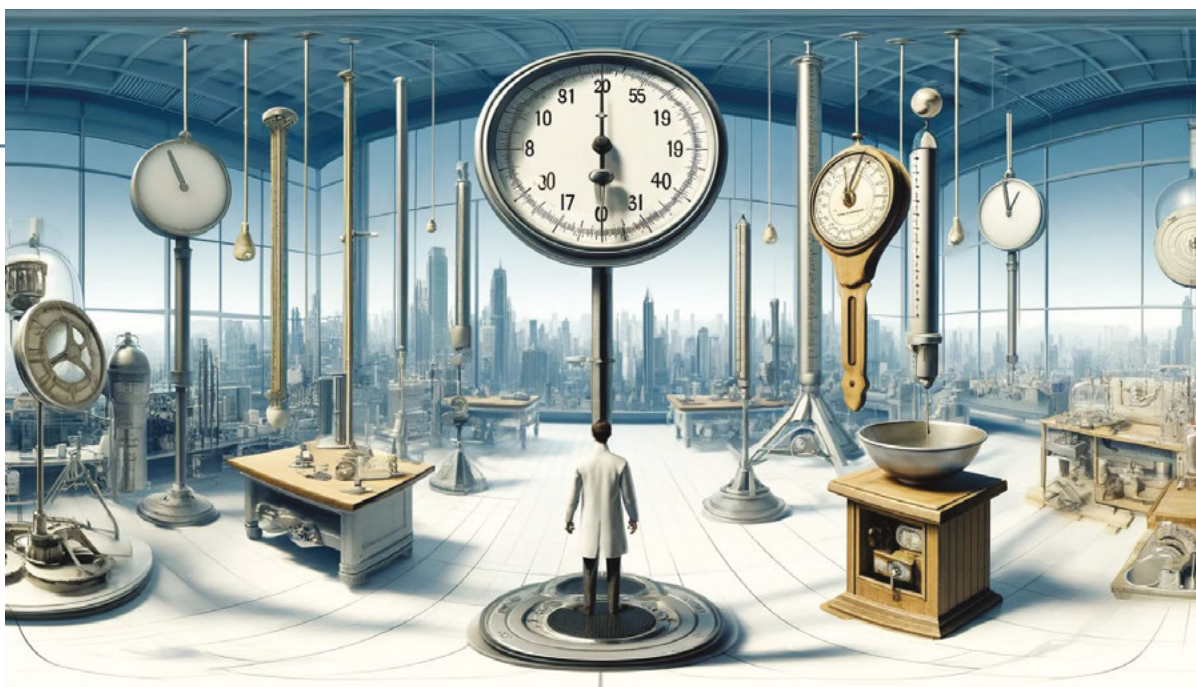
JCGM-WG1, with responsibility for the GUM and related documents, and JCGM-WG2, with responsibility for the VIM. IUPAC takes a close interest in both of the working groups. Guidance on measurement uncertainty is important for working analytical chemistry laboratories; not only because an understanding of the measurement uncertainty associated with results is good practice, but also because laboratories accredited to ISO/IEC17025 are required to evaluate measurement uncertainty and to report it where relevant [3]. Vocabulary for metrology is important because it provides a consistent set of concepts, terms and definitions for use across all fields of measurement. For IUPAC, this is important because chemists, and particularly analytical chemists, need to understand standardised terms as they apply to chemical measurement. In addition, close involvement in the development of generic terminology helps to make sure generic terms can be applied in chemistry and in IUPAC’s own terminology guides. For example, the most recent edition of the IUPAC Orange Book [4] adopts many terms from the current version of the VIM.

IUPAC currently has three representatives on JCGM-WG1: Stephen Ellison (LGC, UK) has recently been joined by two very welcome new representatives, Ivo Leito (University of Tartu, Estonia), and Francesca Pennecchi (INRIM, Italy). Ellison has also recently joined JCGM-WG2, supporting established WG2 members Zoltan Mester (NRC, Canada) and Jeremy Frey (University of Southampton, UK).

Work in WG1 has for some time focused on reshaping the series of JCGM guidance documents on measurement uncertainty. Although still a key

*The eight members organizations of JCGM are

- the Bureau international des poids et mesures (BIPM),
- the International Electrotechnical Commission (IEC),
- the International Federation of Clinical Chemistry and Laboratory Medicine (IFCC),
- the International Laboratory Accreditation Cooperation (ILAC),
- the International Organization for Standardization (ISO),
- the International Organization of Legal Metrology (OIML),
- the International Union of Pure and Applied Chemistry (IUPAC), and
- the International Union of Pure and Applied Physics (IUPAP).



document, the GUM has long been supported by documents on the use of Monte Carlo methods for measurement uncertainty evaluation [5], on measurement uncertainty for the multivariate case [6], and on measurement uncertainty in conformity assessment [7]. In 2017, WG1 agreed to restructure the measurement uncertainty documents in its portfolio. The whole suite of documents is now known as the “Guide to the expression of uncertainty in measurement”, and as documents are updated or developed, documents will be re-numbered to fit into the new structure. The first of these was the relatively recent guide on developing and using measurement models [8]; this was published in 2020 as JCGM GUM-6.

An important new edition in the portfolio is the recent release of the Introduction to the series of documents [9]. Formerly JCGM 104, this new edition of the Introduction fulfils two purposes. First, it forms a very basic introduction to measurement uncertainty, giving the rationale for its evaluation and introducing the main processes and approaches now available for measurement uncertainty evaluation, leaving detail for the different parts of the portfolio. Second, it gives an overview of the portfolio of documents, including future planned documents. Accordingly, the new Introduction acts as both a short introduction and a signpost to detailed guidance; an ideal first document when approaching the JCGM measurement uncertainty suite. It is fittingly numbered JCGM GUM-1.

At the most recent meetings—most of which have been online since 2020—JCGM has been busy on other documents. Working Group 1 is working on a revised edition of the Monte Carlo document, which will give updated guidance and which will bring some of the procedures more closely in line with best practice in statistics. In particular, the present direction

places less emphasis on the ‘maximum entropy’ basis for some distributions. This will improve the internal consistency of the guide, which currently uses a mixture of Bayes’ rule and maximum entropy to justify distributions. Further effort is being put into a new compilation of examples of measurement uncertainty. This will widen the range of application examples, making it easier for different measurement sectors to apply the principles of the GUM. It will also provide illustrations of the different evaluation approaches, to better show the advantages and disadvantages of each in different applications. The compendium will also be extended over time, adding to the applications and illustrating more approaches. The intent is to include applications of Bayesian methods in time, taking advantage of the developments in Bayesian Statistics and increasing availability of supporting software tools for Bayesian analysis.

WG1 is also actively reviewing terminology and definitions associated with measurement uncertainty. In part, this is driven by a need to encompass the wider range of approaches in use. For example, uncertainty intervals in the GUM are formed by multiplying a standard uncertainty by a “coverage factor” to give an “expanded uncertainty”, very similarly to the construction of the well-known statistical confidence interval. By contrast, intervals can be taken directly from the quantiles of Monte Carlo output. It is then not sensible to define a coverage interval merely in terms of expanded uncertainty; rather, it is important to seek a definition that applies well to both approaches.

A second reason for renewed interest in terminology is the current activity of JCGM Working Group 2, which has been working for several years to develop a substantial revision of the VIM. The intent is in part to provide more coherent and simpler terminology, and in

part to add terms related to qualitative (“nominal”) properties. Determination of properties such as chemical or biological species identity (for example, confirmation of identity of drugs of abuse or of pathological bacterial species) are covered by different accreditations standards, and IUPAC has published a vocabulary relating to nominal properties [10]. The aim of the VIM revision is to adapt this vocabulary to a wider range of measurement fields. Other topics for the VIM revision include changes leading from the most recent edition of the SI Brochure, in particular on units for “dimensionless quantities” (those for which all SI units cancel, like mass fraction or other ratios) and from the recent redefinition of the SI, and revision of concepts related to the idea of physical quantities (length, time, *etc.*) and their values. Some of these changes have proven contentious and generated a considerable volume of comments; WG2 accordingly expect to provide a further consultation draft later in 2024 after addressing the most recent comments.

Finally, it is worth pointing out that for IUPAC to form a clear view of IUPAC members’ needs and views on these key documents, and for those views to carry weight in the working groups, it is vital that individual members take time to check the drafts and to lodge comments. Both WG1 and WG2 always issue draft documents to member organisations, including IUPAC, and allow generous timescales for comment. Both JCGM and IUPAC want documents to serve their communities well; that cannot be done unless members participate actively in their development.

References

1. JCGM 100:2008, Evaluation of measurement data — Guide to the expression of uncertainty in measurement. BIPM (2008)
 2. JCGM 200:2012, International vocabulary of metrology — Basic and general concepts and associated terms (VIM) 3rd edition. BIPM (2012)
 3. ISO/IEC 17025:2017, General requirements for the competence of testing and calibration laboratories. ISO, Geneva (2017)
 4. Compendium of Terminology in Analytical Chemistry, IUPAC Orange Book, prepared for publication by D Brynn Hibbert, The Royal Society of Chemistry, 2023 [ISBN 978-1-78262-947-4]; <https://doi.org/10.1039/9781788012881>
 5. JCGM 101:2008, Evaluation of measurement data — Supplement 1 to the “Guide to the expression of uncertainty in measurement” — Propagation of distributions using a Monte Carlo method (BIPM, 2008)
 6. JCGM 102:2011 Evaluation of measurement data — Supplement 2 to the “Guide to the expression of uncertainty in measurement” — Extension to any number of output quantities (BIPM, 2011)
 7. JCGM 106:2012 Evaluation of measurement data — The role of measurement uncertainty in conformity assessment (BIPM, 2012)
 8. JCGM GUM-6:2020 Guide to the expression of uncertainty in measurement — Part 6: Developing and using measurement models (BIPM, 2020)
 9. JCGM GUM-1:2023 Guide to the expression of uncertainty in measurement — Part 1: Introduction (BIPM, 2023)
 10. Nordin, G., Dybkaer, R., Forsum, U., Fuentes-Arderiu, X. and Pontet, F. “Vocabulary on nominal property, examination, and related concepts for clinical laboratory sciences (IFCC-IUPAC Recommendations 2017)” *Pure and Applied Chemistry* 2018, 90(5), 913-935; <https://doi.org/10.1515/pac-2011-0613>
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IUPAC and Wikipedia (cont. from page 18)

privileges, such renaming, deleting or protecting some pages, or blocking some users. They are volunteers selected by the community among its more trust-worthy and experienced editors. A Wikipedia editor is anyone who contributes to it by writing and editing its contents. Wikipedia has some well-defined rules but, unlike a scientific journal, it has no official and centralized “editor’s office” that decides what is publishable and what is not.

5. See, for example: Jan Kaiser, David Brynn Hibbert, and Jürgen Stohner. “Preparation, formatting and review of IUPAC Technical Reports and Recommendations, IUPAC-sponsored books, or other items carrying the IUPAC label” *Pure App. Chem.* 2022, 94(11-12), 1257-1267; <https://doi.org/10.1515/pac-2022-1106>
6. See <https://creativecommons.org/licenses/by-nc-nd/4.0/> (accessed on 25 March 2024).

7. See <https://creativecommons.org/licenses/by-sa/4.0/> (accessed on 25 March 2024).
8. See <https://goldbook.iupac.org/> (accessed on 25 March 2024).
9. <https://en.wikipedia.org/wiki/Polymer> (accessed on 25 March 2024).
10. https://en.wikipedia.org/wiki/Chain_transfer (accessed on 25 March 2024).

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A brief guide to measurement uncertainty (IUPAC Technical Report)

Antonio Possolo, David Brynn Hibbert, Jürgen Stohner, Olha Bodnar and Juris Meija

Pure and Applied Chemistry, 2024

Vol. 96, no. 1, pp. 113-134

<https://doi.org/10.1515/pac-2022-1203>

This *Brief Guide* reintroduces readers to the main concepts and technical tools used for the evaluation and expression of measurement uncertainty, including both classical and Bayesian statistical methods. The general approach is the same that was adopted by the Guide to the Expression of Uncertainty in Measurement (GUM): quantities whose values are surrounded by uncertainty are modeled as random variables, which enables the application of a wide range of techniques from probability and statistics to the evaluation of measurement uncertainty. All the methods presented are illustrated with examples involving real measurement results from a wide range of fields of chemistry and related sciences, ranging from classical analytical chemistry as practiced at the beginning to the 20th century, to contemporary studies of isotopic compositions of the elements and clinical trials. The supplementary material offers profusely annotated computer codes that allow the readers to reproduce all the calculations underlying the results presented in the examples.

<https://iupac.org/project/2015-024-2-500/>

Definition of the pnictogen bond (IUPAC Recommendations 2023)

Giuseppe Resnati, David L. Bryce, Gautam R. Desiraju, Antonio Frontera, Ingo Krossing, Anthony C. Legon, Pierangelo Metrangolo, Francesco Nicotra, Kari Rissanen, Steve Scheiner and Giancarlo Terraneo

Pure and Applied Chemistry, 2024

Vol. 96, no. 1, pp. 135-145

<https://doi.org/10.1515/pac-2020-1002>

This recommendation proposes a definition for the term “pnictogen bond”; the term pnictogen bond designates a subset of the attractive interactions between an electrophilic region on a pnictogen atom in a molecular entity and a nucleophilic region in another, or the same, molecular entity.

<https://iupac.org/project/2016-001-2-300/>

IUPAC Distinguished Women in Chemistry and Chemical Engineering Awards 2023— Preface of the special collection of invited papers by recipients of the 2023 Awards

Mary J. Garson

Pure and Applied Chemistry, 2024

Vol. 96, no. 1, 2024, pp. 1-4

<https://doi.org/10.1515/pac-2024-0022>

The 2023 awardees were selected from an impressive list of high achieving and creative women chemists or chemical engineers from all around the globe. In their individual career stories, each of the winners reveals a willingness to share their expertise and experiences with other chemists, and a passion for science. Their activities and outreach advance the chemical and chemical engineering sciences in so many diverse ways. The collection of articles in this January 2024 issue of *Pure and Applied Chemistry* have been specially prepared by some of the 2023 awardees. While some manuscripts explore topics within the awardee's research interests, others chart individual career journeys. This special issue will inspire women scientists worldwide and provide encouragement to all of us to advance the chemistry of the future.

This year collection includes:

- **Yoshihiro Sohtome and Mikiko Sodeoka***
Catalytic oxidative carbon–carbon bond-formations of benzene-1,2-diols
- **Suprotim Koley, Monika Gaur, Nilotpal Barooah, Achikanath C. Bhasikuttan and Jyotirmayee Mohanty***
Supramolecular assemblies with macrocyclic hosts: applications in antibacterial activity
- **Marinda Li Wu***
Women in chemistry: remarkable progress, but are we there yet?
- **Madeleine S. Woodward, Danielle E. Runacres, Julian Grigg, Imtiaz Khan, William Levason, Graeme McRobbie and Gillian Reid***
Automating the production of $[\text{Fe}^{18}\text{FF}_2(\text{BnMe}_2\text{-tactn})]$ and investigating radiostabilisers for use with high-activity $^{18}\text{F}^-$
- **Lidia Armelao*, Maria Rando, Silvia Carlotto, Irene Motta, Gregorio Bottaro and Marzio Rancan**
Bridging two worlds: $(\text{DABCO-H})\text{CuKI}_3$ a hybrid copper iodide phosphor with a perovskite structure



Eleven of the twelve awardees of the 2023 Distinguished Women in Chemistry recognized in 2023 in Den Haag during the IUPAC World Chemistry Congress Meeting (L to R): Javier García-Martínez (IUPAC President), Mary Garson (Chair, selection jury), Jyotirmayee Mohanty, Marcia Foster Mesko, Laura McConnell, Marinda Wu, Nguyen Thi Kim Thanh, Chunying Chen, Mikiko Sodeoka, Annette Beck-Sickinger, Gill Reid, Lidia Armelao, and Tatjana Parac-Vogt. Award recipient Bin Liu was unable to attend the award ceremony.

- **Ann Van der Jeugd and Tatjana N. Parac-Vogt***
Empowering women in science through role models, mentors, and support groups: a personal perspective
- **Chiara Ruggirello, Karin Mörl and Annette G. Beck-Sickinger***
Peptides for therapeutic applications – challenges and chances

<https://www.degruyter.com/journal/key/pac/96/1/html>
<https://iupac.org/iupac-2023-distinguished-women/>

Special issue of POLY-CHAR 2023 and in memory of Professor Melissa Chan Chin Han

Jiayong Jin and Holger Schönherr
Pure and Applied Chemistry, 2024
 Vol. 96, no. 2, 2024, pp. 147-148
<https://doi.org/10.1515/pac-2024-0202>

The IUPAC-endorsed conference POLY-CHAR [Auckland] was held at Auckland, New Zealand from the 22nd to the 26th of January, 2023. POLY-CHAR is a nonprofit, non-governmental organisation fostering a

friendly environment for sharing information, establishing student exchange and strengthening international cooperation. An important goal of POLY-CHAR is offering a forum for PhD students and young researchers to create their own scientific networks and experience a vested scientific community.

After postponement from January 2021, POLY-CHAR [Auckland] 2023 was the first live conference to be hosted since the two purely digital events of POLY-CHAR [Venice] 2021 and POLY-CHAR [Halle-Siegen] 2022. The POLY-CHAR regular attendees and newcomers were able to gather in-person after years of suspension during the pandemic. About 180 scientists attended POLY-CHAR 2023 from 29 countries and the conference programme consisted of a total of seven plenary speakers, 15 showcase speakers, 27 keynote speakers, 43 oral speakers and 19 poster presenters. The four-day conference plus one-day pre-conference workshop covered the following technical topics:

- Advances in polymer physical and structural characterisation
- Advances in synthetic polymer chemistry
- Biological functional polymers
- Polymers additive manufacturing (3D/4D printing)
- Polymers for molecular separation, energy, and environment

This special issue in *PAC* includes contributions presented at POLY-CHAR 2023 collectively showcasing the recent advance in polymer research from synthesis to applications.

Furthermore, the present special issue is complemented with selected papers that honor late Prof. Dr. Melissa Chan Chin Han (Faculty of Applied Sciences of University Teknologi MARA, Malaysia) and her invaluable contributions to polymer science and the wider community through her very active role in IUPAC and in POLY-CHAR. During the opening ceremony obituary to Prof. Dr. Melissa Chan Chin Han was observed. Her dedication and tireless efforts to develop POLY-CHAR as an inclusive organization spanning all continents with a focus on providing opportunities especially for young scientists and to actively support their education is unsurpassed. With a balanced mix of tutorial contributions on central aspects of polymers and polymeric materials as well as highlights of recent developments, we bow to honor Melissa Chan Chin Han and dedicate this issue to the memory and legacy of our dear colleague, companion and friend.

From water to chemicals: vision and opportunities of a sustainable hydrogen society

A special issue of *PAC* dedicated to the 5th edition of *Avogadro Colloquia* "From water to chemicals: vision and opportunities of a sustainable hydrogen society" was released as Volume 96, Issue 4, April 2024.

Preface by Lidia Armelao, Elio Giamello, Gaetano Guerra, and Maria Chiara Carrozza; <https://doi.org/10.1515/pac-2024-0229>.

The Avogadro Colloquia conference represents a forum of discussion on challenging and urgent topics relating to chemical sciences, the environment, and the needs of society. It is jointly organized periodically by the National Research Council (CNR), Department of Chemical Sciences and Materials Technologies and the Italian Chemical Society. The 5th edition was one of the first important events for the celebrations of CNR centenary and was held at the CNR headquarters in Rome on 15-16 December 2022. This edition of the Colloquia was focused on the technologies for hydrogen production and use in the so-called "green transition" towards a society with reduced CO₂ emissions. Such technologies fit well the objectives suggested by the United Nations and by

Mission EU2030 for the mitigation of the climate change.

Greeting addresses were given by the IUPAC president Javier García Martínez, the elected president of the European Chemical Society (EuChemS) Angela Agostiano, the CNR president Maria Chiara Carrozza, the director of *Dipartimento Scienze Chimiche e tecnologie dei Materiali* DSCTM CNR Lidia Armelao, and the president of *Società Chimica Italiana* (SCI) Gaetano Guerra. All the representatives of the national and international chemical societies underlined the key role of chemical sciences and innovative materials in the green transition.

The conference was organized in four thematic sessions:

- production and uses of green hydrogen, in which the topics relating to water electrolysis processes and the materials used in these processes and in fuel cells were discussed;
- transport and storage, both through chemical approaches and physical methods and the presentation of case studies;
- production of chemicals with high added value and with green methods, such as the so-called "e-fuels"; and finally
- decarbonization policies, analyzing both the political-regulatory aspects of the issue and the strategic ones.

Finally, particular attention was paid to the most difficult industrial sectors to decarbonize, such as steel, ceramics, glass and cement, which constitute a first, crucial challenge ground for the use of green and blue hydrogen.

The special issue collects some of the reports presented at the conference, and includes:

- "H₂ in the energy transition" by Vito Di Noto *et al.* University of Padova,
- "Rethinking chemical production with green hydrogen" by Gabriele Centi *et al.* University of Messina,
- "Hydrogen storage and handling with hydrides" by Marcello Baricco *et al.* University of Torino,
- "Hydrogen as an energy carrier: constraints and opportunities" by Nicola Armaroli *et al.* National Research Council - Bologna,
- "In-situ and operando Grazing Incidence XAS: a novel set-up and its application to model Pd electrodes for alcohols oxidation" by Alessandro Lavacchi *et al.* National Research Council – Firenze,
- "Watching atoms at work during reactions" by Stefano Agnoli *et al.* University of Padova,

Making an imPACt

- “Hydrogen production and conversion to chemicals: a zero-carbon puzzle?” by Mario Marchionna SAIPEM – Milano,
- “Shaping the future of green hydrogen: De Nora’s electrochemical technologies for fueling the energy transition” by Michele Perego *et al.* De Nora Industries – Milano,
- “Perovskite: a key structure for a sustainable hydrogen economy” by Alessandra Sanson National Research Council – Faenza,
- “Advanced polymer electrolyte membrane water electrolysis for power to gas applications” by Antonino Salvatore Aricò *et al.* National Research Council – Messina.

The proceedings in Italian are published in a dedicated issue of “La Chimica & l’Industria” edited by the Italian Chemical Society (issue 5/2023) <https://www.soc.chim.it/it/riviste/chimica_industria/catalogo>.

<https://www.degruyter.com/journal/key/pac/96/4/html>



Lectures and session discussions of the Avogadro Colloquia took place in the iconic Marconi Hall of the Consiglio Nazionale delle Ricerche (CNR), Piazzale Aldo Moro, in Roma.

IUPAC Provisional Recommendations

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

Glossary of Terms for Mass and Volume in Analytical Chemistry

A glossary of terms and definitions for concepts in the use of mass and volume in analytical chemistry is presented. These include definitions for analytical methods of measurement (gravimetry, volumetry, and titrimetry) and supporting terms. Terms are updates of earlier recommendations or Orange Book entries.

Comments by **31 August 2024**

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Definition of materials chemistry

Materials chemistry is focused on the design, preparation and understanding of innovative materials with useful properties. It is an emerging area of research where definitions are not well established. This document defines the area of materials chemistry for the benefit of chemistry communities and the general public worldwide interested in this discipline. This Recommendation defines the term “materials chemistry” as “Scientific discipline that designs, synthesizes and characterizes materials, with particular interest upon processing and understanding of useful or potentially useful properties displayed by such designed materials.”

Comments by **31 July 2024**

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Systems Thinking and Sustainability— A Workshop at 5th ACRICE

by Marietjie Potgieter and Ghada Bassioni

The Fifth African Conference on Research in Chemistry Education (ACRICE2022) was held at the Ain Shams University in Cairo, Egypt, from 6-10 December 2022. The objectives of the conference were to emphasize the importance of chemistry education for sustainable development and to promote partnerships between those in charge of teaching chemistry in Africa and world experts in this field to further this cause. The conference provided an opportunity for the presentation of chemistry education research and the exchange of experiences in curriculum development to align chemistry education with the imperatives of sustainability. The conference was endorsed and financially supported by IUPAC. IUPAC president Javier García-Martínez attended the conference and delivered a plenary address during the opening ceremony.

The IUPAC Committee on Chemistry Education (CCE) accepted an invitation by the organizers of ACRICE2022 to present a one-day workshop on Systems Thinking in Chemistry Education (STICE) as the feature activity of the conference. The workshop was presented on Wednesday, 8 December 2022 in three 2-hour sessions and was led by Felix Ho and Marietjie Potgieter, the chair and secretary of the CCE, respectively. It was attended by approximately 40 participants: Chemistry educators from different faculties at Ain Shams University—professors, lecturers,



assistant lecturers and demonstrators—and secondary school chemistry teachers. Before the event, all participants received access to a reading pack consisting of 20 key articles on the topic. The workshop consisted of presentations during which the basic tenets of STICE were explained, alternating with interactive hands-on activities where participants applied these principles to a relevant contextual challenge in Egypt. Eight self-assigned small groups were formed at the start of the workshop for participants to exchange ideas and collaborate on activities. A trademark of the workshop was the lively debate and active participation of all members which was enabled by this configuration.

Workshop outcomes

- The workshop provided an opportunity for participants to engage experts on the principles of STICE and its relevance to sustainability. They applied these principles to the design of a learning sequence on the chemistry involved in the sustainable provision of clean water for all inhabitants in Cairo which would be suitable to implement in their teaching.
- Participants acknowledged the need for global collaboration to move urgently towards new educational systems that can prepare the next generations to be systems thinkers able to solve global systemic problems and crises. Systems thinking is essential not only for deep learning of chemistry but also to prepare students for the future professions of the 4th Industrial Revolution.
- Attendees were introduced to the limitations of traditional teaching approaches as compared



Project team: Felix Ho (CCE secretary, presenter), Nadia Kandile (project chair, ACRICE scientific chair), Marietjie Potgieter (CCE chair, project chair and presenter), and Ghada Bassioni (chair of ACRICE organizing committee)



to the potential of STICE to prepare chemistry graduates to contribute meaningfully in multidisciplinary teams working on sustainability challenges. In addition, STICE encourages students to take personal responsibility for lifestyle choices that contribute to sustainability.

- The conference highlighted the need to distinguish between STICE and a systemic approach to the teaching and learning of chemistry (SATL). STICE represents an area of active development in chemistry education internationally and is supported by IUPAC (<https://iupac.org/project/2017-010-1-050/>, <https://iupac.org/project/2020-014-3-050/>, <https://iupac.org/project/2023-004-2-050/>). SATL was pioneered and refined by Farouk Fahmy, Emeritus Professor

of Chemistry at Ain Shams and conference chair for ACRICE2022.

- Several participants, especially high school chemistry teachers, were inspired by the potential of STICE to demonstrate the relevance of chemistry to everyday contextual problems and were empowered to infuse that in their chemistry teaching. Tertiary educators were similarly convinced of the need to infuse STICE but acknowledged the constraints imposed by fixed curricula and the unavailability of textbooks in which STICE is made explicit.

or more information and comment, contact Task Group Chairs Marietjie Potgieter <marietjie.potgieter@up.ac.za> or Nadia Kandile | <https://iupac.org/project/2022-013-1-050/>

Worldwide Nurturing Green Chemistry Innovators

**The 15th Green Chemistry
Postgraduate Summer School
2023, dedicated to the memory of
Prof. Pietro Tundo**

*by Soulaima Chkirida, Géraldine
Chanteux, and Sherwin Hugo T. Lu*

In memory of Professor Pietro Tundo, the founder of the Green Chemistry Postgraduate Summer School and the Green Sciences for Sustainable Development Foundation and one of the leading scientists in the field of Green Chemistry, whose recent passing has left a profound void in the world of Green Chemistry:

Pietro Tundo's remarkable leadership and commitment to fostering global collaboration in Green Chemistry have left an indelible mark on all who had the privilege of working alongside him. As we reflect on the transformative experiences of the 15th Green Chemistry Postgraduate Summer School, we fondly remember Pietro Tundo, who has graced us with his presence despite battling illness. Despite his physical absence, Prof. Tundo's unwavering commitment to the Summer School and the principles of Green Chemistry was still felt even from afar. He was fully engaged, ensuring that every detail was meticulously taken care of. While we mourn his loss, we also celebrate his enduring legacy and the countless lives he touched through his pioneering work in Green Chemistry. In honoring Prof. Tundo's memory, we rededicate ourselves to advancing the principles of Green Chemistry and building a more sustainable future, and we pledge to carry forward his passion and dedication, ensuring that his vision for a more sustainable world continues to thrive for generations to come. Now, as we move forward, we honor his memory by continuing in his footsteps, striving for greatness as we are a community of environmentally conscious green chemists.

In the pursuit of a sustainable future, the realm of chemistry stands at the forefront of innovation and change. Within the realm of Green Chemistry, scientists and scholars converge, seeking eco-friendly solutions and eco-conscious alternatives, harnessing the power of nature to solve some of the world's pressing global challenges.



Professor Pietro Tundo

Against this backdrop, the 15th Green Chemistry Postgraduate Summer School held in the wonderful city of Venice, Italy, from 2-7 July 2023, emerged as a beacon of inspiration and education for emerging researchers in the field of Green Chemistry. The summer school was organized by the Green Sciences for Sustainable Development (GSSD) Foundation in collaboration with IUPAC's Interdivisional Committee of Green Chemistry for Sustainable Development (ICGCSD) and Ca' Foscari University of Venice, Italy. This annual event provided a unique platform for like-minded researchers and talented peers to engage in meaningful discussions about

sustainable solutions, develop collaborations, and delve into the depths of green chemistry for a more sustainable future. As a highlight on the calendar of green chemists worldwide, this serves as a melting pot of minds willing to push the boundaries of what is possible in the realms of renewable energy, eco-friendly synthesis, and waste reduction. Participants were prepared for a week of intense learning and knowledge exchange with a carefully crafted program that included notable keynote speakers and vibrant poster sessions.

The event brought together well-known scientists and leading experts worldwide, with 148 students hailing from 40 different nationalities. The Summer School embraced a hybrid format, blending online and in-person participation, facilitated by the Green Sciences for Sustainable Development Foundation.

Notably, the Foundation provided financial support to students from developing countries, underscoring the universality of green chemistry and science and collaboration across borders. Acknowledging the generous support of sponsors spanning across continents, the GSSD Foundation emphasizes the universal language of science, transcending political boundaries. This 15th edition follows a legacy of 14 previous successful editions, with the in-person sessions hosted at Ca' Foscari University of Venice's "Gradoni" auditorium, and accommodations were provided at the Campluss Santa Marta Apartments.

This article, authored by **Soulaima Chkirida**, **Géraldine Chanteux**, and **Sherwin Hugo T. Lu**, the three on-site poster awardees, chronicles personal journey through this transformative experience. From the anticipation and preparations preceding the

summer school to the invaluable insights gained from distinguished experts, we culminated in the unexpected honor of receiving a total of six Best Poster Awards, three on-site and three online via Zoom.

Reflecting on the event's success, it is evident that every detail was scrupulously attended to. This level of quality reflects the devotion and hard work of the organizers who worked behind the scenes. Collaborating alongside Prof. Tundo were the members of the organizing committee, each bringing their unique expertise and passion for Green Chemistry for sustainable development to the forefront. Fabio Aricó, representing Ca' Foscari University of Venice, Aurelia Visa, from the Romanian Academy "Coriolan Drăgulescu" Institute of Chemistry in Timisoara, Mirabbos Hojamberdiev from Technische Universität Berlin, Graziana Gigliuto, and Beatrice Tassotti from the Green Sciences for Sustainable Development Foundation, and ensuring the seamless maintenance of the online platform. This dedication guaranteed full participation, extending the reach of the event.

Sherwin Lu: One way that I'd describe my experience is the feeling of standing by the feet of giants. The whole summer school was such a gratifying experience to have conversed with great academics and colleagues from all around the world. Before this, I had just come from a slump in my academic progress and it still boggles me how I eventually got to attend the Green Chemistry Summer School 2023. Truth be told, I was initially hesitant to join since I was only a master's student, but I was encouraged as a student in the Green Chemistry and Sustainability program of Chulalongkorn University, Thailand. I had only been studying for a year and this felt like a mix of luck and generosity that my adviser had encouraged me to attend this event. It was a great opportunity, especially with the physical attendance of Nobel Laureate Jean-Marie Lehn and the remote attendance by Pietro Tundo, who was at the forefront of promoting green chemistry.

Entering the summer school, I didn't feel as nervous as I was excited up until we started introducing ourselves

to each other. I found myself in a room with professors and Ph.D. students from all around the world. Initially, I only knew Nan, my lab mate, who also attended the summer school, but later on, I had met new friends such as Eunice, a fellow Filipino who's studying in France, and Pa, a Thai student from Sweden. Over the next few days, the open forum-like design of summer school had made interactions a lot easier like the communal lunch tables, where we were simply people who had knowledge in green chemistry. If not for the nametags and the lectures, I don't think I could've distinguished the students and lecturers. What was enjoyable was the after 4 pm trips to anywhere in Venice that sometimes included late-night walks by the riverside with my additional friends, Gamze and Azime from Turkey.

As the latter half of the summer school happened, I found myself being more interested in not just learning, but also engaging and interacting with everyone. During the poster sessions, so many works from different fields using different approaches were presented, all with the common goal of abiding by the 12 principles and UN SDGs. Coming from a green chemistry program in its infancy, it was inspiring to learn about these to say the least. During the lectures, I was really glued to my seat about the myriad of perspectives on green chemistry. Out of these, I personally think two lectures were truly inspiring: one by Philip Jessop and another by Alessandra Quadrelli. Jessop's way of delivery and method of teaching allowed me to see his perspective on the potential of their work's material. Jessop showed how a switchable material, which could have just as easily only been a research work, was actually placed into commercial reality. As for Quadrelli's data-backed approach and style of presentation, this truly flipped my understanding of how to see green chemistry. It was not only the science of being green that mattered, but also the social aspects of it; essentially situated green chemistry. Admittedly, I was so captivated by Quadrelli's talk that I had written close to nothing; I was fully preoccupied with the philosophical and scientific questions posed by her talk. A last addition to my experience was an impromptu conversation with Mirabbos Hojamberdiev during our boat ride to Burano Island. It pretty much affirmed my desire for an academic career and also to broaden my outlook on opportunities. Applying for a master's degree abroad and coming to the summer school already felt like climbing giants' steps, but I was motivated even more to climb higher and higher steps just from that exchange with Mirabbos Hojamberdiev.

As the summer school ended, I realized this place was more than just sharing our academic works, but



Sherwin Lu

also the journey and history of our works. It made me realize that Green Chemistry, as it is now, may only exist through the community it creates and the goal we collectively aim for. It is nice that we have greener alternatives and research being done, but its future potential can only be realized together with our peers. In questioning and sharing each other's work, we gain perspectives into what green chemistry means to each field and how we each put the principle into our own works. These events help to invite, inspire, and involve people in the discussion of green chemistry and, eventually, prompt people to simply call it chemistry."

Géraldine Chanteux

reflects on her experience: The 2023 in-person Green Chemistry Summer school was, to me as a PhD candidate, a unique opportunity to delve into the goals and challenges of chemistry towards a more sustainable world. Indeed, questioning fundamental challenges such as 'how to make chemistry green?', 'how to develop chemistry processes compatible with ecological principles and in line with our living system?' stands as an imperative stride towards developing the green and sustainable world of tomorrow.

Expecting nothing more than learning knowledge about alternative chemistries and looking for inspiring scientific discussions, I ended up the week fascinated by the variety of discussions and topics shared all together, which raised new perspectives and will certainly guide my future researches and choices.

Sustainability and green chemistry are ever-growing topics in social media and have boomed in the last years, particularly since the coronavirus crisis in 2020. The week at the Summer School in Venice brought keys to develop a sustainable approach in chemistry, based on past, present and future developed researches. Awareness that the Earth's limits are already surpassed (for 6 over 9) is critical to change mindset, and has, to me, been put in exergue during the summer School week in Venice. After being aware of the problems engendered by past developments in chemistry, the current attempts for sustainable processes were exposed as well as strategies behind. Importantly, the next challenges were enumerated and some solutions were detailed in terms of the use of



Géraldine Chanteux

water-based solvents reactions, biomass valorization, circularity in the chemical processes, waste treatment and so on. Notably, the share of chemistry projects between the young researchers during the poster sessions complemented the courses by including fresh and new ideas and was, for sure, an invaluable and insightful moment. These shared moments were very inspiring because it raised new ideas for the development of on-going or future research projects with more sustainable approaches.

From the courses held during the week, Jean-Marie Lehn defined the Periodic Table's elements as "the Matter that matters." As chemists, we play a crucial role in manipulating this matter to develop lifestyle comfort and facilitate the lives of human beings. Therefore, the study of chemistry is at the core of new sustainable technologies and acts as a tool to create new technologies that actually impact a lot our development as human beings. As judiciously depicted by Paul Anastas: "Today's chemical sector is about depleting and degrading. Tomorrow's chemical sector will be renewable and restoring. This is what we necessarily need to target and achieve." The discussion on alternative pathways to perform organic synthesis was raised. Particularly interesting idea considering the current global economic/ecological transition mandatory to be well adapted to environmental changes. To be noted, the accessibility to connect with open-minded teachers such as Alessandra Quadrelli was greatly appreciated all during the week. I am grateful for sharing ideas and being able to debate on important subjects like energy transition with her.

Following the same end goal, it was taught in the summer school that connecting disciplines one to another is one key factor for practical and efficient sustainable technologies in the future. To do so, life cycle assessment is a tool that considers the cost of a chemical process as a whole instead of one step isolated from the whole synthesis-industrialization process. One illustrative example, taught by Philipp Jessop, consists of the life cycle assessment of a synthesis reaction. The systematic evaluation of different factors by LCA tools (E factor, amount of CO₂ and other greenhouse gases released...) depends on the input considered into the calculations. In a chemical reaction, the chemist considers the quantities of reagents and the volume of solvents used, as well as the energy consumed to heat up a reaction, the volumes of washing solvents needed post reaction, *etc.* But also, if looking before and after the synthesis reaction (*i.e.* extraction and transport of metal resources, the energy to regenerate the solvents or chemical waste's treatment, the recycling of the



chemicals *etc.*), these aspects not only concern the chemist's work but also engineering branches, production chain, merchants and so on. These parameters, globally, are forming the major factors that are impactful in the final calculation of the LCA report and must be included for an accurate estimation of the environmental cost of the whole process. For sure, LCA-related technologies will help in raising solutions in making chemistry greener and sustainable in the near future.

To conclude on the experience, the Summer School brings together scientists, in raising the understanding and goals of sustainability and green chemistry. This event permitted to share ideas, insights, perspectives, tools to a vast community of "green chemists" to go towards a more sustainable way to work in the chemistry's world. As a chemist, this week gave me new perspectives on how to work in chemistry in a sustainable and more responsible way, to respect the world despite ever-growing technologies. The spreading of the chemistry's perspectives by brilliant professors and researchers is very precious for the young generation of scientists on solving challenges related to current technologies, *i.e.* climate change objectives, energy related questions, pollutions, resources use. The emulation around green chemistry topic was a real source of inspiration for me and I am so grateful of taking part of the event. The balance between classes, poster sessions and informal relaxing events (such as the boat tour) was enriching to create connections, and friendships with the students from different horizons, with a desire to share advancements and different mindsets on green chemistry and sustainability. I really hope this experience will encourage many more students to build and integrate the vast community of green chemists,

for a smooth transition towards a future world hopefully becoming sustainable and environment-friendly."

As for the experience of **Soulaima Chkirida**: attending the summer school in Green Chemistry in Italy, as a resident of a developing country, was nothing short of a dream come true. I had applied for the scholarship before completing my Ph.D. thesis, hoping for a chance to immerse myself in the world of sustainable chemistry. When I received the acceptance notification in March 2023 "on my birthday," it was an unforgettable moment. Attending the Summer School right after completing my thesis was the icing on the cake, and being recognized as one of the best poster awardees was truly the highlight of my academic journey.

Italy had always been my dream destination, and experiencing the Summer School amidst the breathtaking beauty of Venice was a life-changing experience. Every moment, from the stimulating sessions at the school to the leisurely walks along the picturesque streets of Venice, filled me with immense gratitude. In the midst of July, a time when staying in Italy would have been financially out of reach for me, I found myself living a dream, thanks to the generosity of the organizing committee.

While all the lectures were captivating and each



Soulaima Chkirida

professor demonstrated remarkable talent, there were two presentations that left an indelible mark on my experience: the lecture by Nobel laureate Jean-Marie Lehn and the enlightening insights shared by Paul Anastas, Director of Green Chemistry at Yale University.

Meeting Nobel Laureate Jean-Marie Lehn was an extraordinary privilege and a moment of immense excitement for me. His lecture on supramolecular chemistry, which delves into chemistry beyond the molecule, was truly enlightening. Lehn's insights into this fascinating field opened my eyes to the boundless possibilities of molecular assembly and interaction. Having the courage to ask Lehn a question and engage in a face-to-face interaction with him was a pivotal moment in my academic journey. Standing beside such a towering figure in the scientific community filled me with a profound sense of awe and admiration. It was an honor to have the opportunity to converse with someone of his caliber and to gain further insights into the intricate world of supramolecular chemistry.

Paul Anastas, Director of Green Chemistry at Yale University, delivered a captivating lecture on green chemistry and green engineering that left a lasting impression on me. One quote in particular stood out: *"It's not about what to do with the chemistry, but how you do your chemistry and why?"*. Anastas's emphasis on the process and purpose of chemistry challenged conventional thinking and underscored the importance of sustainability and ethical considerations in scientific practices. His lecture highlighted the pivotal role of green chemistry and engineering in addressing global environmental challenges while fostering innovation and progress. His lecture, overall, inspired me to reevaluate my approach to chemistry and to consider the broader implications of my work. By prioritizing environmentally conscious practices and understanding the underlying motivations behind our scientific endeavors, we can contribute to a more sustainable and equitable future for generations to come.

Moreover, beyond the academic realm, the summer school provided us with a unique opportunity to explore the enchanting island of Burano. This day trip was not just a delightful escape from the rigors of our academic pursuits but also a profound opportunity for cultural exchange and networking. As we wandered through the vibrant streets adorned with colorful houses, we forged connections that transcended borders and languages. It was a remarkable experience witnessing individuals from diverse nationalities come together, sharing stories, and building camaraderie.

This experience underscored a profound truth: while researchers from developing countries may

face challenges in accessing advanced scientific infrastructure, our passion, talent, and knowledge are second to none. The opportunity provided by the Summer School is a testament to the transformative power of granting access to education and resources. It serves as a reminder that given the right opportunities, researchers from all backgrounds can contribute meaningfully to scientific research and innovation. I am deeply grateful to the organizing committee for making this experience possible and for recognizing the potential of researchers from developing countries. Their commitment to inclusivity and opportunity has left an indelible mark on my academic journey.

As we reflect on the completion of this article, we cannot help but feel a sense of regret that Professor Pietro Tundo is no longer with us to read it. We believe he would have been proud to see the culmination of our experiences at the Green Chemistry Summer School captured in this piece. His vision and dedication to the advancement of green chemistry will continue to inspire generations of researchers, and we are honored to contribute to his legacy through this article. Additionally, this Summer School serves as a beacon of education and inspiration for young researchers worldwide, fostering a deeper understanding of the principles and practices of Green Chemistry. It is imperative that such initiatives continue to thrive, providing invaluable opportunities for future generations to contribute to a more sustainable world. By instilling a sense of environmental stewardship and fostering innovation in sustainable practices, initiatives such as this Summer School play a pivotal role in shaping a more sustainable future for all.

Last but not least, we would like to express our gratitude to Mirabbos Hojamberdiev for his unwavering belief in us and for entrusting us with the opportunity to write this article. His guidance and support have been invaluable throughout this process, and we are deeply grateful for the confidence he has shown in our abilities.

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See details at <https://iupac.org/brief-from-the-2023-summer-school-on-green-chemistry/>

Digital Standards: A Path to Sustainable and Interoperable Chemical Data Exchange

by Fatima Mustafa, Dana Vanderwall, Leah McEwen, Ray Boucher, Richard Hartshorn, Ian Bruno, Greta Heydenrych, and Gerd Blanke

In today's rapidly evolving digital landscape, the importance of standardized data exchange cannot be overstated, especially in fields as critical as chemistry that contribute hugely to many related disciplines. Recognizing this urgency and having the drive of applying Sustainable Development Goals (SDGs) especially strengthen global partnerships, IUPAC has led a workshop in collaboration with the InChI Trust, and the Cambridge Crystallographic Data Center (CCDC). This effort was in the form of a focused invitation-only workshop [1] that was held at the CCDC, Cambridge, UK during 25-26 March 2024 with the aim of charting a course for the development, adoption, and maintenance of digital standards within the Chemistry community. The workshop was held under the umbrella of the WorldFAIR Chemistry project coordinated by CODATA and RDA [2]*. It gathered participants from diverse backgrounds and areas of

expertise—academia, industry, standards organizations, publishing, and cheminformatics—who rarely have the opportunity to collaborate and be in one room. Using the FAIR (Findable, Accessible, Interoperable, and Reusable) data principles [3], the workshop sought to address fundamental questions surrounding sustainability, stakeholder and user engagement and the future of chemical data standards in an increasingly complex digital world.

The Importance for Digital Standards

For over a century, the Chemistry community has relied on established standards to communicate complex chemical information accurately and efficiently. IUPAC has played a key role in setting and disseminating these standards. Yet, with the advent of digital technologies, the landscape is shifting dramatically. Digital standards play a crucial role in enabling interoperability and data exchange across diverse scientific domains [4], and reinforce the digital economy as it is significantly enhanced by digital data [5]. While these technologies offer unprecedented opportunities for data exchange and collaboration, they also present new challenges, particularly in terms of implementation and scale. The need for consistent, machine-readable data exchange is more pressing than ever, necessitating a

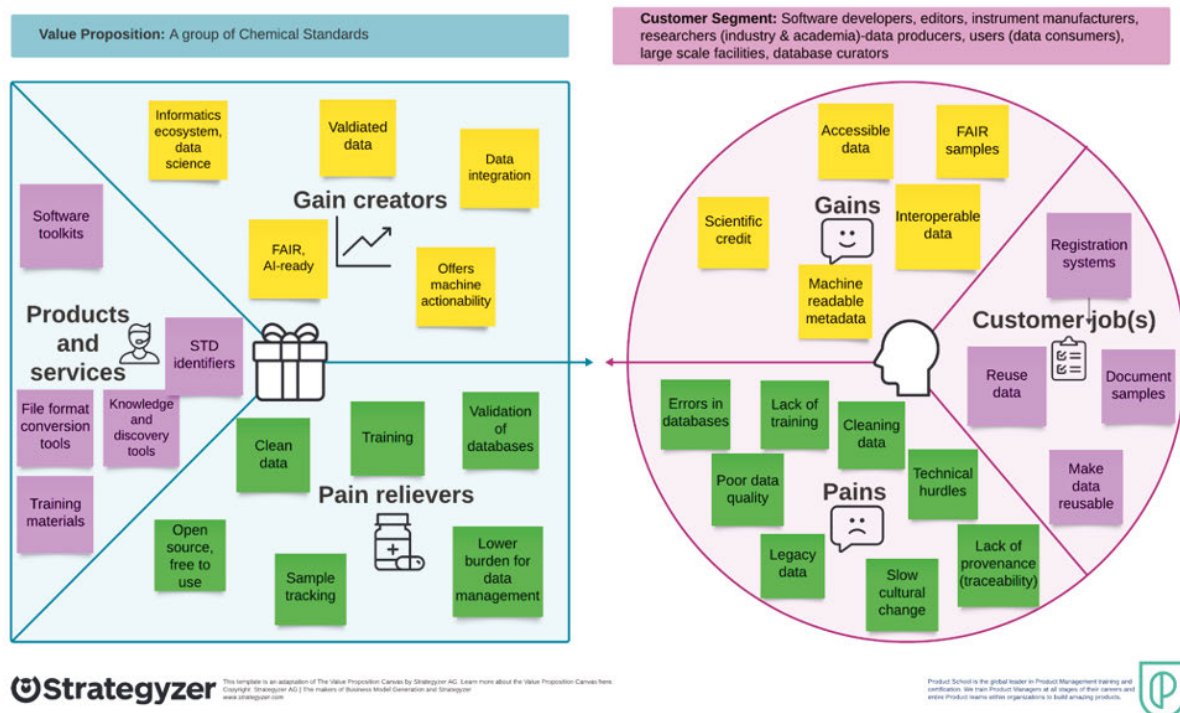


Figure 1. Business Model Canvas based on hands-on exercises in which participants examined multiple existing Chemical standards.



Participants of the “Sustainable Business Modeling for Digital Standards Development” workshop, CCDC, Cambridge, UK, 25-26 March 2024. Image credited to Michael Webb ©University of Cambridge

robust and proactive approach to standards development and adoption.

Paving the Path for Sustainability

While numerous valuable standards have emerged from collaborative efforts in Chemistry and the Life Sciences, many of these projects have lacked a sustainable plan or resources for long-term viability. Establishing a sustainable framework for projects targeting specific demands around digital standards for chemistry, thorough comprehension of the economic landscape, operational dynamics, and resources essential for developing, sustaining, and maintaining a solution (digital standard and supporting tools). This area may frequently be unfamiliar to scientists or developers who initially conceive solutions for common problems. Based on Peter Drucker's definition, a good business model answers the questions: “Who is the customer? And what does the customer value? It also provides the fundamental questions every manager must ask: How do we make money in this business? What is the underlying economic logic that explains how we can deliver value to customers at an appropriate cost?” [6].

A critical focus of the workshop was the challenge

of sustainability. Developing and maintaining digital standards requires significant ongoing investment of resources and expertise, making long-term sustainable business models a pressing concern. Through hands-on exercises, participants examined multiple existing standards such as:

- InChI - Identifier for chemical structures
- IGSN - Persistent identifier for samples
- HELM - Notation for biological macromolecules
- SMILES - Notation for chemical structures
- MOL/SDfile - Representation format for chemical structure
- UDM - Unified data model for chemical reactions
- CIF - Exchange format for crystallographic data + checkCIF
- ChEBI - Ontology for chemical entities of biological interest
- IDMP-o - Ontology for identification of medical products
- ADF - Allotrope Data Framework for analytical data.

Throughout the activity, the business model (**Figure 1**) and value proposition canvas were used to define community, contributors and users, and

other stakeholders; define parameters around values, both open and revenue-generating; articulate target resources and services to serve the broader community in using standards; initiate market analysis and identify funding streams which will feed into the IUPAC roadmap for digital Chemistry standards.

The main themes derived from these discussions were:

- **Value Proposition:** at first standards might seem similar in benefits; however, it would be helpful to communicate with potential adopters to help differentiate the utility of each one in certain use cases.
- **Relationships with customers:** It was common to require extra activities and resources to build and keep relationships, bring more awareness and understanding which are a precondition to adoption.
- **Resources:** All the standards we studied commonly require technical resources, although to a lesser degree for operational support tasks.
- **Activities:** Various aspects such as payment innovation, operational support including licenses, travel, and software development alongside strategic planning, software development sustainability, and infrastructure maintenance and construction are crucial considerations. Additionally, efforts directed towards driving adoption through innovation workshops and bringing subject matter experts together. These activities collectively contribute to the comprehensive ecosystem supporting advancement and adoption.
- **Revenue Models:** There's a widespread interest in assessing license and revenue models that achieve a balance between accessibility and sustainability.

Stakeholder Engagement

Central to the workshop's agenda was the exploration of strategies to maximize the opportunities presented by digital technologies. Participants delved into questions of stakeholder engagement, identifying key players in the Chemistry data economy, and fostering collaborative approaches to standards development. Stakeholder engagement is essential for the effective development and implementation of digital standards, ensuring that they meet the diverse needs of the user community [7]. By aligning efforts across disciplines and sectors, the workshop aimed to ensure that digital standards remain relevant, accessible, and interoperable in an increasingly interconnected world.

Looking Ahead

The collective goals for Chemistry digital standards encompass building relationships, establishing new partnerships, enhancing outreach and engagement, managing technical and coordination resources, and understanding business models. The discussions reflected a shared interest in clarifying common objectives and limitations of collaborative efforts, identifying key stakeholders, and extending the reach of the initiative. Participants emphasized the importance of a well-articulated mission, potentially through an extended white paper [8] (which was initially drafted to outline the scope of the workshop), to guide future actions and recruit additional contributors. Additionally, there was a recognition of the need to address resource challenges, explore alternative models for sustainability, and connect with relevant international organizations such as CODATA and RDA, as well as national organizations, the private sector, and funding organizations. The dialogue also touched on the potential impact of digital standards on related disciplines and industries, particularly in the context of artificial intelligence and machine learning applications.

Following the workshop, there will be an 18-month plan, involving contributions from various participants to continue working on the white paper and to convene for another workshop. The plan includes the establishment of a coalition, association, or federation dedicated to sustaining digital standards in the chemical sciences and adjacent disciplines. Workstreams will be discussed in June 2024, and a workshop focusing on the sustainability of standards organizations themselves will be in near future.

Overall, the focus was on fostering collaboration, defining strategic priorities, and leveraging collective expertise to advance the development and adoption of Chemistry digital standards. The sustainability of chemical informatics standards depends on active engagement, collaboration, and support from the broader community of stakeholders. By following best practices in standards development, collaboration, adoption, and long-term planning for maintenance and resourcing, we can ensure that these standards continue to support research, education, and innovation in Chemistry and related fields for years to come.

References

1. Vanderwall, D., & Leah, M. (2024). Workshop: Sustainable Business Modeling for Digital Standards Development. Zenodo. <https://doi.org/10.5281/zenodo.10966075>
2. WorldFAIR Chemistry: making IUPAC assets FAIR, <https://iupac.org/project/2022-012-1-024/>

3. Wilkinson, M., Dumontier, M., Aalbersberg, I. *et al.* The FAIR Guiding Principles for scientific data management and stewardship. *Sci Data* 3, 160018 (2016). <https://doi.org/10.1038/sdata.2016.18>
4. NIST (2018), The Role of Standards in Digital Transformation. National Institute of Standards and Technology
5. OECD Roadmap Towards a Common Framework for Measuring the Digital Economy (2020)
6. <https://hbr.org/2002/05/why-business-models-matter>
7. OECD Roadmap Towards a Common Framework for Measuring the Digital Economy (2020)
8. Vanderwall, D., & Leah, M. (2024). Workshop: Sustainable Business Modeling for Digital Standards Development. Zenodo. <https://doi.org/10.5281/zenodo.10966075>

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The organizing team extends heartfelt gratitude to all workshop participants, and panelists whose enthusiastic engagement and insightful contributions were crucial to the event's success. Many of them have expressed their willingness to further collaboration and commitment.

Workshop organizing team and authors

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Feature Articles Wanted

Contact the editor for more information at <edit.ci@iupac.org>.

GREEN CHEMISTRY POSTGRADUATE SUMMER SCHOOL

In memory of Professor Pietro Tundo

30th of June - 5th of July 2024

Venice, Italy

Organizers:

Francesco Trotta Chairman

Fabio Aricò

Aurelia Visa

Mirabbos Hojamberdiev

Graziana Gigliuto Secretary

Topics:

Benign synthesis routes

Green catalysis

Alternative solvents

Renewable and green raw materials

Green chemistry for energy

Clean processes

Green Chemistry education

Info:

www.greenchemistry.school

www.gssd-foundation.org

Contacts:

postmaster@pec.gssd-foundation.org

secretariat@gssd-foundation.org

2024 (starting 1 July)

30 Jun - 3 Jul 2024 - Biotechnology - Maastricht, The Netherlands

19th International Biotechnology Symposium - "Biotechnology for the Grand Challenges of our Society", joint with the 19th European Congress on Biotechnology (ECB2024) and the Annual Dutch Biotechnology Meeting (NBC-24)

Co-chair: Aldrik Velders, Wageningen University; contact: ecb@tfigroup.com • <https://www.ecb2024.com/>

30 Jun - 5 Jul 2024 - XVI Postgraduate Summer School on Green Chemistry - Venezia, Italia

General information: secretariat@gssd-foundation.org • <https://www.greenchemistry.school/>

1-4 Jul 2024 - MACRO2024 - Coventry, UK

50th World Polymer Congress—Sustainability: improving lives whilst preserving our planet

Chair: Dave Haddleton, University of Warwick, Coventry, UK, d.m.haddleton@warwick.ac.uk

<https://www.macro2024.org/>

8-12 July 2024 - Science, Technology, Society and WIKIPEDIA

Contact: Raos Guido and Fabio Parmeggiani Dept. of Chemistry, Materials and Chem. Eng. "G. Natta"

Politecnico di Milano • guido.raos@polimi.it, fabio.parmeggiani@polimi.it

14-19 Jul 2024 - Photochemistry – Valencia, Spain

29th IUPAC Symposium on Photochemistry

Symposium co-chairs: Gonzalo Cosa <gonzalo.cosa@mcgill.ca> and Maria Marín <marmarin@qim.upv.es>

<https://www.photoiupac2024.com/>

15-19 Jul 2024 - Chemistry Education - Pattaya, Thailand

27th IUPAC International Conference of Chemistry Education (ICCE2024) - The Power of Chemistry Education for Advancing SDGs

Chair: Supawan Tantayanon, Faculty of Science, Chulalongkorn University, Supawan.T@chula.ac.th;

Contact: icce2024@gmail.com • <https://www.icce2024thailand.com>

23-26 Jul 2024 - Congreso de Química Costa Rica - Heredia, Costa Rica

Chemistry: a solution for global changes

Chair of the IAB and of the Local Organizing Committee: Carlos Vega Aguilar, Carlos.vegaaguilar@ucr.ac.cr

<https://eventoscqcr.com/congreso/>

29 Jul - 2 Aug 2024 - Soft Matter - Raleigh, North Carolina, USA

8th International Soft Matter Conference (ISMC2024) - Blurring Boundaries Between Fields

Contact: Daphne Klotsa, Department of Applied Physical Sciences, University of North Carolina in Chapel Hill,

dklotsa@email.unc.edu • <https://soft-matter.com/ismc2024/>

11-16 Aug 2024 - Novel Aromatic Compounds - Toronto, Canada

20th International Symposium on Novel Aromatic Compounds

Chair: Dr. Thomas Baumgartner (he/him) York University, Toronto, ON, Canada; isna2024@outlook.com

<https://www.isna2024.com/>

12-16 August 2024 - Transforming Chemistry and Interdisciplinary Research to Innovation

The Virtual Conference on Chemistry and its Applications (VCCA-2024)

Contact: Ponnadurai Ramasami, Chair of VCCA-2024, vccamru@uom.ac.mu

<https://sites.google.com/uom.ac.mu/vcca-2024>

18-22 Aug 2024 - Physical Organic Chemistry - Beijing, China

26th IUPAC International Conference on Physical Organic Chemistry

Chair: Jin-Pei Cheng, Centre of Basic Molecular Science (CBMS), Tsinghua University, Beijing, China;

icpoc26@mail.tsinghua.edu.cn • <https://www.icpoc26.tsinghua.edu.cn/>

9-13 Sep 2024 - Solubility Phenomena - Novi Sad, Serbia,

21st International Symposium on Solubility Phenomena and Related Equilibrium Processes

Chair: Slobodan Gadžurić, University of Novi Sad, Faculty of Sciences, Novi Sad, Serbia; slobodan.gadzuric@dh.uns.ac.rs; contact: issp2024@dh.uns.ac.rs • <https://issp2024.pmf.uns.ac.rs/>

18-20 Sep 2024 - Isoprenoids - Naples, Italy

The 25th Congress on Isoprenoids

Contact/Chair: Orazio Taglialatela-Scafati, University of Naples Federico II, Naples, scatagli@unina.it; contact: secretariat@isoprenoids25.org • <https://isoprenoids25.org/>

25 Sep 2024 - 3rd Global Conversation on Sustainability - virtual

A joint project between the IYCN and IUPAC • <https://www.gcs-day.org/>

7-12 Oct 2024 - General and Applied Chemistry - Sochi, Russian Federation

XXII Mendeleev Congress on General and Applied Chemistry

Contact: Yulia Gorbunova, Professor A.N. Frumkin Institute of Physical Chemistry and Electrochemistry of RAS; yulia@igic.ras.ru or MendeleevCongress@mesol.ru • <http://mendelevcongress.ru/>

24-29 Oct 2024 - Green Chemistry Towards Carbon Neutrality - Beijing, China

10th IUPAC International Conference on Green Chemistry

Zhimin Liu, Program committee chair, liuzm@iccas.ac.cn • <https://greeniupac2024.org>

7-9 Nov - Pesticides and Related Emerging Organic Pollutants

International Conference Pesticides and related emerging organic pollutants — Impact on the Environment and Human Health and Its Remediation Strategies

Conference Convener: Sreenivasa Rao Amaraneni, drsreenivasa.chem@eastpoint.ac.in, East Point College of Engineering & Technology, Bengaluru 560049, India <https://epcet.edu.in/international-pesticides-conference-2024/>

11-15 Nov 2024 - Solutions in Chemistry

Co-Chairs: Ernest Meštrović and Vladislav Tomišić, President of the Croatian Chemical Society

Contact: Andrea Usenik, Secretary, Faculty of Science, University of Zagreb • solutionsinchemistry@hkd.hr

19-21 Nov 2024 - Chemistry, a lever for sustainable development of African countries - Dakar, Senegal

Annual Days of Chemistry of Senegal & 9th FASC Congress (FASCIJACS 2024)

General contact: Modou Fall; modou.fall@ucad.edu.sn, PO Box 15756, Dakar-Fann, Senegal, Tel: +221775557200 • <https://csc.ucad.sn> (under Congrès and FASCIJACS 2024)

10-12 Dec - International N.I.C.E. Conference on Bioinspiration & Biobased Materials—Winter 2024

Organizing chair: Frédéric Guittard • Contact: contact@nice-conference.com

Save the dates!

11 Feb 2025 – IUPAC Global Women Breakfast – Global all around and Virtual

In 2025, the GWB will actually be held on the International Day of Women and Girls in Science <https://iupac.org/gwb>

13-18 Jul 2025 - IUPAC World Chemistry Congress 2025 - Kuala Lumpur, Malaysia

<https://iupac2025.org/>

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is the global organization that provides objective scientific expertise and develops the essential tools for the application and communication of chemical knowledge for the benefit of humankind and the world. IUPAC accomplishes its mission by fostering sustainable development, providing a common language for chemistry, and advocating the free exchange of scientific information. In fulfilling this mission, IUPAC effectively contributes to the worldwide understanding and application of the chemical sciences, to the betterment of humankind.

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