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Global Women's Breakfast 2021

FAIR and Open Data in Science ▶

Ethical Advice across Scientific Borders ▶

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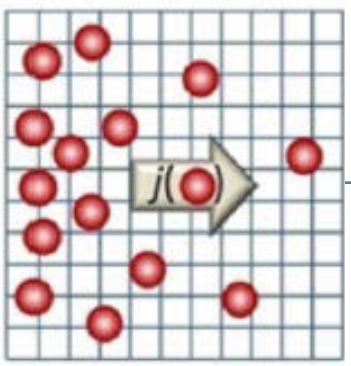
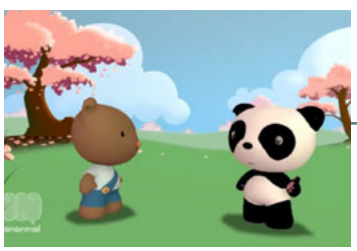
Cover: In a year marked by unprecedented challenges, IUPAC hosted the largest ever Global Women's Breakfast (GWB2021) on 9 February 2021, bringing together more than 20 000 people around the world to celebrate the achievements of women scientists, to strengthen and expand professional networks, to inspire the next generations, and to challenge the status quo with respect to equality for women scientists in the workplace. **See more p. 8.**





IUPAC first Virtual World Chemistry Congress and General Assembly

by Neil Burford

On behalf of the Organizing Committee for IUPAC|CCCE 2021, I am delighted to invite you to the 51st IUPAC General Assembly (GA) and 48th World Chemistry Congress (WCC), in conjunction with the 104th Canadian Chemistry Conference and Exhibition (CCCE). The IUPAC|CCCE 2021 events will be hosted by the Canadian Society for Chemistry (CSC), the Canadian National Committee for IUPAC (CNC-IUPAC) and the National Research Council Canada (NRC). Canada has previously hosted the IUPAC GA & WCC in Vancouver (1981) and Ottawa (2003). The original plans for IUPAC|CCCE 2021 were for the events to take place in Montréal, QC, Canada, 13-20 August 2021. Unfortunately, as travel to Montréal are impeded by the global pandemic, all events associated with IUPAC|CCCE 2021 will occur virtually. As chemical sciences professionals, we know conferences are a key venue for professional development, networking, and scientific advancement, and we will work to ensure that these principles stand true for the virtual event as well. While not a replacement for in-person events, this new endeavour will synthesize the best of our in-person events, with the convenience and accessibility of a virtual event. Beyond that, a virtual experience provides unique opportunities to engage a global audience, reach more young professionals, reduce our environmental impact, and stay safe.

For details, see iupac2021.org and program details at https://www.cheminst.ca/conference/ccce2021/program/program-overview/

I am grateful for the dedication, hard work, skills, and commitment of the Organizing Committee (listed below), which is composed of members of the CSC, NRC and staff of the Chemical Institute of Canada (CIC):

- Bruce Lennox (McGill University, Chair of the WCC)
- John Polanyi (University of Toronto, Honorary Chair of the WCC)
- Kim Baines (Western University, Co-chair of the WCC Technical program)
- Jeremy Melanson (National Research Council, Co-chair of the WCC Technical program)
- Marc Janes (NuChem Therapeutics Inc., Liaison with industry partners for the WCC)
- Shan Zou (National Research Council, Coordinator of the GA)
- Thomas Baumgartner (York University, CSC Director of Conferences)
- Joan Kingston (CIC Director of Finance and Administration)
- Paul Smith (Xerox Canada, Chair of the CIC and Interim Executive Director)
- Claire Duncan (CIC Manager of Membership, Communications and Marketing)
- Keith Lapierre (CIC Program Coordinator)

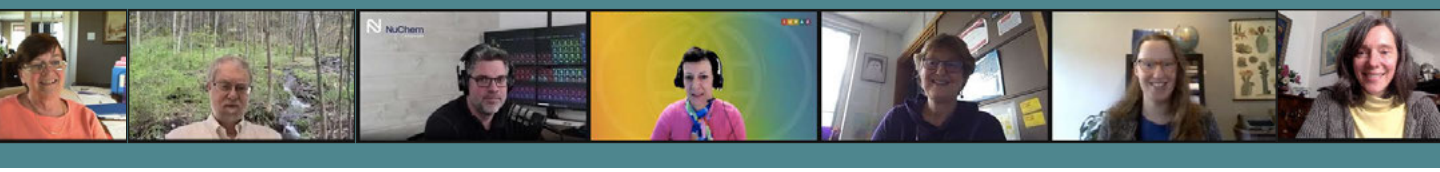
I have very much appreciated the guidance and support of the IUPAC executives Lynn Soby and Fabienne Meyers, and the IUPAC Bureau Member Chris Ober. As well, the Committee has enjoyed coordinating and collaborating with representatives of the IUPAC Division Presidents and Committee Chairs.

The Congress emphasizes the vital role of chemistry in the future of society under the title of "**Solving Global Challenges with Chemistry.**" The program is coordinated under five themes that collectively offer 86 symposia. Plenary lectures by world-class scholars will punctuate each of the themes:

- **Chemistry for Energy** (Plenary speaker: Donald R. Sadoway, MIT)
- **Chemistry for Health** (Plenary speakers: Petra Fromme, Arizona State University; Margaret Brimble, University of Auckland)
- **Chemistry for Society** (Plenary speakers: Zafra M. Lerman, Malta Conferences Foundation; Alison Thompson, Dalhousie University)
- **Chemistry for Sustainability** (Plenary speaker: Paul Anastas, Yale University)
- **Chemistry at the Frontiers** (Plenary speaker: Makoto Fujita, University of Tokyo)

The 51st General Assembly meetings of Divisions and Committees and the IUPAC Council are scheduled in advance of the Congress and all will occur virtually (https://www.cheminst.ca/conference/ccce2021/general-assembly/). The next generation of chemists is represented by the International Younger Chemists Network (IYCN), who will also hold a virtual IYCN General Assembly, and has identified the United Nations Sustainable Developments Goals as a focus for a symposium during the WCC. In addition, the participation of Young Observers during the General Assembly is encouraged.

The World Chemistry Leadership Meeting (WCLM) will take place over a 24-hour period beginning in



Montréal and with events in Malaysia (host of IUPAC 2025) and the Netherlands (host of IUPAC 2023) before returning to Montréal. The theme of the WCLM is **Applications of Artificial Intelligence to Chemistry**, addressing the education, teaching and skills required for the researcher of the future. (see details p. 48) Professor Yoshua Bengio (Université de Montréal) will present a lecture at 8:00 am EST on August 17 to open the event. Analogous events will occur 8 hours later in Kuala Lumpur and 16 hours later in the Hague and will conclude at 8:00 am EST on August 18 back in Montréal.

The hosts of IUPAC 2021 are CSC, CNC-IUPAC, and the NRC. The NRC is the Canadian National Adhering Organization (NAO) for IUPAC, the Government of Canada's premier research organization supporting industrial innovation, the advancement of knowledge, technology development and fulfilling government mandates. The NRC plays a unique role in Canada, undertaking large-scale mission-oriented research and development programs. NRC provides a national network of experts and facilities, and its world-class research capacity in diverse areas of engineering, life sciences, quantum technology, metrology, astronomy, and emerging and disruptive technologies, makes the organization a wealth of resources and knowledge. The NRC celebrated a hundred years of science excellence in 2016, and has been a pillar of federal science and support for innovation. The NRC has continually made beneficial contributions to the needs and challenges of Canadians for decades. Throughout the 20th century, the NRC provided fertile ground for many Nobel Prize-winning ideas, and to date a dozen Nobel laureates have spent most or part of their careers at NRC.

The CSC is a national, not-for-profit, professional association that unites chemistry students and professionals who work in industry, academia and government. The CSC is one of the three constituent societies of the Chemical Institute of Canada (CIC), along with the Canadian Society for Chemical Engineering (CSChE) and the Canadian Society for Chemical Technology (CSCT). Collectively, these organizations are funded by the more than 5000 members and are managed by a dedicated office located in Ottawa. The CSC organizes the annual Canadian Chemistry Conference and Exhibition (CCCE), Canada's premier annual conference for the chemical sciences, which celebrated the 100th edition in May 2017 in Toronto. The CSC and members of the CSC have an excellent record for organizing international conferences with impressive scientific programs. Examples include the IUPAC WCC and GA 2003 in Ottawa (3000+ participants, 40+ countries), World Congress of Chemical Engineering 2009 (2800+ participants, from 60+ countries). The CSC is also a Founding Society of the Pacifichem Congress that attracted 16 000+ delegates in December 2015.

Canadian chemical scientists interact with IUPAC in a number of ways. The formal relationship is through the NRC, which represents the NAO for Canada. The CNC-IUPAC was formed in 1993 in an agreement between NRC and CSC, who share responsibility for appointing committee members and maintaining a balanced representation from university, industry, government and scientific disciplines. The main responsibilities of CNC-IUPAC are to advise NRC on Canadian participation in and activities of IUPAC, to promote IUPAC activities that are of particular importance and relevance to Canada, to inform the Canadian chemical community of IUPAC activities and promote these activities to ensure maximum benefit to Canada.

Chemical research is strongly supported in Canadian universities with funding by a number of government agencies including the Natural Sciences and Engineering Council (NSERC), the Canadian Institutes of Health Research (CIHR), the Canada Foundation for Innovation (CFI), and the Canada Research Chairs (CRC). These organizations encourage collaboration and interdisciplinary research, and promote research collaboration between scientists in academia, industry and government, as well as international collaborations. The impact of Canadians on the discipline of chemistry is evident in the broad spectrum of published chemical research from Canada, the visibility of Canadians at international conferences and the eight Canadians who have been awarded the Nobel Prize for Chemistry (Smith, Marcus, Altman, Polanyi, Taube, Herzberg, Glauque, Rutherford).

With the history of significant contributions that Canadians have made to the broad discipline of chemistry and the Canadian commitment to the discipline of chemistry and to IUPAC, we look forward to hosting a successful GA and WCC. We hope that all scientists and students will enjoy the virtual experience offered for 2021 and that they have the opportunity to engage more broadly with their international colleagues.

Neil Burford, <nburford@uvic.ca>, from the University of Victoria, is Chair of the Organizing Committee of IUPAC|CCCE 2021, the 51st IUPAC General Assembly, the 48th IUPAC World Chemistry Congress and the 104th Canadian Chemistry Conference and Exhibition.

Top banner (from left to right): Present on a call of the IUPAC CCCE 2021 Organizing Committee, 7 May 2021: (from left to right) Shan Zou, Thomas Baumgartner, Zhongxin Zhou, Middlé Lemoine, Bruce Lennox, Neil Burford, Joan Kingston, Chris Ober, Marc Janes, Lynn Soby, Kim Baines, Claire Duncan, and Fabienne Meyers.

Strategies for Success as an Industrial Chemist[1]

by Carolyn Ribes

Chemists find careers in the chemical industry very rewarding. The focus is on applied chemistry and in delivering solutions that meet customer needs, whether the customers are other industrial companies or individual consumers. Chemistry provides solutions to the global challenges facing our society, including the need for clean water, nutritious food, improved healthcare and wellness, affordable housing, and sustainable infrastructure. Within industry, chemists serve in a wide variety of roles. The largest fraction may be in research and development (R&D), although opportunities in manufacturing, technical service and development, supply chain, marketing, intellectual property protection, sales and commercial functions, and many other options are also open to chemists who want to apply their skills [1]. I was drawn to a career in industry because I'm results oriented and I wanted my work to be applied immediately and have an impact.

Brilliant technical skills and an outstanding dissertation are great assets when graduates look for their first job. However, a successful career in industry requires strengths in three areas: business acumen, technical skills, and interprofessional skills. This has been described as a three-legged stool, and each leg must be strong for a successful career. "Interprofessional skills" defined as the combination of interpersonal and communication skills required for effective teamwork [2]. Most formal education programs emphasize the development of technical knowledge and skills; the focus is on cognitive development. Skills in the other areas are either learned through specific training courses offered by the employer or developed informally as on-the-job training.

Since each of us has a different definition of a successful career, it's important to understand yourself and how you define success. As an industrial chemist, you should have an individual professional development plan that outlines your skills, experiences, vision, and desired career path. It is more effective if you can describe particular roles you want to achieve at future stages, skills you want to develop, and opportunities or experiences you seek [3]. Keep that development plan updated; share it with your leader, your mentor, and others that may be able to help you achieve your professional goals. Understanding your strengths is critical as is identifying how you can fully utilize your strengths in a given role. Formal and informal feedback as well as self-assessments [4] are very useful for this. Your unique combination of strengths and skills will distinguish you from others.

Business acumen

Business acumen implies understanding what value you provide towards impacting the profitability bottom line. Chemical companies exist to bring value to their stakeholders, including customers, shareholders (for public companies), employees, and their communities. Competitive advantage may arise from having advantaged technology over competitors, superior or differentiated products, lower prices due to scale of manufacturing, operational excellence that results in lower operating costs, or access to lower cost raw materials. Chemists in industry need to understand the value proposition for the projects they are working on and how the project will impact the bottom line for the company [2-6]. Not all research projects are successfully commercialized and R&D chemists need to understand the risks involved in reaching their final goal and be prepared to modify projects to ensure a strong return on investment. A basic understanding of financial principles, awareness of global markets, and appreciation for the entire process (from ideation to delivering a product to customers) is recommended. Industrial chemists should be aware of the importance of intellectual property and ways to protect ownership of innovations in products, processes, and applications. Awareness of global drivers and trends and how this impacts your business and market is essential for growth. Understanding and appreciating the differences in markets and applications across geographic regions may be critical for evaluating opportunities for your products [2]. As an example, since materials of construction for residential housing in the US are often different than those for houses in Europe, developing products for residential infrastructure may require a different approach in these geographies. Learn how to define and utilize work processes to drive standardization and efficiency when needed, and simplify and streamline when appropriate.

Chemistry students interested in a career in industry would be well served by a course or two in business or

1. First published as *Pure and Applied Chemistry*, vol. 91, no. 2, 2019, pp. 327-330; https://doi.org/10.1515/pac-2018-0718, part of the special issue titled 'Distinguished Women in Chemistry and Chemical Engineering'

economics during their undergraduate years. Earning a MBA degree (Masters in Business Administration) is one way to expand business acumen and is sometimes recommended for advancement in industry, especially along the commercial or managerial career paths [7]. You may find this more useful for roles that require understanding market trends, business development, strategic portfolio management, finance, or innovation management. There may be specific roles within a corporation that require both formal business and technical education credentials. There are a variety of options available, including executive, part-time and Open University programs. Some employers provide tuition support or flexible work schedules for employees that pursue a MBA as part of the development plant. For part-time students who are earning a degree while working, you may identify a thesis project that relates to your role or provides information relevant to your employer, and demonstrates the value of your new knowledge to the employer.

Another aspect of business acumen is being able to understand, appreciate, and communicate the value you, as an individual, contribute to the company and how your contributions impact the strategies and goals of your organization. You will be accountable for setting and achieving goals and articulating how your accomplishments impact the bottom line. You may need to consider the short-term and long-term consequences of decisions and the broader impact they may have. Even if you don't pursue any formal education, take the time to learn as much as you can about the businesses you support, the markets, and how your work/function contributes and interacts with other functions within your organization.

Technical knowledge and skills

Most chemists will expect that their technical expertise is key to success in industry. In addition to technical and general knowledge learned as an undergraduate and the focused knowledge developed doing research, we also learned how to practice the scientific method: how to formulate hypotheses, investigate relevant literature, design and conduct experiments, evaluate results, draw conclusions, document our work, and develop recommendations for the future. These skills are highly transferable to any business project or situation. The research we performed in graduate school may or may not be relevant to our industrial responsibilities initially. Over time, chemists must either continue to develop deeper knowledge in a particular subject matter or broaden their knowledge to become a generalist, perhaps with an emphasis in a particular area. However, success either way depends on the chemist's ability to continue to learn throughout their careers, keeping up with technological advances and leveraging developments in other areas so that their skill sets continue to be relevant ten, twenty, thirty, or perhaps forty years after graduation [5, 6, 8]. Your industrial role may require that you keep up with literature across diverse areas, participate in conferences both focused on your sub-discipline and broad in nature, and perhaps take short-courses or continuing education courses. Learning concepts and principles from other disciplines, such as engineering, statistics, or information technology may be beneficial [2]. Enhance your ability to move up the knowledge pyramid by having the right data, converting that to information, developing knowledge from that, and finally creating wisdom. Knowledge management and transfer are also important skills since they ensure that the expertise and knowledge of one individual can be communicated, leveraged, and sustained across an organization. That's required for successful commercialization of a product, global implementation of a technology, or for training your successor so you can move to new challenges or roles.

Industrial chemists will need than just technical skills. Collaboration, communication, networking, mentoring and working with people from around the globe are all important as well.

Interprofessional skills

These skills, also called interpersonal skills, are probably the most important and highly prized skills in industry [1, 13]. They are a critical part of determining your career trajectory. Surveys of industrial employers have reported that over 90% value "soft skills" over technical skills when making hiring decisions [6, 10]. It is less common for academic programs to include specific training or development opportunities within their curriculum. Many industrial employers provide their own in-house training or hire consultants. Teamwork, the ability to work collaboratively with a group with diverse expertise, experience, and backgrounds in a way that enhances the outcome is a very important skill in industry [10, 11]. Some university programs may include projects that involve a team of people contributing to a combined outcome, but the work is often done individually and the pieces combined at the end. That may be the first step in learning teamwork, but the ability to synergistically work together, developing ideas, approaches, and solutions beyond what an individual can do, is much more valued. This requires that the team members, who may have very diverse educations and experiences, be able to communicate and collaborate across functions and disciplines.

As the chemical enterprise has become global, the ability to work across geographies has become another required skill. Understanding the cultural differences and strengths, and the ability to communicate effectively regardless of language, time zone, or other barriers is a necessity. There are multiple ways to gain cultural awareness, including books, workshops, and international work experiences [12, 13]. Opportunities to develop these skills are becoming available in graduate and undergraduate research programs [2].

The value of strong communication skills, written and verbal, cannot be overemphasized [6, 9]. This includes understanding your audience, how they want to be communicated with, what they want to hear, and the frequency they expect. Consider the purpose and desired outcome of your message since you may structure your presentation differently if you want to share information or influence a decision [11]. Realize that your audience may have a different background and will filter your communications through their own experiences; they may not have any technical training. You will need to assess if the audience is internal to the company or external stakeholders, including customers, suppliers, or regulatory agencies. Recognize the amount of detail that you should provide with each communication; an executive summary followed by a more thorough explanation may be better received by some audiences. The reality is that a poor presentation may mask the excellence of the work described [5].

Two skills that have been important for decades, and continue to be important, are networking [14] and mentoring [15]. Since most successful industrial projects require collaboration across multiple functions, developing a broad network is vital. Employees with strong networks may be considered as "hubs" since they can connect problems and challenges with solution providers within their company. They may develop

a reputation as the go-to person and be drawn into a wide range of projects. Mentors are trusted advisors outside of your leadership chain. They may serve as a listening board, ask probing questions to help you better assess a decision, or provide career guidance. You may want to have a few methods for different aspects of your career. An inner circle of trusted colleagues is extremely important. They listen when you are having problems, provide authentic feedback, help you recognize hard truths, and celebrate your accomplishments.

Most industrial chemists begin as individual contributors. However, after a few years, you may have the opportunity to take on a leadership role, either as a technical leader or organizational (people) leader. As an organizational leader, you'll still be involved with technology but not as a hands-on practitioner. That role will likely include some managerial aspects. However, true leadership is focused on people, not things. You'll need to define a clear vision, develop a strategy to achieve it, and communicate the vision and strategy [8]. Emotional intelligence may be more important than IQ or technical expertise in these roles [16].

The sweet spot

Be sure to take the time to develop financial acumen, technical skills, and interprofessional skills and invest in your own professional growth. While your employer may provide courses or support, it's your career and you should own your development. A job that you are very good at and provides value to the company, but you don't enjoy easily becomes a chore. If you enjoy the work and do it well, but it is not valued by the company, then you really have a hobby. The best advice I've received is to aim for that sweet spot: a job that makes the most of your strengths and skills, provides value to the company, and is a job you really enjoy.

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Carolyn Ribes <cribes@dow.com> is the Business Analytical Leader for Industrial Intermediates and Infrastructure at Dow Chemical. She earned her B.S. in Chemistry at the University at Buffalo, SUNY, and a Ph.D. in Chemistry at the State University of New York at Buffalo in 1989. She joined the Dow Analytical Sciences R&D group in Plaquemine, Louisiana where she developed and implemented on-line analyzers for process control and monitoring. In 1997 she relocated to Freeport, Texas, as part of dual-career move within Dow, and expanded her responsibilities in process analysis to global projects. In 2006, Carolyn moved to Terneuzen, the Netherlands, as the process analytical technology leader for Europe. In 2009, she became a Business Analytical Leader; in this role she defines and implements the business manufacturing analytical strategy to support quality control and manufacturing operations. Carolyn is active in WIN, Dow's Women's Innovation Network. She was a member of the IUPAC Committee on Chemistry and Industry (COCI) from 2008-2019 and Chair of COCI in 2018-2019, and a member of the US National Committee to IUPAC 2005-2011. She served as Co-Chair of the IUPAC Distinguished Women in Chemistry and Chemical Engineering Award Committee from 2012-2019. Carolyn has been a volunteer leader in the American Chemical Society, serving local sections, the Analytical Division, and several national committees and task forces. She was recently elected to the ACS Board of Directors. She is a Fellow of the American Chemical Society (2014), received the 2019 Award for Volunteer Service to the American Chemical Society, and was named one of the 2011 Distinguished Women in Chemistry and Chemical Engineering by IUPAC.

Diversity in Science at the Global Women's Breakfast Network

by Mary J. Garson, Laura L. McConnell, and Lynn M. Soby

In a year marked by unprecedented challenges, IUPAC hosted the largest ever Global Women's Breakfast (GWB2021) on 9 February 2021, bringing together more than 20,000 people around the world to celebrate the achievements of women scientists, to strengthen and expand professional networks, to inspire the next generations, and to challenge the status quo with respect to equality for women scientists in the workplace.

Building upon the success of earlier GWB events, men and women from more than 300 events in 70 countries joined together around a theme of *Empowering Diversity in Science*. A large majority of breakfast events were held virtually due to the COVID-19 pandemic, but organizers took advantage of virtual platforms like Facebook Live and Zoom to collaborate with other groups, to expand their audience, and to exhibit flexibility in event scheduling to meet the needs of their communities.

GWB2021 was launched in New Zealand, with University of Waikato in Waikato and the Manawatu Branch of the New Zealand Institute of Chemistry (NZIC) in Palmerston North sharing the honour of first breakfast. As each breakfast event began, the map pins turned from white hearts to red, moving as a wave from east to west. The final breakfast occurred about 33 hours later with an evening event hosted by the Alaska Chapter of the American Chemical Society.

The most easterly and most southerly events were also in New Zealand in Palmerston and Dunedin (NZIC Otago), respectively. The northernmost breakfast was held in Tromso (Norway) hosted by the Nordic Consortium for CO_2 Conversion, and the westernmost breakfast was hosted by Bayer Crop Science on the Hawaiian island of O'ahu.

The IUPAC GWB website (iupac.org/gwb) served as a networking hub for event organizers to connect with each other and for attendees to discover events happening in their region. GWB promotional materials were provided to organizers to make marketing their events easier. A welcome video was created and shared via the website along with a PowerPoint slide deck about IUPAC. The welcome video included short clips created by organizers around the world (https://youtu.be/StbLcIpTyUM). IUPAC used social media platforms: Twitter, Facebook, LinkedIn, Instagram with the hashtag #GWB2021 to promote the event. A Flickr group (https://www.flickr.com/groups/iupacgwb2021) was set up as an archive for photos and videos from the 2021 event. Breakfast organizers and attendees were invited to upload their photos and videos from both before and during the event.

Participation in GWB has increased over the last three years from 203 events in 2019, 244 in 2020, and 324 this year. The countries of Algeria, Benin, Cambodia, Cyprus, Ecuador, Finland, Iraq, Israel, Kazakhstan, Kenya, Jamaica, Norway, Sri Lanka, Zambia, and Zimbabwe joined for the first time. Countries with the greatest number of events were Australia (15), Canada (14), India (61), Mexico (40),

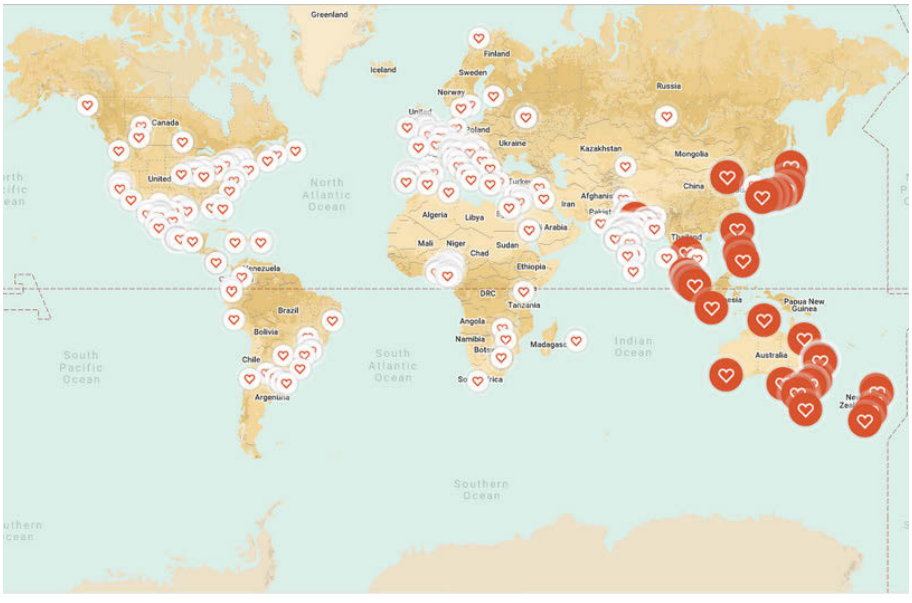

Figure 1- The GWB2021 Global Breakfast Map as events began in Asia.

Figure 2- Collage of photos from the GWB2021 welcome video

Nigeria (21), United Kingdom (10) and United States (30). Notable was the increased number of events in Mexico and India over previous years.

Universities made up approximate 70% of host organizations, Chemical Societies hosted 15% of events, Industry hosted 12% of events. Bayer Crop Science organized 17 events in 7 countries, and Dow Chemical organized 15 events in 12 countries. Government research institutes and high schools organized a number of events.

GWB2021 benefited from the creation of an IUPAC project #2020-010-2-020 entitled "Creation of IUPAC Global Women's Breakfast Series and a Global Network in Support of Eliminating the Gender Gap in the Chemical Sciences" with a large multi-national task group of country champions to help publicize GWB, to recruit new organizers, and to provide feedback and suggested improvements. A small number of organizers acknowledged that they had not known much about IUPAC prior to becoming involved in the GWB task group, and through their participation, the aims and objectives of IUPAC, and its global role, were shared to a new audience.

What has been the impact of GWB?

Importantly, 62% of respondents indicated that hosting an event resulted in increased attention to diversity issues in their organization (Table 1). Many reported new connections with groups internal or external to their organization. Indeed, the virtual format adopted for the 2021 event favoured an increased emphasis on remote in-country or regional interactions. Respondents also commented favourably on the event providing leadership development opportunities within their organization. The opportunity to raise awareness of gender gap issues in an informal setting was welcomed and was highlighted as an important topic of conversation for future events.

What activities were organized at GWB events?

Each GWB event was independently organized to meet the needs of the local organization. Some were quite simple gatherings of five or ten scientists over a cup of coffee. Others were more formal events with hundreds of attendees including scientific presentations or panels of distinguished scientists. Some events included attendees from a single organization. Others collaborated with breakfast events in their region or in other countries. Some took the opportunity to connect with companies in their regions or invited high school students to attend. Many GWB events have made a special effort to welcome male participants, both as attendees and as speakers, and it is a welcome objective fully in line with the values of IUPAC, and the UN SDG, to increase the diversity of attendees at future GWB events.

Organizers used fun activities like Periodic Table Bingo and chemistry-themed trivia, some awarded prizes and certificates. The group in Instituto Superior de Engenharia do Porto had fun making a wonderful short video that captures the humor of using Zoom for social events (https://www.youtube.com/watch?v=rHUPN2ejxec).

Each event across the world was unique, but a cross-section of events from different regions are highlighted as examples.

Benin: The first ever GWB event in Benin was held at the government's flagship Sèmè City hub which aims to create a world-class knowledge and innovation center in Africa. Ten attendees from academic

institutions and the drug company Pharmaquick shared a self-introduction session and then brainstormed on "Empowering diversity in science." Participants provided key words or sentences that were converted into a Word Cloud (Figure 3).

Japan: The Gender Equality Committee of the Chemical Society of Japan and the Society of Chemical Engineers, Japan arranged a set of six online lunchtime meetings at major cities throughout the country. The various groups used breakout rooms to brainstorm how to expand the research network across genders.

A separate event at Kyoto University brought together academics, professional staff, and students from several nations, including Canada, Egypt, Iran, Mongolia, India, China, Italy, France, Thailand, and the USA, and from bio-related fields including biopolymers, bioimaging, chemical biology, and biosensors. Participants were encouraged to discuss work-life balance in a breakout session. The legacy of this event was the promotion of new bonds between young and more established women in chemistry.

Mexico: In Mexico, 40 virtual events of the Global Women's Breakfast were registered, of which 21 were held in the state of Chihuahua where 689 people participated (352 university level and 337 of secondary and high school level). Event organizers reached out to participants in remote areas of Mexico. Invited panellists shared, "What woman inspired you in science?" And, "What do you propose to promote diversity in science? How can we inspire women, men, boys, and girls, to increase their interest in science?"

India: There were attendance numbers in the hundreds at many of the 61 events held in India. Outreach to the Chemistry Teachers of India at their Annual Meeting was highly effective at generating interest prior to GWB. For example, at a virtual webinar jointly arranged with the Shri Vaishnav Vidyapeeth Vishwavidyalaya Indore, over 100 participants from all over India watched presentations on the role of gender diversity in innovation and scientific discovery. Eminent space scientist and alumna Seetha Soma Sundaram gave a presentation to 250 attendees at Hindu College in Delhi, followed by a poster competition. Many breakfast events welcomed significant interactions with overseas participants. An audience of 300 participants at Maghav Science PG College heard presentations delivered by speakers based in Australia and the Philippines. Small group meetings were equally successful. Over 40 students from Primus Public School (which first participated in 2019) held a joint session of talks and a quiz with MS Ramaiah University. A student in Hyderabad organized singing games and a periodic table quiz for 14 participants, while a group of 7 at the Sage Institute, Indore, held a discussion over their breakfast.

Nigeria: In 2021, a total of 21 breakfasts were held at locations throughout Nigeria. For example, at an event hosted by the Chemical Society of Nigeria (CSN) at Atiba University, Oyo, there were over 80 women and men participants including academics and students. Presentations by both men and women speakers covered mentor-mentee relationships, achieving work-life balance, and gender equality in the workplace. A group of ~20 at the University of Nsukka listened to a presentation on COVID-19. Other breakfasts arranged by CSN chapters included presentations on women, career development and healthy lifestyles, and included presentations by women chemists working in industry. A number of venues made plans to continue local women chemist's networks.

Philippines: The University of San Agustin, Iloilo City in the Western Visayas region, has joined in three Global Breakfasts meetings, using the events as an opportunity to build overseas connections. The 2021 breakfast was co-hosted by the regional chapter of the Philippine Association of Chemistry Teachers (PACT)

"How has the IUPAC Global Women's Breakfast event influenced women scientists in your organization?"

Answer Choices	Positive Responses
Increased attention to diversity issues	62%
New connections between groups	56%
New connections outside my organization	48%
Leadership development opportunities for women	44%
Open discussions on need for more diversity	55%
New groups formed in support of diversity in science	27%

Organizer survey response to the above question.

with 48 participants. There were talks from diverse fields of science, including "Pandemic Response from the Bottom-Up", and "Aquaculture for You and Me" (highlighting gender equality in the field of fisheries and aquaculture). A final presentation on "Transdisciplinary Research from the Perspective of a Young Chemist" was given by a representative from Universiti Teknologi MARA (Malaysia).

United Kingdom: The UK nationally coordinated 10 events in 2021. A virtual breakfast event was arranged by the Royal Society of Chemistry involving international as well as UK-based registrants. After a welcome from Acting CEO Helen Pain and from Mary Garson in Australia, participants undertook "Meet and Greet" networking in breakout rooms. This was followed by short presentations from Dr. Marina Resmini (University of London) and Dr. Laura Knowles (Dow Chemicals) describing gender parity initiatives. Samantha Peralta (WomChemSheffield) then hosted a short quiz on women in chemistry, and the event was summarized by Dr. Ale Palermo from RSC.

Figure 3. Word Cloud results from brainstorming "How to Empower Diversity in Science"; image provided by Dr. Essé Agossou (Benin).

What next for the Global women's Breakfast Series?

The next GWB will be held on **16 February 2022**, with Empowering Diversity in Science continuing as the overall theme. We invite organizers to begin planning now for next year's event. It is never too early to begin reaching out and networking with other universities and industry organizations in your country or region or even on the other side of the globe.

The GWB project team is seeking to increase interaction with umbrella organizations such as the Federation of Asian Chemical Societies and the Federation of African Chemical Societies with the aim of extending the network further in developing country networks, and to grow regional cooperation on diversity issues.

We look forward to strengthening the bonds that have been formed within the GWB network, and we look forward to progress on closing the gender gap in science.

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The task group organizers for 2021 were Ghada Bassioni (Egypt), Karla Susana Bernal (Mexico), Vanderlan Bolzani (Brazil), Cristina Delerue-Matos (Portugal), Fun Man Fung (Singapore), Hooi Ling Lee (Malaysia), Fatima Mustafa (USA), Mei-Hung Chiu (China-Taipei), Lori Ferrins (USA), Hemda Garelick (UK), Sandra Gonzalez Gallardo (Wiley VCH, Germany), Carla E. Giacomelli (Argentina), Rachel Hevey (Switzerland), Cynthia Ibeto (Nigeria), Francesca Kerton (Canada), Mary Kirchhoff (American Chemical Society, USA), Ekaterina Lokteva (Russia), Sadhna Mathura (South Africa), Alessandra Mosca (Dow Chemicals, Italy) Bailey Mourant (USA), Lars R. Öhrström (Sweden), Bipul Behari Saha (India), Fani Sakellariadou (Greece), Hina Siddiqui (Pakistan), Mallika Pathak (India), and Supawan Tantayanon (Thailand).

Mary Garson is an Emeritus Professor of Chemistry at The University of Queensland. She is an elected Member of the Bureau of IUPAC, and a co-leader of the Global Women's Breakfast Network. Laura McConnell is a Bayer Science Fellow at Bayer Crop Science, an Emeritus member of Division VI, and a co-leader of the Global Women's Breakfast Network. Lynn Soby is Executive Director of IUPAC.

FAIR and Open Data in Science: The Opportunity for IUPAC

by Ian Bruno, Simon Coles, Wolfram Koch, Leah McEwen, Fabienne Meyers, and Shelley Stall

At the start of 2020, IUPAC's Committee on Publications and Cheminformatics Data Standards (CPCDS) formed a Task Force to propose guidelines for the dissemination and sharing of machine-readable chemical data. These guidelines would be for IUPAC to adopt internally and recommend to the wider chemistry community.

The FAIR Data Principles were to be central to these guidelines with the aim to ensure that scientific data management and stewardship will make chemical research data findable, accessible, interoperable, and reusable by **both** humans and machines [1].

In a digital context, FAIR means describing data outputs such that they are *machine-actionable*, for example in applications such as modelling and machine learning. Data outputs are **findable** through unique and persistent identifiers that are associated with basic machine-actionable metadata to distinguish different outputs. Data outputs are **accessible** through systems that employ universal Internet protocols and allow for authentication to access sensitive content. Data outputs are **interoperable** through formats that incorporate authoritative and referrable domain vocabularies that are syntactically and semantically parsable. Data are **resuable** through rich metadata that enable linking and compiling, provenance trails that establish authority and open licenses [2].

The membership of the task force includes high level experts supporting chemistry research endeavours and those with leadership positions in scientific organisations active in FAIR initiatives. A key focus was on IUPAC's own data outputs and the opportunity there is for these to be managed in a FAIR manner so they become more readily available for consumption by digital technologies and provide an exemplar in best practice for the wider community.

Whilst the FAIR Principles are central to many discussions pertaining to policy and practices surrounding research data, the extent to which they penetrate the horizons of most chemists in industry and academia may be limited. One of the first questions the Task Force thus contemplated was why the FAIR Principles might matter to chemists and to IUPAC. To answer this, we turned to a range of broader principles, provocations, and reports that help frame the practical utility of the FAIR Principles, and to initiatives that demonstrate their practical application in other disciplines. The following section highlights some of the landmarks identified as we undertook our tour of the landscape surrounding the FAIR Principles.

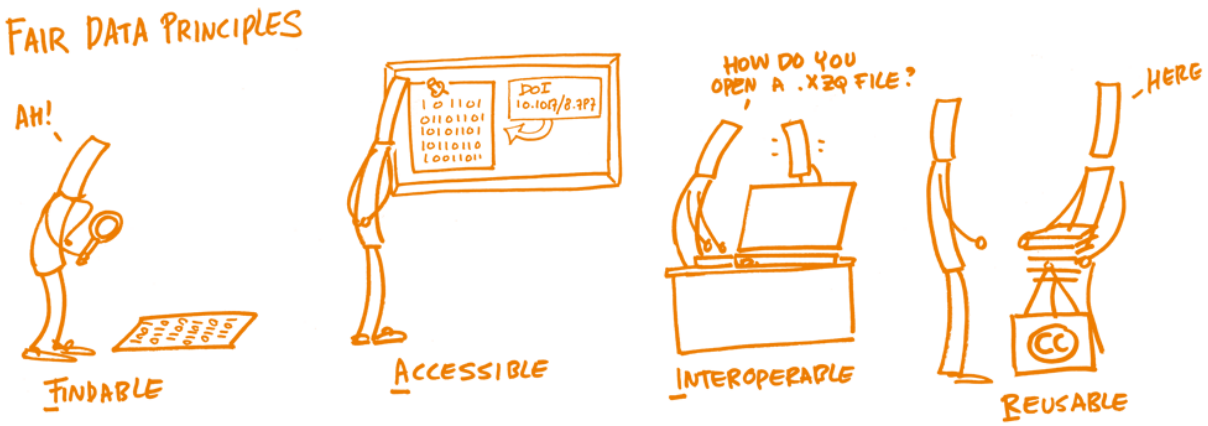
Taking in the Scenery

We began our review with "Science as an Open Enterprise,", a report published by the Royal Society in 2012 which highlights the enormous potential modern digital technologies have for exploring massive amounts of data to address matters of public policy and business [3]. The report identifies six key areas for action that are very much focussed on data. These include publishing data in reusable form, cultivating experts in the management of digital data, and establishing common standards for sharing information—an area of activity very much aligned with IUPAC's core mission.

A parallel report on "Open Science By Design," published by the U.S. National Academies in 2018, specifically calls out the sharing and preservation of research results under FAIR principles whilst highlighting the need to prepare data and tools to support reproducibility, replicability, and reuse [4]. The importance of the availability of well-managed research data to support reproducibility and replicability in science, and the role that the FAIR Principles have in enabling this, is further emphasised in other National Academies reports specifically focused on this area [5,6].

A policy driver for adoption of the FAIR Principles comes from research funders across regions and domains [7-11]. Their policies recognise research data as a public good and increasingly expect data management plans that reflect elements of the FAIR Principles to ensure data are adequately identified, described, licensed and attributed. Publication policies are also key and a recent International Science Council report articulating principles for publishing in the digital era offers a comprehensive argument for open publication of data in support of claims in articles [12]. It further notes that datasets need to "intelligently open" through procedures formalised by the FAIR Principles.

The economic case for supporting the FAIR Principles is laid out in a report published by the European Commission which estimates the cost to the EU member states of not having FAIR research data to be a minimum of € 10.2 billion per year with a significant portion of this (around 96 %) being due to duplication of effort and storage [13].



(Reproduced from https://book.fosteropenscience.eu/en/02OpenScienceBasics/02OpenResearchDataAndMaterials.html)

Whilst the FAIR Principles have their roots in academic communities, they have also been adopted within the life sciences industry to help shape strategies that support digital transformation and accelerate the application of AI and deep learning to industry data [14]. The opportunity to apply FAIR principles to chemical data within industry to enable interoperability outside of localised silos has further been highlighted [15]. The principles espoused by FAIR become critical when we envisage future laboratories where experimental data are automatically captured and analysed, conceivably in real time, to generate actionable insights that inform subsequent experimental choices [16-18].

The FAIR Principles are central to various European infrastructure activities supporting research in chemistry and beyond. NFDI4Chem for example is a German initiative that aims to build an open and FAIR infrastructure for research data management in Chemistry [19]. More broadly, the EU-sponsored FAIRsFAIR project is producing a range of recommendations in support of FAIR data policies, practices and services [20]. The output of FAIRsFAIR will contribute to the rules of participation in and governance of the European Open Science Cloud, a virtual environment being developed with funding from the European Commission to underpin data-driven science in Europe [21].

Internationally, the FAIR Data Principles are found at the heart of the CODATA Beijing Declaration, a statement of core principles to encourage global cooperation around research data [22]. They also feature in the recently published UNESCO draft Recommendation on Open Science [23] which, in common with the Beijing Declaration, has at its heart the UN Sustainable Development Goals [24] and the reliable and efficient exchange of information and data needed to address the complex and interconnected global challenges facing the world today.

Successful implementation of the FAIR Principles requires input from stakeholders and service providers across and around the research life cycle. A Commitment Statement adopted by the Coalition for Publishing Data in the Earth and Space Sciences outlines commitments for researchers, funding agencies, publishers, repositories and institutions in support of open and FAIR data [25, 26]. The Royal Society report [3] extends a similar list to include business investors in research, government and regulators. Both highlight a role for societies, academies, and other professional bodies, such as scientific unions, that includes:

- Exploring how enhanced data management could benefit their constituency and how habits, credit and recognition might need to change to achieve this;
- Supporting the promulgation and development of FAIR data principles and educating their communities about these;
- Participating in the development of community standards, infrastructure, tools, and services to enable open and FAIR data practices.

These and other key themes that emerged align well with IUPAC's mission to develop tools that enable the application and communication of chemical knowledge, including:

- The relevance of FAIR for enabling robust reproducibility;
- The importance of establishing trust in research data across sectors;
- The need for infrastructure that enables the long term stewardship of research data;
- Opportunities FAIR offers to underpin improvements in the publication of research data;
- The opportunity for collaboration around FAIR across academia and industry.

Cover of the recently published UNESCO draft Recommendation on Open Science [23] which, in common with the Beijing Declaration, has the FAIR Data Principles at the heart, along with the UN Sustainable Development Goals.

IUPAC Opportunities

IUPAC's more than a century of work on projects and initiatives to define a common language for chemistry position it well to embrace FAIR and other related principles that facilitate exchange of scientific information. Implementing FAIR is an opportunity for the wider community to benefit from prior work undertaken over many years to develop digital representation formats such as JCAMP-DX [27] chemical structure identifiers such as InChI [28] and IUPAC terminologies published in *Pure and Applied Chemistry* and various colour books aggregated in digital form as the GOLD Book [29]. It is also an opportunity to identify requirements for new standards and to develop metadata profiles that provide machine-readable descriptions of standard atomic weights [30], spectroscopic data [31], and critically evaluated solubility data [32]. Incorporating FAIR practices into these efforts will enable IUPAC standards to be more readily reusable and interoperable across domains.

A key factor for the success of FAIR is engaging with communities of researchers to identify and raise awareness of solutions that can enable the FAIR publication of their data. The Chemistry Implementation Network (ChIN) of the GO FAIR initiative aims to move forward the practical implementation of FAIR within the broader chemistry community through such engagement [33]. This will firstly involve facilitating and advocating the development of FAIR standards, materials and software specific to our discipline. Having developed a critical mass of tools and approaches, the second aim of the ChIN is to use these to help drive a culture change across the discipline so that the goal of FAIR chemistry data can be achieved. Set within the landscape of a range of GO FAIR Implementation Networks covering many disciplines, the ChIN is also well placed to reach beyond the chemistry community and support the use of chemical information in other disciplines. Critical to these activities are domain-based standards and IUPAC has demonstrated support through endorsement of the Chemistry GO FAIR Implementation Network Manifesto [34].

Engagement across stakeholder groups is also key and this was a prominent feature of a 2018 NSF-sponsored workshop organised with input from CPCDS members to establish publishing guidelines for chemical structures and spectra [35]. This brought together researchers, publishers, data organisations, software developers, librarians, and standards bodies and led to practical initiatives to encourage the FAIR publication of machine-readable representations of spectra alongside journal articles [36].

FAIR provides a focal point for bringing together communities from across disciplines to explore various aspects of the management and publication of chemistry research data. As part of International Data Week in 2018, IUPAC joined forces with the International Union of Crystallography (IUCr) to organise a symposium that specifically looked at the challenges of interoperability across disciplines including chemistry, biology, crystallography, and the earth sciences [37]. The opportunities for growing the FAIR community at the intersection of the Geosciences and Pure and Applied Chemistry have further been explored [38]. Currently, IUPAC is engaging in the delivery of a Data Sharing Seminar Series for Societies in collaboration with the American Geophysical Union and other societies [39]. This aims to help communities understand

more about how they can help enable publication of data in line with guidelines such as FAIR.

Challenges Ahead

Over the years, IUPAC has been responsible for generating data assets that are highly valuable to the scientific community. In a digital age, the value of these assets potentially grows but so does the question of how prepared IUPAC's processes and infrastructure are to fully realise this value for its mission and role. The importance of ensuring that IUPAC is producing standards that become embedded in the core digital infrastructures used in research across the chemical sciences has been previously articulated as part of a vision for a Digital IUPAC [40]. Embracing and adopting FAIR Principles will help accelerate progress towards this essential vision.

A challenge for IUPAC currently is where to host its outputs in machine-accessible form such that they are readily discoverable now and into the future. Any data repository option would need to be one that IUPAC could envisage sustaining for a number of years, including considerations of infrastructure, storage, and resources to oversee ongoing curation. It would also need to enable access to chemical objects that are born digital and machine-actionable. Such requirements are unlikely to be provided by traditional publishing platforms or partnerships. A related challenge is identifying licensing terms that can support broad reuse of outputs whilst also ensuring that integrity is preserved and opportunities for IUPAC to develop revenue streams based on these assets are retained.

The processes adopted while defining, executing, and reporting data related to outputs of projects will also impact the FAIR availability and reuse of IUPAC's assets. Many of IUPAC's outputs to date are published in forms that did not anticipate the digital expectations of today and effort will be required to transform these so they become actionable by machines. We can avoid creating the same challenge for future assets by establishing plans for disseminating outputs digitally early in a project and evolving these throughout. CPCDS are currently in the process of developing guidance that can be applied by IUPAC to ensure that its future outputs are born FAIR-ready and prepared for a digital existence that persists beyond the lifetime of a project.

Central to realising FAIR Chemical Data in IUPAC is the bringing together of "standards" and "community"—two words that strike to the very core of IUPAC's essence. Indeed, bridging these is something that IUPAC is uniquely placed to do. It has the standards and it has an authoritative voice—now is the time to combine these to advance the adoption of FAIR data principles across the global chemistry community. Doing so will unlock the opportunity of a step change in the provision and supply of quality-assured scientific data that can be used to further enable the application of the chemical sciences in tackling critical global issues facing the future of our societies and our planet.

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IUPAC Focus on Digital Health

by Helle Møller Johannessen and Ulla Magdal Petersen

The G-Science Academies of Science and of Medicine published a statement in 2020 titled "Digital Health and the Learning Health System." The statement is interesting and relevant to the work of the Div. VII Chemistry and Human Health, and especially to the Subcommittee on Nomenclature for Properties and Units (SC-NPU).

The G-Science Academies

The G-Science Academies of Science and of Medicine is a group of national science academies, regularly issuing statements to address some of the world's greatest challenges through the use of science and technology. In 2020, leaders of the national science academies of Brazil, Canada, China, France, Germany, Global Young Academy, India, Indonesia, Italy, Japan, Nigeria, South Korea, the United Kingdom, and the United States signed a statement on "Digital Health and the Learning Health System" (found at https://www.nationalacademies.org/our-work/joint-science-academies-statements-on-global-issues) that seems especially relevant to the work done in IUPAC. The scope of the document is impressive, describing the many aspects and needs of future Digital Health technology. The statement stresses the need for extensive individual, organizational, national and international collaboration. Some of these aspects have been a concern of IUPAC for decades, especially via IUPAC Division VII, Chemistry and Human Health, and the Division welcomes cooperation with G-Science Academies on these aspects.

Future development of digital technologies

The development of digital technology is not only ongoing, it is accelerating. There is a need to address uses and risks of digital applications and infrastructure we cannot really imagine today. We (the authors) have for decades been active in various parts of the digitalizing of Danish health care, and while its state today is far beyond what we imagined possible at the start, even the latest and best of health care applications and infrastructure have demonstrated risks and flaws not imagined by the designers. Health care data are very personal, but they are also very valuable in many fields both inside and outside the health care sector. With Health care data being communicated both nationwide and worldwide, it is certain that unplanned access to, recombination of and use of data, and automatic decision making on basis

Infrastructure requirements for progress in digital health. Source: The G-Science Academies of Science and of Medicine published a statement "Digital Health and the Learning Health System" in 2020

of these data, both in and outside the health care field, will happen. There is a need to evolve not only international technology standards, allowing us to improve the functionality of our tools. We also need ethical and legal standards, economic and political tools, and international agreements for the use of our information. This calls for international participation. But more important, we need to think outside the traditional risk management concepts, because despite all technical improvement over decades, health data can still be lost, inaccessible, misunderstood, misused and stolen.

The G-Science statement recognizes this in the section ***Data reliability, storage and access:***

> Structure and maintenance guidelines as well as international cooperation is essential. Equally important are protocols for data storage, access, control, sharing, and use. In principle, authority over individual data lies with the individual from whom they derive, and access to and control of use belongs to the individual or their designee. Every step in the use of information, however, generally requires an element of ceding control, as well as the potential for value to be added. Economic, legal, philosophical and practical issues must be addressed. The differences that exist among nations concerning data access, control, and monetization clearly present limiting circumstances for the contributions of digital health. Thus, mechanisms for ongoing cooperative exchange are needed.

Relevance to IUPAC Division VII Chemistry and Human Health

The G-Science statement analyzes and describes the present and future benefits of evolving digital applications and infrastructure, and lists key priorities for future development:

- Cybersecurity, safety, and privacy
- Interoperability
- Availability of reliable data and information
- Secure virtual data repositories
- Integrative analytics and predictive modelling
- Mathematics of learning
- Knowledge representation & management
- IT literacy, public understanding, and ethics

These priorities are all extremely relevant, and especially interesting for IUPAC Division VII is the third item:

> Availability of reliable data & information: standards and curation protocols for data and information, including tools to track provenance, and improvements in the amounts and quality of open data.

The work in IUPAC Division VII is concerned with subjects of medicinal chemistry and drug discovery, toxicology, explanatory dictionaries, terminology and nomenclature of properties in clinical laboratory science, and advances in immunochemistry. These activities all are relevant in one way or the other to the aspects of *Availability of reliable data & information* for the purpose of supporting global standardization.

For more than 50 years IUPAC has cooperated with other International organizations, notably the International Union of Pure and Applied Physics (IUPAP), the International Organization for Standardization (ISO), the International Bureau of Weights and Measures (BIPM), and the International Federation of Clinical Chemistry and Laboratory Medicine (IFCC), to develop standards for metrology in general.

IUPAC Div. VII has been aiming at describing and communicating health relevant information, *e.g.*

- International agreement on and publication of descriptions and definitions of the communicated information, based on international scientific nomenclature and classifications, to help solve conflicts and misunderstandings due to differences in tradition and language
- Standards of metrology, especially measurement units, and structured and coded reporting of medical data, to make data safely available for clinical use in communication across time and geography, and to allow for reliable reuse of data for research and statistics.

Results of patient examinations make up the main part of communicated data in health care, and most of the data are concerned with the fields of medication, toxicology, human body chemistry and biochemistry. The nationwide or worldwide digital communication of such data supports individual welfare, research and many kinds of statistical use, but also introduces new risks. The data producers (clinician, clinical laboratory, pharmacology dept. ….) are increasingly unable to control where, in which context and for what purpose these data are used. Data are communicated between many different public and private users via systems using different standards, and are recombined and aggregated for many different purposes, both statistical, scientific, and commercial.

Concern for the safety and privacy of personal data has caused the European Union to issue a General Data Protection Regulation (GDPR) in 2018 (found at https://gdpr-info.eu/), and other nations have expressed similar concerns.

A committee supported by IUPAC and IFCC on 'Nomenclature for Properties and Units' has worked on the issue of definition and identification of personal medical data in a form that can be transmitted between systems and across geography and time, without corruption. The result is the 'NPU Terminology', a set of well-defined and coded 'patient properties' that may be measured or estimated, reported, communicated and reused for many different purposes without loss of meaning.

The NPU terminology

The NPU terminology is a medical terminology for identification of patient examination results, often based on sample material from the patient. These examinations are often called 'laboratory examinations', even if many of them today are performed locally, in direct contact to the patient, not in a separate laboratory. It covers many different medical fields:

- Clinical allergology
- Clinical chemistry
- Clinical immunology and blood banking
- Clinical microbiology
- Clinical pharmacology
- Molecular biology and genetics
- Reproduction and fertility
- Thrombosis and hemostasis
- Toxicology

The terminology is used in the clinical setting, delivering information about examination results for individual patients. It offers a safe way to communicate

and compare patient data between different systems and organizations, both locally and on national basis. In the Scandinavian countries (Denmark, Norway and Sweden) the NPU Terminology is managed by National Authorities, translated into the National languages, and used all through the Health Care systems for both ordering of, reporting on and reimbursement for examinations. Transmission of examination results is usually by direct digital communication from medical laboratory systems into local health care systems. The digital examination results are also stored in National Health Care portals, available to both doctors and patients, enabling comparison of results across both time and geography, and allowing for extracts of data for research.

Metrology standards

The source and definitions for general measurement concepts in the NPU terminology is the 'International vocabulary of metrology – Basic and general concepts and associated terms (VIM)' published by the Joint Committee for Guides in Metrology (JGCM). It ensures International agreement on the meaning of the concepts of the NPU terminology. The International System of Units (SI), commonly known as the metric system, is the international standard for measurement units.

General terminology standards of ISO and the European Committee for Standardization (CEN), and the IUPAC 'Colour books' on Nomenclature have been essential for developing definitions of the specific concepts involved in NPU definitions. In particular important in the field of health terminology and metrology is IUPACs Compendium of Terminology and Nomenclature of Properties in the Clinical Laboratory sciences (The 'Silver Book') [1]. It is produced with the support of both IUPAC and the IFCC (International Federation of Clinical Chemistry and Laboratory Medicine), and makes recommendations on logical standardized nomenclature, symbols, properties, and units in many disciplines of the clinical laboratory sciences. It has been a central source of terms and definitions for health care data.

Units are essential

Collecting, comparing, storing and reusing measurement results across time, geography and culture is not easy. Many different measurement units are in use in the world, and the units we use shape our general understanding of and relating to magnitudes. Expressing a well-known measured concept using an unfamiliar unit may make it difficult to estimate its meaning. (If you are used to describing body height in centimeters, a value expressed in feet may make it difficult to estimate if a person's height is above or below normal, and *vice versa*). The difficulty may be handled technically by converting units for presentation and use in in different settings, or socially by agreeing on using the same system of units everywhere.

The NPU terminology is committed to the International System of Units (SI), held by the BIPM.

Incidentally, while this is being written, the BIPM is preparing for the World Metrology Day on 20 May 2021, commemorating the anniversary of the signing of the Metre Convention in 1875. (worldmetrologyday.org/press_release.html). The theme for this year is Measurement for Health!

Not all patient examinations are measurements, some are observations graded on an ordinal scale, or may be nominal classifications (*e.g.* names of microorganisms identified). But where results are numerical values on a difference or ratio scale, with a measurement unit, the NPU terminology specify either a SI unit or a referenced WHO international unit (IU).

	Enhed	2020 05.08 08:43	05.08 00:00	22.07 07:57	15.07 08:48	13.07 08:41	10.07 08:44	08.07 08:37	06.07 08:57	02.07 07:33	29.06 08:23	24.06 08:30	10.06 08:28
Folat;P	nmol/L			9,5									
Hæmoglobin [MCHC];Erc(B)	mmol/L												
Hæmoglobin;B	mmol/L	7,2↓		5,9↓	7,4↓	6,5↓	6,6↓	8,6	8,9	7,1↓	7,9↓	7,1↓	8,4
Hæmoglobinindhold [MCH];Erc(...	fmol												
Jern;P	µmol/L			18									
Leukoblaster; antalk.;B	× 10^9/L												
Leukocytter;B	× 10^9/L	6,8		3,4↓	9,4 R↑	12,5↑	0,66↓	0,98↓	14,4↑	10,4↑	13,3↑	5,7	8,4
Lymfocytter;B	× 10^9/L	1,9		0,5↓		0,9↓	0,4↓	0,5↓	0,6↓	1,6	3,0	2,3	2,7
Metamyelo.+Myelo.+Promyeloc...	× 10^9/L												
Metamyelocytter;B	× 10^9/L				0,1								
Methæmoglobin;Hb(B)													
Monocytter;B	× 10^9/L	0,6		0,2		0,3	0,1↓	0,0↓	0,1↓	0,3	0,7	0,6	0,6
Myelocytter;B	× 10^9/L				0,35↑								
Neutrofilocytter (segmk.+stavk....	× 10^9/L												
Neutrofilocytter;B	× 10^9/L	3,9		2,5		11↑	0,1↓	0,4↓	14↑	8,5↑	9,5↑	2,5	4,7
Promyelocytter;B	× 10^9/L				0,08								
Store ufarvede celler;B	× 10^9/L	0,11		0,07		0,08	0,05	0,04	0,03	0,03	0,07	0,20↑	0,20↑
Trombocytter;B	× 10^9/L	138↓		123↓	59↓	53↓	31↓	43↓	100↓	139↓	172	183	118↓
Vitamin B12;P	pmol/L			1230									

Danish patient overview available on a national platform. By using the unique NPU code and its definition with the unit, the NPU data can be imported directly into the presentation forms. The 'up arrows' and the red colored numbers indicate that the examinations result is above the upper reference limit value. The 'down arrows' and the blue color indicate that the examinations result is below analysis' lower reference limit value. Links to reference intervals and to supplementing information on the investigated property is available as links. Note that the terms are nor the full NPU definitions, but local/national use names.

This makes results reasonably comparable, even though the uncertainty of measured values may differ. If more than one SI unit or international unit are in use for the same patient property, *e.g.* mmol/L and µmol/L, NPU uses different identifiers for results with each unit, to avoid misunderstanding.

The result values aim at representing the status of the measurand in the patient at the time of sample collection or direct measurement, not the state of the measurand in the test tube after collection, addition of anticoagulant, centrifugation, or other treatment during the analytical procedure (this is why there are no NPU definitions for blood serum samples—there is no serum in patients. When the blood sample left the patient, it contained blood plasma, and turning it into serum happened in the test tube).

Terminology standards

All NPU items consist of an identifier (NPUxxxxx) and a formal definition of the examined patient property.

The NPU item definitions are written with a vocabulary of internationally defined concepts and their terms, and references to international definitions of each concept are filed. The NPU definition has three or four parts, describing

- **The System**—the part of the universe examined. In the medical context usually the patient or a part of the patient, *e.g.* the blood or skin. Definition of the terms is usually from anatomy sources or other authoritative sources of medical concepts
- **The Component**—the part of the system that is investigated, *e.g.* the red blood cells in the blood, or the bacteria on his skin. Definitions are found in relevant international nomenclatures, taxonomies *etc.*
- **The Property** examined of the Component in the System, *e.g.* the number concentration of red blood cells in the blood, or the systematic names (taxa) of bacteria identified in the skin. The definitions of these concepts are found in the IUPAC Color Book series
- **A unit**—If relevant according to the SI system (*e.g.* 10^9/L for the number concentration of red blood cells), or an International Unit (IU) with reference to a specific WHO reference preparation.

An abbreviated form of the NPU definition is used as a name for the NPU item, and users may introduce local or National names in their presentation. The NPU identifier ensures that the complete formal definition can always be found.

Examples:

Full definitions

NPU01132	Plasma—Albumin; substance concentration = ? micromole per litre
NPU18868	Plasma—Immunoglobulin E; arbitrary substance concentration(WHO 68/341; procedure) = ? × 10^3 international units per litre
NPU14049	Secretion(Anus)—Parasite(egg);

	taxon(procedure) = ?
NPU60270	Urine—Mercury; mass concentration = ? microgram per litre

Abbreviated descriptions for general use

NPU01132	P—Albumin; subst.c. = ? µmol/L
NPU18868	P—Immunoglobulin E; arb.subst.c.(WHO 68/341; proc.) = ? × 10^3 IU/L
NPU14049	Secr(Anus)—Parasite(egg); taxon(proc.) = ?
NPU60270	U—Mercury; mass c. = ? µg/L

Terms that may be used in local/National context

NPU01132	Albumin;P
NPU18868	IgE; P
NPU14049	Parasite eggs; Anus
NPU60270	Mercury;U

Information about the analytical procedure is generally not part of the NPU definition. But the specification 'procedure' or 'proc.' added to the 'property' part of the definition indicates that results may not be comparable unless the analytical procedure used is the same.

Information about result uncertainty is considered a property of the result value, not of the NPU definition, and is never included in the definition.

With increasing use of the NPU terminology the need for extra information communicated with the examination results has also increased, *e.g.* on patient condition, sample collection process, methods, instruments, result uncertainty, applied cut-off values etc. It is not feasible to add these very different types of information into the NPU definitions on demand; the definitions would lose their consistency and comparability. But the need for the information is there, and an International standard model and nomenclature for transmitting this kind of supplemental data could be a safe way of handling the problem.

Cooperation with other organizations

IUPAC Div. VII has always cooperated actively with other organizations in the field of metrology and terminology in Health Care, and continues to do so. IUPAC is a project-based organization, and International projects are the main tool for future development. The NPU terminology continues to evolve and adapt as medical science develops, and the IFCC-IUPAC Subcommittee on Nomenclature, Properties and Units will welcome suggestions for projects in the field.

Cooperation in the field of *Availability of reliable data & information* could benefit the work of both the GSA and IUPAC.

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COMEST: Ethical Advice across Scientific and Geographic Borders

by Leiv K. Sydnes

COMEST, an acronym for the French name of the World Commission on the Ethics of Scientific Knowledge and Technology [1], is an advisory body within United Nations Educational, Scientific and Cultural Organization (UNESCO) and a forum of reflection, "mandated to formulate ethical principles that could provide decision-makers with criteria that extend beyond purely economic considerations." [2] Over the years, the Commission has addressed ethical issues in many areas where science and technology have an impact on people, nature, and society. The deliberations result in reports, which are put forward to the biannual General Conference of UNESCO for discussion and adoption. The outcome has often been ethical recommendations and guidelines to consider and hopefully abide to so that science can interact with society in a responsible way and without adverse consequences.

Formation

The United Nations Charter, signed 16 November 1945 [3], contained references to several specialized agencies, which, according to paragraph 57, were envisaged to deal with "economic, social, cultural, educational, health, and related fields" as would be decided by intergovernmental agreements. It is interesting to note that the original listing did not include science, but when the planning of the agencies started, not only science, but also the ethics of science were inserted and paved the way for the establishment of UNESCO.

Initially, the focus of the organization was mainly on rebuilding schools, libraries, and other cultural institutions that had been destroyed during World War II, but as the years passed, first education at various levels and then the impact of scientific and technological developments on society received increasing attention. An indication of the shift of focus to the latter was the publication of *Recommendation on the Status of Scientific Researchers* in 1974 [4], which outlined a framework for putting science into service of society in a fair way. In the following decades, tremendous progress in science and significant technological innovations transformed the world considerably and changed the way we live and how we work. Many changes were indeed beneficial, but other developments raised concerns about ethical aspects associated with "science and technology and the principles on which a knowledge society might be built."[5] As a result, UNESCO acknowledged the need to pay more attention to "possible adverse consequences of scientific development in general and certain scientific advances in particular. If left unattended, this concern could undermine popular support for, and trust in, the whole enterprise of modern science."[5] After thorough consultations, UNESCO decided to establish COMEST in 1997 with a mandate to advise on ethical principles and guidelines related to science and technology and the consequences of their applications in society (see Box) [6]. The commission was set up with 18 appointed members, with very different professional backgrounds and coming from all parts of the world, and 10 *ex-officio* members from major international scientific organizations.

United Nations Educational, Scientific and Cultural Organization · World Commission on the Ethics of Scientific Knowledge and Technology (COMEST)

The symbol/text used on all COMEST correspondence.

Code of Conduct

The first major assignment was to undertake studies, in collaboration with the International Council for Science (ICSU, now ISC), into the possibility of creating a code of conduct for scientists. The work led to a two-tier approach: Codes should be disciplinary and be worked out by disciplinary scientific organizations, whereas UNESCO should develop the ethical framework, on which the codes should be based. This solution had direct consequences for IUPAC, because

The COMEST tasks according to the commission's homepage. [6]

- To advise the Organization [UNESCO] on its programme concerning the ethics of scientific knowledge and technology;
- To be an intellectual forum for the exchange of ideas and experience;
- To detect on that basis the early signs of risk situations;
- To perform the role of advisor to decision-makers in this respect;
- To promote dialogue between scientific communities, decision-makers and the public at large;
- Finally. It aims at applying such standards into the scientific and policy communities, creating awareness of the ethical issues and building capacities to deal with them appropriately.

when the memorandum of understanding (MoU) between UNESCO and IUPAC was signed, the Union was challenged to develop a code of conduct for chemists. This inspired a group within IUPAC to take on the task, and they went at it with a will. A draft of a code was ready by 2008, and this document became the basis for CHEMRAWN XVIII Conference: Ethics, Science, and Development, which was held during the IUPAC World Chemistry Congress in Glasgow, UK, in 2009. However, the IUPAC leadership at that time was not in favour of a traditional code of conduct, so the working group modified the proposal and came up with a Living Code of Conduct for chemists. However, attempts to have the final version approved as a formal IUPAC recommendation failed, but the working group was allowed to publish the Living Code in an article in *Chemistry International* in 2011 [7].

Societal impact

When the two-tier solution had been adopted, COMEST broadened the scope and started to work on ethics in areas where many ethical issues emerged form the interplay between scientific disciplines and technologies on one hand and society on the other. The result of the work has always been published in well-referenced reports, which are available on the UNESCO homepage (unesco.org). Some of the themes addressed have been quite general and have had implications for science and technology at large; such topics include the clarification of the precautionary principle [8], the teaching of ethics [9], and Recommendation on Science and Scientific Researchers [10]. However, other topics have been more concrete and closer to the natural sciences; among the topics are the nanotechnologies and ethics [11], water ethics [12], the ethics of energy [13], and the ethics of land use, which is a study currently in its final stage. Particularly in the more concrete cases, discipline-specific issues frequently become quite relevant, and in this context, chemistry has a special position because chemicals are everywhere and impact the environment and the society in important ways. Elements of the IUPAC Living Code of Conduct can be recognized in many of the study reports, but the impact is amplified by the wider perspective and the synergy with ethical thinking from other disciplines.

During the last three to four years, COMEST has worked extensively with ethical aspects related to integration of digital technologies in society. By interconnecting electronic devices such as computers, sensors, and control systems, enabling technologies (Internet of Things; IoT [14]) are almost invading us and

Example of a report published by UNESCO on the basis of work done by COMEST. Copied from the UNESCO homepage (see ref. 10)

already surround us and make it possible to use artificial intelligence (AI) [15] to handle intricate situations and complex systems quickly and predictably "without human error." Such technologies have already started to transform the health-care landscape in many parts of the world and have the potential to do the same with all sorts of monitoring, including environmental monitoring, which often is based on automated chemical analyses. This development has raised the need to establish "international and national policies and regulatory frameworks to ensure that these emerging technologies benefit humanity as a whole." [16] Important parts of these policies are related to chemistry. There are two main reasons for that: many parts of the devices used in IoT and AI systems have a complex chemical composition, and many of the components applied contain elements that are available in limited quantities. The chemical complexity issue makes the recycling of IoT devices challenging, and such pieces of equipment already contribute significantly to the stream of E-waste. Although the recycling of such waste is steadily improving, its handling is a global problem, [17-19] which will be addressed at *CHEMRAWN XXII Conference E-waste in Africa* in Lagos, Nigeria, in

November this year [20]. The other chemical aspect is related to element depletion because many advanced devices integrated in IoT and AI systems contain parts made of elements that are predicted to be in short supply in foreseeable future [21]. Most of these elements, termed Critical Materials, are rare-earth elements, but even an element as common and technologically important as lithium may run the risk of becoming scarce [22]. It is therefore crucial to assess if the supply of critical materials is sufficiently large to maintain IoT systems and technologies in a sustainable way for years to come. If the answer is no, the introduction of such systems should be postponed and undergo serious ethical considerations.

The future

Proposals for new topics to be studied by COMEST are coming from commission members, other UNESCO bodies, and international organizations. So far, no suggestions have come from IUPAC despite the level of ethical reflection the Living Code of Conduct suggests chemists should be engaged in. But that may change if the IUPAC Council approves the proposal to form a standing Committee on Ethics, Diversity, Equity, and Inclusion (CEDEI) and if the committee becomes more extrovert than the terms of reference indicate it might become. With conspiracy theories blowing in the wind and gaining support, it is increasingly important that science, technology, and ethics move forward hand in hand. In this movement the scientific unions should support COMEST wholeheartedly and pay attention to the reports published by the commission.

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More Than Just a Random Walk?

by Jörg Kärger, Douglas M. Ruthven, and Rustem Valiullin

Owing to their potential for eco-friendly matter upgrading by molecular sieving and shape-selective conversion, nanoporous materials are among the pioneers of green chemistry. The performance of their application is often controlled by diffusion, *i.e.* the rate of mass transfer within these materials. This mass transfer, however, is rather complex and subject to numerous influences. Unambiguous diffusion measurement has thus remained a challenge to this day with errors in the interpretation of experimental data being all too common. The present feature reports the efforts of an IUPAC initiative to overcome these limitations.

1. An omnipresent phenomenon

Diffusion, meaning the random movement of objects, is an omnipresent phenomenon. The fact that it is a topic of scientific consideration can be traced back to Heraclitus of Ephesus and his *„panta rei"* (everything flows) in the sixth century BCE. Random movement may be observed with real objects, typically atoms and molecules, the constituents of matter. In fact, our understanding of diffusion is mainly based on the observation of atomic and molecular diffusion. These "conventional" diffusion studies have served as the main source for the development of theoretical concepts for the description of diffusion phenomena.

Diffusion, however, may also be observed with larger objects such as the spread of viruses as pathogens, of which we have become painfully aware during the current pandemic. However, random movement may even be observed with objects as large as plants and animals, *e.g.* during their "invasion" into novel biotopes. The complexity of such phenomena increases the difficulty of making reliable predictions.

We are presently witnessing this complexity worldwide with the spreading of the coronavirus pandemic—and it is particularly true for the spreading of non-physical objects, such as rumors, linguistic features, or jokes. The study of the extent to which these phenomena may, in some of their features, be reasonably well interpreted within the framework of "conventional" diffusion concepts is a fascinating topic of current research [1].

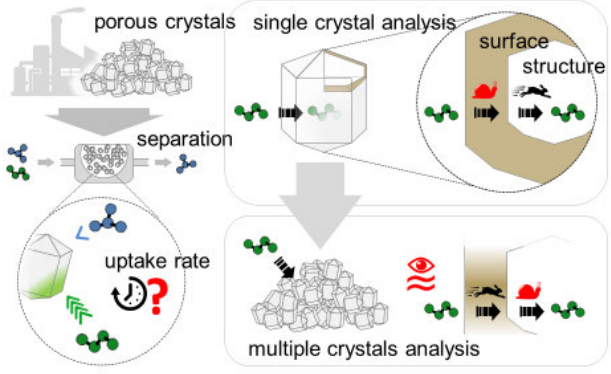

Figure 1: *Mixture separation by selective adsorption (after [5]). Left: Separation principle. Right: Example of misguided reasoning about the limiting process (see section 5 for details)*

2. A process of economic relevance

Diffusion is an important step in the process of value enhancement in many areas such as metallurgy and semiconductor production. This holds, in particular, for matter upgrading by molecular sieving and/or shape-selective conversion in nanoporous materials (see, *e.g.,* chapters 10 and 11 of [1] and [2, 3]). Following an IUPAC recommendation [4], *nanoporous* is the term used for characterizing materials with pore widths up to 100 nm. More specifically, materials with pores up to 2 nm are called *microporous*, from 2 to 50 nm *mesoporous* and beyond that *macroporous*.

With pore sizes of typically the same order as the sizes of the molecules under consideration, microporous materials offer particularly favorable conditions for target-oriented separation and transformation of the guest molecules. This is a basic prerequisite for their resource-conserving and environmentally friendly use.

The left side of Fig. 1 shows, schematically, the principle of operation when using microporous materials for mass separation. It takes advantage of the fact that the critical diameter of one component (here shown in blue) is sufficiently large, thus allowing (if at all) only a very slow penetration into the zeolite, while the smaller diameter of the molecules of the other component (shown in green) results in their rapid capture. Hence, during "filling" of the bed of zeolites, the permeate contains an excess of the blue molecules. Subsequently, in a "rinsing" phase, the other component is provided in abundance. Performance, *i.e.* the gain in value-added (*i.e.* separated) products per unit time, increases with increasing adsorption and desorption rates. Transport acceleration, as a consequence, leads to productivity enhancement. Note that this principle becomes particularly important when the boiling points of the mixture constituents are close to each other so that separation by distillation, the method of common choice, becomes extremely energy- and cost-intensive.

With the widespread exploitation and extension of this principle, microporous materials, including zeolites as their economically most important representative, were, in the second half of the last century, among the first to foster "Non-Waste Technology and Production" and/or "Pollution Prevention", as a predecessor and promoter of today's "Green Chemistry" [6]. For example, the annual benefit worldwide from their exploitation in petroleum refining has been estimated to be at least 10 billion USD ([1] pp. 171/172).

As a matter of course, the gain in value-added products can never be faster than what is allowed by the rate of exchange between the interior of the microporous particles of the host material and their surroundings. This process of exchange includes, in particular, the rate of propagation (diffusion) of the guest molecules within the space of the micropores. The intimate contact between the guest molecules and the internal surface of the host material, which is a prerequisite for its functionality for matter separation and/or conversion results in a dramatic reduction in the mobility of the guest molecules. Ways out of this dilemma include the use of small particles or thin membranes, and of particles with a hierarchical pore structure where, ideally, the micropore space is traversed by a network of "transport" (i.e. meso- or macro-) pores.

Acceleration of mass transfer between the nanoporous material and its surroundings as a main route towards performance enhancement in their application in matter separation and conversion has to be based on the knowledge of all contributing processes and, notably, the assessment of their relative importance for overall mass transfer.

3. In search of the rate-determining step in mass transfer

For decades, it was assumed that the mitigation of mass transfer upon confinement in the micropores within the zeolite bulk phase would inevitably lead to the dominance of intracrystalline diffusion (also referred to as micropore, configurational or zeolitic diffusion) as the limiting process of molecular uptake and release by beds of zeolite crystallites. This was at least implied in experiments with sufficiently small beds of crystallites so that any significant resistance of mass transfer through the bed of crystallites could be excluded. Hence, over many years, rate measurements of molecular uptake and release were taken as the main source of information about intracrystalline diffusion.

It came, therefore, as a big surprise when the pulsed field gradient (PFG) technique of nuclear magnetic resonance (NMR, see, *e.g.*, [2, 3, 7] and chapters 10 and 12 of [1]) allowed the *direct* observation of molecular diffusion within the interior of the individual crystallites and, for a number of zeolitic host-guest systems, the diffusivities determined in this way notably exceeded the values deduced from uptake and release measurements with apparently identical zeolite specimens [8]. Uptake and release were thus shown, in many cases, to be controlled by processes other than genuine intracrystalline diffusion.

It thus became clear that, in the study of sorption kinetics, it is necessary not only to determine the intra-crystalline diffusivity but also to establish the rates of other potentially rate controlling processes in order to assess their significance under the relevant conditions.

4. The "various diffusivities" and their measurement

Molecular uptake and release is, obviously, a consequence of the stochastic movement of the guest molecules upon entering or leaving the nanoporous particle. With Fig. 2a, under the influence of this random movement a concentration gradient is immediately seen to give rise to a diffusion flux j which is proportional to the concentration gradient (Fick's 1st law, eq. (1)), with the factor of proportionality D_T referred to as the transport (resp. collective, chemical or Fickian) diffusivity.

Random movement of molecules occurs, as a matter of course, also under equilibrium conditions. This may be investigated by considering, *e.g.,* a mixture of two isotopes (as indicated by the two shades of color in Fig. 2b) of essentially identical mobility. Then, in complete analogy with eq. (1), the flux j^* of either of the two isotopes may be noted as being proportional to the respective concentration gradients (eq. (2)). The factor of proportionality D is now referred to as the self- or tracer diffusivity.

In general, the coefficients of transport and of self-diffusion cannot be identical since the physical situations under which they are defined, are different. They do, however, coincide at sufficiently low concentrations, where the mutual interaction between different molecules becomes negligibly small.

With eqs. (1) and (2), the diffusivities may be determined by the measurement of fluxes either directly or by recording the *effect* of fluxes on considering, *e.g.,* uptake and release or, more generally, the variation in local concentration (Fick's 2nd law [1-3]).

There are also a number of techniques (including PFG NMR) by which it becomes possible to obtain information about the diffusion path of the individual molecules. In this case (Fig. 2c and eq. (3)) one is able to determine the coefficient of self- or tracer diffusion

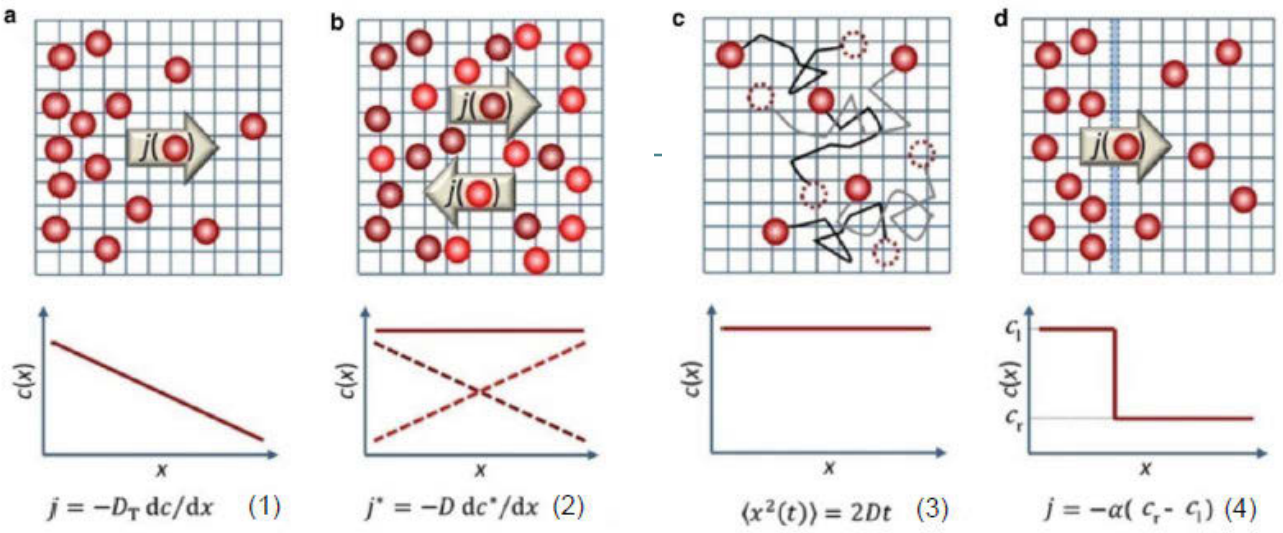

Figure 2: *Definitions and conditions of measurement of the "various diffusivities" (reproduction of Fig. 1 in the Introductory paper by Kärger, Ruthven, Valiullin to [9])*

as the factor of proportionality between the observation time and the mean square displacement covered, during this time, by the molecule. In this proportionality, there appears an additional factor of 2 (4 or 6) for measurement of the displacement in one (two or three) dimensions. Coincidence of the definitions of the self-diffusivity by eqs. (2) and (3) is one of the messages of Einstein's famous diffusion equation [1-3].

Fig. 2d refers to the situation with additional transport resistances ("barriers") crossing the interior of the nanoporous particle. The permeability of these barriers is quantitated by their permeance, which is defined as the factor of proportionality between the flux through the barrier and the difference in the local concentrations on either side. For transport resistances on the particle surface ("surface barriers") one rather has to consider the difference between the guest concentration in equilibrium with the surroundings and the actual boundary concentration.

5. An example of misguided reasoning

Let us consider the two limiting cases in which molecular uptake and release is exclusively determined by intracrystalline diffusion (case of diffusion control) or by penetration through the surface barrier (barrier control). In these two cases, mass increase during molecular uptake or decrease during release follow different, well-defined time dependences. Analysis of the respective time dependences would, accordingly, be expected to provide immediate information about the limiting process in mass transfer.

One must have in mind, however, that the uptake curves are also affected by the crystal size and the intracrystalline diffusivity and/or the surface permeability (*i.e.* the intensity of the surface barrier), as well as by heat transfer. Hence, on considering uptake by a bed of crystals as the common scenario for, *e.g., gravimetric* measurements of adsorption/desorption kinetics, the uptake curve results as only the sum of various single-crystal uptake curves. The shape of the sum of these uptake curves, however, may be notably different from the shape of each individual one and may even, for a "suitable" distribution of the crystal properties, approach the other limiting case.

This is indeed the case on considering, *e.g.,* molecular uptake under barrier limitation with a bed of crystals with appropriately distributed surface permeabilities, but otherwise identical properties [5]. The right side of Fig. 1 refers, in a cartoon-like manner, to such a situation. Analyzing the time dependence of molecular uptake as recorded with a single crystal (top right) will correctly suggest that permeation through the crystal surface is the rate-determining process during uptake (when the guest molecules become "snails"). However, by using the same type of analysis, with beds of crystals (bottom right) intracrystalline diffusion will erroneously appear as the rate-determining step in the overall uptake.

This misinterpretation obviously results from the fact that the information provided by the experiment is still insufficient for a clear reflection of the transport phenomena taking place in the system. For the rate data to be quantitatively useful, the experiment must be designed in such a way that it will provide clear evidence concerning the rate limiting process.

6. A plethora of mechanisms and conditions

Section 4 already introduced two different ways in which diffusion phenomena become accessible by experimental measurement, namely via Fick's laws by recording molecular fluxes and/or the time dependence of molecular concentrations or via the Einstein relation by recording molecular mean square displacements. The distances over which, during the measurement, the molecules typically migrate are clearly a function of the applied method of measurement. This suggests, in addition to the above introduced distinction between equilibrium and non-equilibrium

measurement, a further, material-related classification of the measuring techniques. Thus techniques of diffusion measurement sensitive for displacements of the order of or smaller than the micropores are referred to as submicroscopic, for displacements within the particle as microscopic and for displacements within the bed/pellet as macroscopic. Mesoscopic techniques are focused on a single crystal/particle without allowing a spatial resolution of its interior.

Table 1 provides a survey of the techniques which, so far, are in common use for studying molecular transport in nanoporous materials. The given classification cannot be more than a general guide. Deviations from the assessment include quasi-elastic neutron scattering which, under favorable conditions, allows the recording of displacements into the range of nanometers, and PFG NMR which, for sufficiently large observation times, is also applicable for macroscopic diffusion measurements. If performed with only a small amount of adsorbent particles the information attained by some of the techniques mentioned in the bottom right may be referred to as meso- rather than macroscopic. It is also worth mentioning that the equilibrium techniques may also be applied under non-equilibrium conditions and that, by the application of suitably chosen isotope mixtures, the non-equilibrium techniques may be applied for studying diffusion under equilibrium conditions.

There are two more classification features that do not appear in table 1. One of them refers to the potential of a given measuring technique for providing selective information about the diffusivity of a single component within a mixture. In fact, in most cases of their practical application, nanoporous materials are contacted by mixtures rather than by a single component and it is the behavior of the individual components of the mixture that is mainly of interest. While in some techniques, including single-particle tracking and microimaging via IR microscopy, the selectivity towards a certain molecular species is inherent to the technique, with other techniques selective diffusion measurement is only possible with extreme additional effort or sometimes not at all. Furthermore, it makes a big difference whether a measuring technique is applicable only to a bed of crystals, like PFG NMR or common measurement of the adsorption/desorption kinetics, or whether it may be applied to a single crystal.

With this last example we are back to the "example of misguided reasoning" that we considered in section 5. Misguidance arose because we considered uptake by a bed of crystals rather than by a single crystal. It is true, however, that the option of making measurements with a single crystal might not be available. It is therefore important to be aware that, in the given situation, it is often possible to distinguish between diffusion and surface barrier control even from conventional uptake and release measurements. This option is provided by the so-called partial loading experiment which consists of an adsorption measurement followed, before saturation is reached, by a desorption experiment. A reduction of the time interval between these two experiments leaves, under barrier limitation, the (normalized) desorption curve unaffected while it becomes increasingly steeper under diffusion limitation (see Ruthven *et al.* in [9]).

Measurement	Equilibrium	Non-Equilibrium
Submicroscopic	Solid-State NMR Quasi-Elastic Neutron Scattering (QENS)	
Microscopic	Pulsed Field Gradient (PFG) NMR Single-Particle Tracking (SPT)	Microimaging
Mesoscopic	Dynamic Light Scattering (DLS)	(Single-Crystal) Membrane Permeation
Macroscopic		Adsorption/Desorption Kinetics Liquid-Phase Batch Kinetics Column Breakthrough Dynamics Zero Length Column (ZLC) Technique Frequency Response (FR) Technique NMR Imaging (MRI) X-Ray Computed Tomography (XCT)

Table 1: *Classification of the various techniques of diffusion measurement with nanoporous host-guest systems with reference to the scale of observation ("Microscopic vs. Macroscopic") and the conditions, under which the measurements are (generally) performed ("Equilibrium vs. Non-Equilibrium"). These techniques are in the focus of the activities of an IUPAC task group that has been established for providing a "comprehensive set of guidelines for measurements and reporting of diffusion properties of chemical compounds in nanoporous materials". Details of the various techniques are presented in a Thematic Issue of the Adsorption Journal [9]. Following preceding versions, such as those in [3], the table is adapted from [10], where also complete citations for the table entries may be found.*

7. The random walk of diffusion research

In view of the variety of influences and the limitations in the significance of each of the measurement techniques as appearing from table 1, it is not surprising that the literature of this subject is replete with contradictory statements on mass transfer in nanoporous materials. This tendency is further exacerbated by the fact that nanoporous materials are often far from inert. Their structure and composition are known to be highly sensitive to the conditions of synthesis, storage and pretreatment. They may vary, furthermore, during their technical application and may even change during their preparation for the diffusion measurement and during the diffusion measurement itself.

All these changes, as a matter of course, affect the mass transfer within the systems. Most importantly, however, various constituents of mass transfer may be affected quite differently. This refers, *e.g.,* to an inhibition of mass transfer in either the microporous bulk phase or through surface barriers as discussed in sections 5 and 6. Examples of such seemingly contradictory studies may be found in the text books [2] and [3]. Recording of the "apparent" diffusivities attained in such studies might thus sometimes appear as a random walk on its own.

8. Wanted: A set of guidelines for diffusion measurement

Quantification of the various aspects of mass transfer, as appearing from table 1, necessitates the use of a wide range of different experimental techniques which are only accessible in an extended collaborative network. In 2015 an IUPAC task group dedicated to "Diffusion in Nanoporous Solids" (https://iupac.org/project/2015-002-2-100) has come together for the launch of such an activity, with its final goal "To provide a first comprehensive set of guidelines for measurements and reporting of diffusion properties of chemical compounds in nanoporous materials serving for catalytic, mass separation and other relevant purposes." As a first step, the group initiated the launch of a Thematic Issue of the Adsorption Journal [9] dedicated to the measurement of guest diffusion in nanoporous host materials.

This issue, which has just appeared, will serve as a basis for a first draft of what this "comprehensive set of guidelines" should look like. As a highlight in this discussion, we are happy to invite researchers in the field to attend the upcoming 9th Diffusion-Fundamentals Conference in September 2022 in Krakow, Poland (Diffusion Fundamentals IX - Diffusion Fundamentals - Faculty of Physics, Astronomy and Applied Computer Science (uj.edu.pl)) where a special workshop will be dedicated to the discussion and finalization of these guidelines.

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We sincerely thank the German Research Foundation, the Alexander von Humboldt Foundation, and the Chemical Industry Fund for long-standing support of our work and collaboration, which eventually ended up in the present IUPAC network.

Jörg Kärger, <kaerger@physik.uni-leipzig.de>, Leipzig University, Germany, and Douglas M. Ruthven, University of Maine, Orono, USA, are professors emeriti and authors of the standard textbooks on "Diffusion in Zeolites and Other Microporous Solids" (Wiley, 1992 [2]) and (jointly with Doros N. Theodorous) on "Diffusion in Nanoporous Materials" (Wiley-VCH, 2012 [3]). Rustem Valiullin came to Leipzig University as a Humboldt Fellow from the University of Kazan, Russia, and is now a professor there at the Felix Bloch Institute for Solid State Physics.

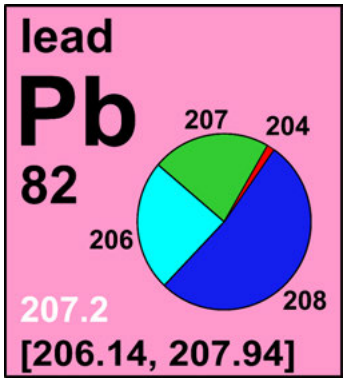
Standard Atomic Weight of Lead Revised

Following the recent publication of the IUPAC Technical Report on the variation of lead isotopic composition and atomic weight in terrestrial materials [1], the IUPAC Commission on Isotopic Abundances and Atomic Weights (CIAAW) is recommending changes to the standard atomic weight (*i.e.* relative atomic mass) of lead:

lead: to [206.14, 207.94] from 207.2 ± 0.1

The assignment of an interval for the new standard atomic weight reflects the common occurrence of variations in the atomic weights of lead in normal terrestrial materials which have been known for over a century [2]. If a single atomic-weight value is needed, the Commission recommends using 207.2 ± 1.1, which corresponds to the common lead with a symmetric uncertainty covering normal materials.

The isotopic composition and atomic weight of lead are variable in terrestrial materials because its three heaviest stable isotopes are stable end-products of the radioactive decay of uranium (^{238}U to ^{206}Pb and ^{235}U to ^{207}Pb) and thorium (^{232}Th to ^{208}Pb). These variations in isotope ratios and atomic weights provide useful information in many areas of science, including geochronology, archaeology, environmental studies, and forensic science. While elemental lead can serve as an abundant and homogeneous isotopic reference, deviations from the isotope ratios in other lead occurrences limit the accuracy with which a standard atomic weight can be given for lead. In a comprehensive review of several hundred publications and analyses of more than 8000 samples [1], published isotope data indicate that the lowest reported lead atomic weight of a normal terrestrial material is 206.1462 ± 0.0028, determined for a growth of the phosphate mineral monazite from the Lewisian complex in north-western Scotland, which contains mostly ^{206}Pb and almost no ^{204}Pb [3]. The highest published lead atomic weight is 207.9351 ± 0.0005 for monazite from a micro-inclusion, also from the Lewisian complex in north-western Scotland, which contains almost pure radiogenic ^{208}Pb [3].



The CIAAW continues to evaluate literature data which leads to identification of developments in the measurement science, recognition of new discoveries, and remains committed to modernize its technical guidelines and work towards further expansion of its website to include more historical databases.

These changes and considerations will be published in *Pure and Applied Chemistry* and can be found online at the website of the IUPAC Commission on Isotopic Abundances and Atomic Weights (ciaaw.org).

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https://iupac.org/standard-atomic-weight-of-lead-revised/

PAC Cheminformatics Special Issue

***Pure and Applied Chemistry Special Issue*—Call for Papers: Cheminformatics: Data and Standards.**

IUPAC has long helped advance cheminformatics and chemical data standards. Examples include the development of the InChI chemical identifier and the JCAMP-DX family of spectroscopic data formats. These formats continue to evolve based on current needs of the community, and new cheminformatics standards initiatives are launching within IUPAC and related organizations, which seek to address gaps in, for example, chemical file formats, chemical metadata standards, and machine-readable data sharing. Cheminformatics standards advance research and teaching, and also facilitate the implementation of chemical processes.

This special issue seeks to continue the conversation around cheminformatics standards development, with the aim to review current standards available, as well as discuss future needed standards. Clearly identifying our current successes and limitations in

cheminformatics standards will serve to inform the community and help coordinate further standards development.

Example topics appropriate for this *Cheminformatics: Data and Standards* special issue may include:

1. Cheminformatics standards use-cases and workflows across disciplines.
2. Discussions around how cheminformatics standards advance research and teaching.
3. Perspectives related to current cheminformatics standards and future needs, for example interoperability and metadata considerations.
4. Cheminformatics datasets useful for teaching and/or validation.
5. Standardization needs related to infrastructure (*e.g.,* repositories), cheminformatics toolkits, or data sharing.
6. Conference, symposia, or workshop based outcomes related to cheminformatics standardization.

If you are interested in contributing to this Special Issue, please send a provisional title, together with the name and email address of the submitting author to Vincent Scalfani vfscalfani@ua.edu.

Guest Editors:

- Vincent Scalfani, University of Alabama
- Jonathan Goodman, University of Cambridge
- Ian Bruno, Cambridge Crystallographic Data Centre

Please see the *Pure and Applied Chemistry* Author Guidelines for specific manuscript preparation information at https://www.degruyter.com/journal/key/PAC/html. Note that typically articles in Pure and Applied Chemistry occupy 6-12 journal pages, however, we will also consider shorter discussions appropriate to the special issue. Manuscripts are due by September 30.

IUPAC Periodic Table Challenge 2020: Top Schools Announced

Following the success of the IYPT2019 [10.1515/ci-2020-0204], IUPAC continued the Periodic Table Challenge which not only had more questions, but also welcomed more participants! Since its start in 2019, more than 100 000 tests have been taken by keen players from 155 countries/territories all over the world. Since, the PT Challenge saw not only continued popularity but was translated into Arabic, Chinese, Russian, and Spanish. Countless schools have participated throughout the year and we are proud to announce the list of 15 most active schools that have showed great and sustained interest in the IUPAC Periodic Table Challenge:

TOP7 SCHOOLS

- Bal Bharati Public School, Navi Mumbai (India)
- Colegio Interamericano, Bogota (Colombia)
- Covenant University, Ota (Nigeria)
- STEM High School Qalyubia, Al Obour (Egypt)
- St. Francis English Medium High School, Machilipatnam (India)
- Tarlac State University, Tarlac (Philippines)
- Universidad Central del Este, San Pedro (Dominican Republic)

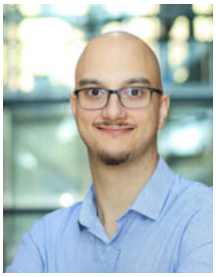
HONORABLE MENTION

- Anglo Sanskrit College, Khanna (India)
- Cluster School of SMK Methodist, Sibu (Malaysia)
- DAV Public School BRS Nagar, Ludhiana (India) Instituto "La Candelaria" Olmos, Buenos Aires (Argentina)
- National Public School Yeshwanthpur, Bangalore (India)
- STEM High School Dakahlia, Belkas (Egypt)
- SMK Ora et Labora BSD, Tangerang Selatan (Indonesia)
- Universidad del Valle de Atemajac, Guadalajara (Mexico)

The highlighted TOP7 SCHOOLS will receive the Periodic Table posters signed by chemistry Nobel Laureates which is made possible by the generous participation from 13 Nobel laureates. We thank Roald Hoffmann (Nobel Prize 1981), Jean-Marie Lehn (1987), Barry Sharpless (2001), Kurt Wüthrich (2002), Peter Agre (2003), Robert H. Grubbs (2005), Martin Chalfie (2008), Ada Yonath (2009), Robert J. Lefkowitz (2012), Ben Feringa (2016), Sir Fraser Stoddart (2016), Joachim Frank (2017), Frances Arnold (2018) for their support!

Winners of the 2021 IUPAC-Solvay International Award For Young Chemists

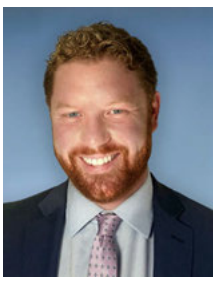
The International Union of Pure and Applied Chemistry and Solvay announce the winners of the 2021 IUPAC-Solvay International Award for Young Chemists, presented for the best Ph.D. theses in the chemical sciences, as described in 1000-word essays.


Gabriele Laudadio


Justin Andrews


Kaibo Feng


Kelly Brown


Austin Michael Evans

The five winners are:

- Gabriele Laudadio (Italy), Ph.D., Eindhoven University of Technology (NL); *New synthetic methods enabled by photochemistry and electrochemistry in flow*
- Justin Andrews (USA), Ph.D., Texas A&M University; *Corralling Electrons in Metastable Vanadium Oxides: Implications for Neuromorphic Computing, Electrical Energy Storage, and Photocatalysis*
- Kaibo Feng (China/Beijing), Ph.D., University of Illinois at Urbana-Champaign; *Late-Stage C(sp3)–H Hydroxylation, Amination, and Methylation in Nitrogen-Containing Molecules*
- Kelly Brown (UK), Ph.D., University of Strathclyde; *Development of Electrochemiluminescent Sensors as Screening Tools for the Identification of Drug Species within Complex Matrices for Forensic Investigations*
- Austin Michael Evans (USA), Ph.D., Northwestern University; *Two-dimensional polymers and polymerizations*

The winners will each receive a cash prize of USD 1000 and are invited to present a poster at the 48th IUPAC World Chemistry Congress describing his/her award-winning work. Because this year the IUPAC Congress is planned as a virtual event, the winners will also be invited the 2023 IUPAC Congress to be held in The Netherlands. Each winner is invited to submit a short critical review on aspects of his/her research topic, to be published in *Pure and Applied Chemistry.*

There were 46 applications from individuals receiving their Ph.D. degrees from institutions in 18 countries. The award selection committee, chaired by Qi-Feng Zhou, IUPAC Past President, comprised members of the IUPAC Bureau and a senior science advisor from Solvay, all of whom have a wide range of experience in chemistry.

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

- Irene Regeni (Germany), Ph.D., TU Dortmund University (Germany)
- Ni Kaiyuan (China/Beijing), Ph.D., The University of Chicago
- Dusan P. Kolarski (Serbia), Ph.D., University of Groningen

The call for applications for the 2022 IUPAC-Solvay International Award for Young Chemists will open soon. Eligible candidates must have received a Ph.D. or equivalent degree in any of the countries that have National Adhering Organizations or Associate National Adhering Organizations in IUPAC during the year 2021.

Winners of the Inaugural 2021 IUPAC Analytical Chemistry Awards

In 2019, the IUPAC Analytical Chemistry Division established two awards:

- The IUPAC Analytical Chemistry Medal—an award to recognize significant lifetime contribution to analytical chemistry and for researchers who have a substantial record of achievements demonstrated by the number and quality of their publications, by being actively involved in international partnerships as well as by their commitment in the training of the next generation of analytical chemists.
- The Emerging Innovator Award in Analytical Chemistry—an award to recognize outstanding work undertaken by researchers who are at the early stage of their independent career.

The inaugural 2021 IUPAC Analytical Chemistry Medal recipient is Joseph Wang.

Wang is a Distinguished Professor of Nanoengineering and SAIC Endowed Chair at the University of California San Diego (UCSD). He also serves as the Director of the UCSD Center of Wearable Sensors.

Wang obtained his higher education at the Israel Institute of Technology (Haifa), being awarded his D.Sc. in 1978. From 1978 to 1980 he served as a research associate at the University of Wisconsin (Madison). Between 1980 and 2004 he was a member of the Chemistry department at NMSU where he held a Regents Professor and a Manasse Chair between 2001 and 2004, and between 2004 and 2008 he served as the Director of the Center for Bioelectronics and Biosensors and a Professor of Chemical Engineering and Chemistry at Arizona State University, and as Chair

of the UCSD Nanoengineering Department between 2014 and 2019.

His research interests include the development of electrochemical biosensors, nanomotors and nanorobots, wearable sensors, flexible stretchable materials, biomedical applications of nanomachines, printable devices, nanomaterials-based sensors, bioelectronics, biorecognition and clinical diagnostics, microfluidic ("Lab-on-Chip") devices, microfabrication, biofuel cells, new interfaces for electroanalysis and electrocatalysis, sensor/recognition coatings, and remote environmental and security sensing. He has authored over 1150 research papers, 11 books, 45 patents, and 35 book chapters. His H-Index (Google Scholar) is 176. Wang has presented more than 400 invited talks, including 200 plenary and keynote lectures in 60 countries. He was been the Founding Editor and Chief Editor of the international journal Electroanalysis (Wiley-VCH) for 3 decades (1988-2018). He has been a member of the Advisory Editor Board of 25 other international journals.

Wang has been a Thomson Reuters Highly Cited Researcher since 2015 and has been included in the Thompson Reuters List of 2015 World's Most Influential Scientific Minds. He has received numerous international awards, honorary doctorates and professorships.

Wang has been a key contributor to IUPAC project "Electrochemical DNA-based biosensors: terms and methodology" (*Pure Appl. Chem*. 82, 1161–1187, 2010).

Professor Wang has mentored 35 PhD students and trained over 350 post-doc and visiting scholar fellows. These trainees currently hold leading academic and industrial positions throughout the globe.

The Emerging Innovator Award in Analytical Chemistry is awarded to Tsuyoshi Minami, PhD.

Minami received his BEng in 2006 and MEng in 2008 from Saitama University, PhD in Engineering from Tokyo Metropolitan University under the direction of Yuji Kubo. Between 2011 and 2013 he was a postdoctoral research associate at Bowling Green State University working with Pavel Anzenbacher, Jr., where he has started his academic career by the appointment as a research assistant professor. In 2014, he moved to Yamagata University as an assistant professor. From 2016 to 2019 he was a lecturer at the University of Tokyo where he was selected as an excellent young independent researcher and since 2019 he is an associate professor. He is also a visiting professor at Yamagata University, Tokyo Metropolitan University, and The University of Technology of Compiègne, France.

His research fields based on analytical chemistry include design and synthesis of artificial receptors, semiconductor materials and nano materials, and device fabrication for sensing applications in solution, solid and gas phases. In his group, two types of research topics are mainly researched: 1) High-throughput Analysis Based on Supramolecular Sensor Arrays and 2) Chemical Sensors based on Organic Thin-Film Transistors Functionalized with Molecular Recognition Materials.

Minami has discovered the self-assembled optical sensor array systems as promising for sensitive detection of analytes (as chiral amines, herbicide glyphosate, saccharides in a soft drink, sulfur-containing amino acids, toxic heavy metal ions) without any synthetic burden. In the field of sensors, he designed and fabricated an extended-gate type organic thin-film transistor for cross-hierarchical detection of various analytes covering a wide range of sizes from small ions to biomacromolecules. Both of his pioneered research topics open a new avenue for practical applications of supramolecular sensors in various fields such as healthcare, environmental assessment, *etc.* His dedication and hard work have earned him 88 publications (53 papers as a corresponding author) including 13 Top10 % papers (Clarivate analytics).

His 32 representative awards cover The Young Scientists Prize, The Commendation for Science and Technology by the Minister of Education, Culture, Sports, Science and Technology (MEXT, 2020), The Chemical Society of Japan Award for Young Chemists (2020), ChemComm Emerging Investigators 2018 (Royal Society of Chemistry, 2018), The Japan Society for Analytical Chemistry Award for Young Researchers (2017).

Minami has succeeded in interdisciplinary studies based on analytical and supramolecular chemistry from the molecular design up to the device fabrication effective for the discovery of a new receptor for drugs, simultaneous detection of multi-analytes, and sensitive detection of analytes in a variety of molecular scale without any labeling. Thus, his research field contributes to the real-world implementation of analytical devices for improve people's quality of life.

Minami's teaching fields are represented by undergraduate laboratory experiments at Yamagata University, supramolecular structural chemistry at Tokyo Metropolitan University, lectures on advanced information system, introductory lecturers for chemistry and biotechnology, polymer and functional materials chemistry, and basic biomedical engineering at The University of Tokyo. Among his students and associates there are 5 postdoctoral researchers, 11 PhD candidates and 5 MS researchers.

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2021 Nominees for Election of IUPAC Officers and Bureau Members

During the 51st IUPAC General Assembly, now to be held online early August 2021, the Council will be asked to elect a Vice President, a Treasurer, and members of the Bureau to fulfill the vacancies created by retiring members. IUPAC National Adhering Organizations have been invited to submit nominations. (see News posted 30 December 2020)

On 1 January 2022, Javier García-Martínez (Spain), Vice President and President-Elect of IUPAC, will become President. Christopher Brett (Portugal), current President, will become Past President and remain an officer and a member of the Bureau for a period of two years, while Qi-Feng Zhou (China), current Past President, will retire. Secretary General Richard Hartshorn (New Zealand) was elected by the Council in July 2019 for a second four-year term and will continue his term until December 2023. Meanwhile Treasurer Colin Humphris (UK) has confirmed that he will retire at the end of 2021.

Vice-President

The Vice-President to be elected at the 51st Council will be President-Elect starting in January 2022, and will become President on 1 January 2024. The nominations received for Vice President are as follows:

- Mary Garson (Australia)
- Ehud Keinan (Israel)
- Ting-Soon Kueh (Malaysia)
- Supawan Tantayanon (Thailand)

Treasurer

The nominations received for Treasurer for the term 2022-2025 are as follows:

- Russell Boyd (Canada)
- Wolfram Koch (Germany)

Elected Members of Bureau

The Bureau consists of the Officers, the eight Division Presidents, Standing Committee Chairs and no less than ten other members elected by Council, who are known as "Elected Members". Elected Members serve a four-year term. No National Adhering Organization shall have more than one Elected Member on the Bureau. The statute also states that: "the principle of fair geographical representation of Members shall be taken into account."

At the conclusion of the 50th Council at Paris, there were ten Elected Members on the Bureau. At the 51st Council this August, the Bureau will make recommendations to Council as to the number of Elected Members (ten or more) who should be on the Bureau for the succeeding two years. At least four Elected Members will be elected at the 51st Council, *i.e.* the minimum number of ten Elected Members less the six Elected Members who continue in office until 2023.

This year and following the special vote by Council on May 5th, 2021, the elections will be held electronically in real time during the virtual General Assembly.

The nominations received for Elected Members of the Bureau are as follows:

- Abeer Al Bawab (Jordan)
- Hemda Garelick (United Kingdom)
- Ting-Soon Kueh (Malaysia)
- Patrick Maestro (France)
- Laura McConnell (USA)
- Zoltan Mester (Canada)
- Greg Russell (New Zealand)
- Ken Sakai (Japan) *reappoint*
- Zhigang Shuai (China/Beijing)
- Supawan Tantayanon (Thailand)
- Pietro Tundo (Italy)

Elected Members of Bureau who remain on Bureau and whose terms end in 2023:

- Ghada Bassioni (Egypt)
- Mei-Hung Chiu (China/Taipei), 2nd term
- Petr Fedotov (Russia)
- Ehud Keinan (Israel), 2nd term
- Gloria Obuzor (Nigeria)
- Bipul Behari Saha (India)

[Note that if any Elected Members of Bureau who are continuing, or any candidates for Bureau, are elected to a position as Officer, Division President, or Standing Committee Chair, they are not eligible to continue or to be elected to the Bureau at this election for the 2022-2023 biennium. Should that occur there may be additional elected positions to be filled.]

https://iupac.org/2021-nominees-for-election-of-iupac-officers-and-bureau-members/

Your Basic Polymer Sciences with the Subcommittee on Polymer Education: From Synthesis to Application!

International conferences, in bringing researchers from different backgrounds and different levels of access to opportunities together, are ideal venues for educational activities to improve the practice of science, particularly in the emerging nations.

Educational Workshop in Polymer Sciences 2016 in conjunction with MACRO2016, Istanbul

Polymer synthesis

Educational Workshop in Polymer Sciences 2018 in conjunction with MACRO2018, Cairns

Polymer processing

25th Short Course on Polymer Characterization in conjunction with 25th POLYCHAR 2017, Kuala Lumpur

Polymer characterization

Educational Workshop in Polymer Sciences 2020+ in conjunction with MACRO2020+, Jeju

Applications of polymers

The Sub Committee on Polymer Education (SCPE) has organized a social series of workshops about Education in Polymer Chemistry on several occasions.

This series of interactive IUPAC Education Workshops in Polymer Sciences (2016, 2017, 2018 and 2020+) on polymer sciences are intended primarily for students or active researchers from emerging countries. The presentation slides from the instructors are accessible from IUPAC project webpages through the QR-codes given below:

The Subcommittee on Polymer Education under IUPAC Polymer Division and IUPAC Committee on Chemistry Education (CCE) wanted to publish the lecture notes of the series workshop as well as the educational materials in polymer sciences in a special issue of *Chemistry Teacher International.*

One of the goals of *Chemistry Teacher International* is to bridge the gap between research and education. Good practices and the basics for some topics in polymer sciences for educational purpose should be helpful educational materials for the teachers or lecturers. In this recently released special issue, three articles on polymer synthesis, five articles on polymer characterization, two articles on polymer processing and three articles on polymer applications are published.

Both SCPE and CCE

acknowledge the work done by the instructors and the contributors of the articles for the benefits of the young researchers and teachers.

This special issue is available through the website of the Open Access Journal *Chemistry Teacher International*: https://www.degruyter.com/journal/key/CTI/html

Chin Han Chan is from the University Teknologi MARA, Malaysia, and is a Titular Member of the IUPAC Polymer Division. Jan Apotheker is from the University of Groningen, The Netherlands, and serves as Chair of IUPAC CCE and editor-in-chief of Chemistry Teacher International.

https://iupac.org/project/2019-035-1-050

Systems Thinking in Chemistry for Sustainability

"Earth Day 2021—April 22—with the theme of 'Restore Our Earth,' along with Chemists Celebrate Earth Week 2021 from ACS with the theme 'Reducing Our Footprint with Chemistry,' provides a rich opportunity to reflect on the extent to which we integrate sustainability into chemistry education."

This is exactly what Peter Mahaffy and colleagues from the IUPAC task group 2020-014-3-050 on "Systems Thinking in Chemistry for Sustainability: Toward 2030 and Beyond (STCS 2030+)" did in a guest editorial published in the *Journal of Chemical Education*, titled "Integrating Sustainability into Learning in Chemistry." [1]

"This editorial highlights how the interdisciplinary work of integrating sustainability into chemistry education can be guided by systems thinking, and by the United Nations Sustainable Development Goals and Planetary Boundaries frameworks. Such systematic approaches can energize educators and learners to situate chemistry within a broader landscape of knowledge and thus tap chemistry's potential to enhance sustainability."

The authors highlight the importance of transforming chemistry education so that it can play a meaningful role in achieving a sustainable future for our planet and its people. By applying systems thinking, the IUPAC STCS 2030+ project working group is highlighting the centrality of chemistry as a sustainability science and developing systems-thinking-oriented activities and approaches that integrate sustainability frameworks into chemistry education. One focus of the working group is to contribute to the goals of the International Year of Basic Sciences for Sustainable Development, IYBSSD-2022, www.iybssd2022.org. (see more page 40)

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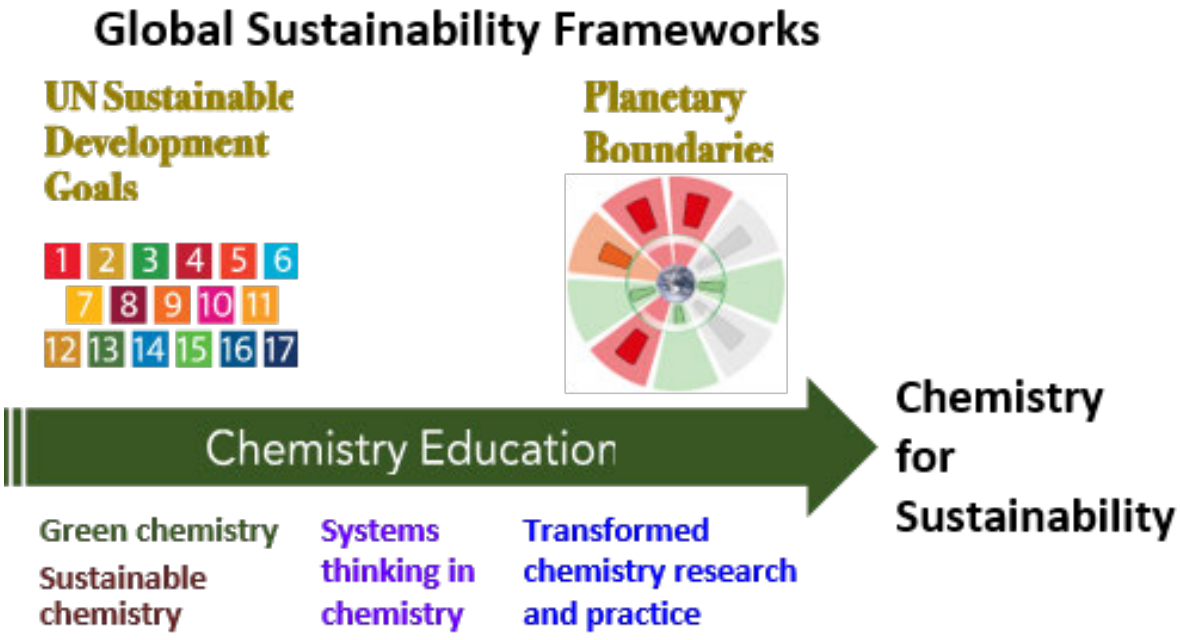
Related IUPAC projects

https://iupac.org/project/2020-014-3-050



The Challenge to establish a definition

by Pavel Karen

Doing chemistry only makes sense if we communicate the results. That is not so simple; the audience has to understand what we mean. It starts by calling things correct names of precise meaning. What are they? Would a plain dictionary help? Partly. A language dictionary often describes a noun with an array of synonyms of subtly varied meaning as a hint about possible contexts. Language is flexible, and that is fine in everyday life. In natural sciences, however, definitions have to be precise. Like having one for each synonym of that explanatory array in the dictionary. We need a proper definition of our term; a short focused description in well-known simple words that delimit the range of applicability of that term (see also [1]). The definition must primarily be: (a) specific, excluding all cases not covered by the term and including all that are covered, and (b) reflective of the current use of that term as a noun, or also as a verb and adjective if applicable.

That is easier said than done. How to recognize an imperfect definition? Say, someone tries to define the metallurgy term "alloy": **Alloy is a solid containing at least one metal and at least one other element (metal or non-metal); showing the properties of metallic crystals**.

It sounds just fine. Until one considers several solids actually "showing properties of metallic crystals". Are these alloys: (1) golden metallic YC_2; (2) AuCu intermetallic compound; (3) golden metallic oxide TiO; (4) silvery metallic perovskite-type $AuNCa_3$; (5) copper colored ReO_3; (6) metallic carbide Fe_3C; (7) austenite, a solid solution of carbon in fcc γ-iron; (8) brass, a solid solution of zinc in copper?

How do these metallic crystals fulfill the above definition? (a) Is the given crystal an alloy? Alloy of what? (b) Can it be prepared by alloying elements (does "alloy" apply as a verb to the synthesis/manufacturing process)? (c) Is it referred to as an alloy in the literature?

Brass, a solid solution of zinc in copper, is made by alloying; adding Zn to melted Cu. The AuCu, Fe_3C and austenite can too be prepared by alloying elements. They are components of an alloy, crystals of own specific structure, each an alloy of a composition with a relatively narrow homogeneity range. The rest are not really alloys: YC_2 is a metallic salt that hydrolyzes in some similarity to CaC_2. TiO and ReO_3 are never referred to as alloys, and we cannot say that they are prepared by alloying Ti or Re with oxygen. The latter would not even form by such a reaction. Neither is the metallic $AuNCa_3$ salt tricalcium auride(1−)nitride(3−) bis[electride(1−)] referred to as an alloy or a component of an alloy.

And then we must ask: Is "showing the properties of metallic crystals" inclusive of all materials typically referred to as an alloy? Does it include amorphous alloys like Vitreloy or metallic glasses in general? No. So our seemingly OK definition is not very good in clarifying what an alloy is.

Another challenge appears when the term to be defined is a quantity, when it has a numerical value. In communication, the term introduces its quantity value [2], yet the value as such does not necessarily define the term. Besides directly measurable "physical" quantities, we have in chemistry several descriptive terms that acquire various numerical values depending on the chemical composition and structure they refer to. Such a term as a quantity concept has a definition. As a quantity value, it obtains via algorithms; often by one approach of several possible, one that suits the target molecule, ion, or compound. Take bond order as an example. Bond order of two atoms is the (integer or fractional) number of their two-electron bonds equivalent to the given bond. This might be a general definition of the term bond order as a simple heuristic concept for any chemist. However, what is its numerical value? That has to be calculated for each bond by a suitable algorithm; preferably heuristic, easy to grasp and think about, not a black box. In this case, several algorithms exist with simple starting parameters for the two bonded elements: For simple molecules, we draw an MO scheme and subtract electrons in antibonding MOs from electrons in bonding MOs to obtain twice the value of the bond order. That algorithm is also nicely illustrative of the bond order as a concept, and, in a more precise form, it appears in the Gold Book entry [3]. Alternatively, we draw a Lewis formula according to rules (8−N rule applied by order of electronegativities, octet, etc.) while counting electrons to obtain bond orders as integers or simple fractions. Or we calculate a decimal bond order, typically fractional, from the bond length. This too is a heuristic approach when based [4] on those two atoms' Allred–Rochow electronegativities, the difference of which correlates with the covalence-based bond shortening versus the sum of the two "ionic" radii that are fit by least squares to many bond lengths of well-defined bond order between these two atoms. Two parameters for each atom are enough; electronegativity and ionic radius. To relate to the result, we must understand how it was obtained and what it means. We thus need the definition to understand the term bond order as a concept, and we need a heuristic

algorithm to calculate its quantity value. Machines need a program code. The heuristic algorithm for human use cannot be just a black box of quantum-chemical program operating with internal parameters that may vary without obvious link to the actual chemistry investigated. However, if such a program is widely used, a normative work about the term should list it after the heuristic algorithms are given.

For the bond-order and similar chemistry concepts, the algorithm is not a definition. None of the three algorithms mentioned above defines in general what the bond order is; for that their practical use is too narrow. The order of the bond is not always seen from the MO scheme; not necessarily well defined by how we set up a Lewis formula; nor by the bond-valence parameters in Ref. 4 that give precise results for extended solids (structural compromises considering) yet less so for bonds of high order in molecules. The algorithm we actually use merely defines the just calculated quantity value.

So, when a chemistry term is not a directly measurable quantity, its quantity value is linked to an algorithm. The current use may allow several heuristic algorithms to calculate it. Whereas the algorithms can build on various specific approaches and sets of parameters, the concept definition should cover the meaning reflected in the current use of the term, free of possible errors. To describe such a concept in a textbook or compendium, both its definition and the algorithms to calculate its value should be listed; definition first, algorithms afterwards.

What can we do to obtain a good definition in a normative IUPAC work? Quite a lot: (a) Analyze the history of the term, of its meaning, of its use. (b) Analyze the current use of the term (the IUPAC principle of reflectivity) in all grammar forms while looking for possible mistakes or inconsistencies in that use. (c) Analyze composed terms related to the term in question. (d) Analyze a lot of examples—those that fit the term and those that do not—in order to identify the validity limits of the term or the algorithm. (e) Have collaborators who cover the needed competence span and have no conflict of interest about the term being defined. And all that can be fun too!

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The International Year of Basic Sciences for Sustainable Development 2022: WE NEED IT MORE THAN EVER

A message from Michel Spiro

For almost a year and a half now, the world has been disrupted by the COVID-19 pandemic caused by the SARS-CoV-2 virus. But how much worse could the situation have been without the progress and results produced for decades, even centuries, by curiosity-driven scientific research?

We deplore the many deaths due to COVID-19, and the future is still very uncertain, especially with the detection of new variants, some of which are spreading more quickly. But, in the first place, how could we have known that the infection was caused by a virus, what this virus looks like and what its genetic sequence and variations are without basic research? Viruses were discovered at the beginning of the 20th century, thanks to the work of Frederick Twort, Félix d'Hérelle and many others. The first electron microscope was built in the 1930s by Ernst Ruska and Max Knoll; and DNA sequencing began in the mid-1970s, notably with research by the groups of Frederick Sanger and Walter Gilbert.

We could continue such a list, with basic research at the root of tests, treatments, vaccines, epidemiological modelling, *etc.* We even owe high-speed, long-distance communications, which allow us to coordinate the fight against the pandemic and reduce interruptions in education, economic activities, and even the practice of science, to the discovery and study of electromagnetic waves and optic fibers during the 19th century, and to the development of algorithms and computers codes during the 20th century. The COVID-19 pandemic is a reminder (so harsh and brutal that we would have preferred to have been spared) of how much we rely on the continuous development of basic sciences for a balanced, sustainable and inclusive development of the planet.

On many other issues, basic sciences have an important contribution to make to progress towards a sustainable world for all, as outlined in Agenda 2030 and its 17 Sustainable Development Goals, adopted in September 2015 by the United Nations General Assembly. They provide the essential means to address major challenges such as universal access to food, energy, and sanitation. They enable us to understand the impacts on the climate, and on life on Earth and in aquatic environments of the nearly 8 billion people currently living on the planet, and to act to limit and reduce these impacts.

Indeed, unlike our use of natural resources, the development of the basic sciences is sustainable *par excellence*. From generation to generation, it builds up a reservoir of knowledge that subsequent generations can use to apply to the problems they will face, which we may not even know about today.

The International Year of Basic Sciences for Sustainable Development (IYBSSD) will focus on these links between basic sciences and the Sustainable Development Goals. It is proposed to be organized in 2022 by a consortium of international scientific unions and scientific organizations led by IUPAP, and including IUCr, IMA, IMU, IUBS, IUGG, IUPAC, IUHPST, IUMRS, IUVSTA; CERN, IRD, IIASA, EPS, JINR, NuPECC, ICTP, ISC, Rencontres du Vietnam, SCOR, SKAO, and SESAME, with the recommendation of a resolution voted by the UNESCO General Conference during its 40th session in 2019. Over 50 national and international science academies and learned societies and around 30 Nobel Prize laureates and Fields Medalists also support this initiative. The Dominican Republic agreed to propose a resolution for the promulgation of the International Year during the 76th session of the United Nations General Assembly, beginning in September 2021.

We very much hope that scientists, and all people interested in basic science, will mobilize around the planet and take this opportunity to convince all stakeholders (the general public, teachers, company managers, policymakers, *etc.*) that through a basic understanding of nature, inclusive (especially by empowering more women) and collaborative well-informed actions will be more effective for the global common interest. We especially invite all chemists and their organizations to create or join national IYBSSD 2022 committees to organize events and activities during this international year.

More information, as well as communication material, can be found at www.iybssd2022.org. This will also be shared through social media accounts (look for @iybssd2022 on Facebook, Twitter, LinkedIn and Instagram). You are also invited to subscribe to the Newsletter at https://www.iybssd2022.org.

Michel Spiro is President of the International Union of Pure and Applied Physics (IUPAP) and President of the Steering Committee for the proclamation of the International Year of Basic Sciences for Sustainable Development in 2022 (IYBSSD 2022)

On good reporting practices for property measurements

by Ala Bazyleva and John P. O'Connell

Have you ever said, "Eureka! This citation should contain precisely the experimental data I need to quantitatively prove my theory and to design the novel process it enables."? But then, when you examine the full article, you find that no numbers are given, only graphs. Or maybe there are tables of values, but the units are not specified. Perhaps the data are not original, but their source is not given. Closer inspection might reveal that derived property values of little interest are tabulated, but no primary data to get properties of your interest are provided. Your frustration grows when you recognize that the experiments were probably done carefully, but the reporting of the results leaves so many omissions and uncertainties that you cannot confidently use the results.

If this has been your experience, you might relate to the scenario of the video, "Data Sharing and Management Snafu in 3 Short Acts" from the NYU Health Sciences Library [1].

Unfortunately, these situations occur far too often in the scientific literature across all disciplines. A huge amount of valuable information has been, and continues to be, lost forever because their publications were incomplete or imprecise. We have gathered a large number of real publications with inadequate data reporting of experiments on thermophysical and thermochemical properties. Here are a few representative examples:

- Researcher A had a research grant to find a solvent for a specific practical application. As part of the research, many solubilities were measured, but no values were published. Rather, only a discussion of the relative suitability of different chemical classes of potential solvents was presented, so no applications could be done.
- Researcher B studied heat capacities of novel substances with precise adiabatic calorimetry having a relative uncertainty of ± 0.1 %. However, all that was published were plots of poor resolution over a wide range of temperature. Digitization could only yield degraded data, so the extra effort for precision was wasted.
- Researcher C measured vapor pressures for several organic compounds yet published only derived enthalpies of vaporization and Antoine equation parameters with no units or the valid temperature range. Moreover, some correlation parameters were misprinted, preventing any reliable use of the work.
- Researcher D measured and published enthalpies of dilution of electrolyte solutions but did not indicate whether they were based on moles of solute, of added solvent, or of something else. All attempts to interpret those data in a meaningful way failed, and research that was potentially valuable for modeling electrolyte solutions was wasted.
- Researcher E studied a mixture of water with a partially miscible deep eutectic solvent (DES) made from compounds A and B in a molar ratio of 1:2. The listed mole fractions of DES in the aqueous solutions did not give a basis for the results (1 mole of {A +2B} or of {1/3A + 2/3B}), resulting in a factor of three ambiguity in the reported compositions. Also, the report did not address the fact that the components of the DES could be nonuniformly distributed between co-existing phases.
- Researcher F published solubilities of industrially important gases in water and organic solvents but did not mention the origin and nature of those values: measured, predicted, or taken from another document. This issue has also been found in reports of thermodynamic properties of explosives where enthalpies of formation, combustion, decomposition are predominantly published without any traceability.
- Expert X has a full-time assistant who digitizes plots of alloy property data from journal articles for use in model development. If the original researchers had published numerical values, not only would the claimed accuracy be preserved, but also a tremendous amount of time and resources would be saved.

Reader: "What I need is the data. Can I have a copy of your data?" Author: "Everything you need to know is in the article." Reader: "No... I think I cannot use your data". Reproduced from [1] by permission from Karen L. Yacobucci (NYU Health Sciences Library)

The sadness of these situations is that though the measurements may have been carefully done, if the data communication is flawed, everyone loses. The original workers, and their sponsors, do not get appropriate credit, while users waste time attempting to uncover needed information that may not actually be in the publication. The result can even be needless replication that is expensive in labor and equipment. Further, as technology advances, data can be useful for purposes beyond the original intention. Thus, chemical engineers can employ them to design chemical processes, build models, assess process safety, *etc.* But incomplete or ambiguous reporting will hamper such practical advances.

The existence of the problem was acknowledged some years ago [2], and specific recommendations were developed [3]. But the efforts did not significantly change the situation. That is why a large group of data users and experts in experimental methods joined an IUPAC project to develop the **Good Reporting Practice Principles** for experimental property data [4] to inform all parties involved in the scientific process (funding agencies, publishers, and researchers). Those principles are:

1. Measured property data should be published in a numerical format (at least in a supplement).
2. Published data should be well defined (including system, state, and property).
3. All published data should be traceable to their origin.
4. Observations should be distinguished from interpretation.
5. Auxiliary (calibration) data should be identified and provided.
6. Necessary details of experimental methods or computation procedures should be given.
7. Uncertainty in each measured value should be reported and justified.
8. Importing reported data into analysis software should be easy and straightforward.
9. Complex mathematical equations should be provided in a machine-readable form.

Also recommended was that corrigenda should be immediately submitted, with prominent visibility from the main publication web page as soon as errors are detected.

Justification for each principle is detailed in the IUPAC Technical Report [4] and its Appendix includes specific examples.

The report also recognizes that well-designed research should solve problems rather than create them. Sometimes problems can be revealed but not immediately solved; however, well-designed research should minimize the number of remaining questions. Therefore, **Elements of Good Research Practice** have also been included in [4] because reporting issues are frequently tied with the design of experiments. Best reporting might require conducting additional experiments before publication. Following these elements can avoid delays and confusion in properties communication. The **Good Research Practice elements** are in the following areas:

- Content (planning): For example, measurements should be made of limiting behavior to provide a basis for consistency checks and model development.
- Methodology (procedure): The accuracy and reliability of the method and apparatus should be confirmed on well-studied test systems over the whole range of conditions of the study. This element also includes material stability, hygroscopicity, and proof of identity of newly synthesized compounds.
- Validation: Thermodynamic consistency of the measured values and comparisons with previously published results should be checked.

The Technical Report [4] is not a checklist to be followed for each publication of experimental results, though some properties journals have instituted this responsibility for authors (see references [18] and [19] in [4]). Rather, it is intended as advice for consideration when developing publications.

The principles and elements were developed for the thermophysical/thermochemical fields, but equally apply to other areas of science, as in the video cartoon about medical literature [1].

The Task Force team is initiating efforts to publicize the report, to encourage journals that publish data to educate their authors and reviewers about these techniques of good reporting and research practices, and to suggest that funding agencies include the principles in their proposal materials.

The report [4] concludes, "Acceptance of the Principles would assist in more complete transfer of the knowledge acquired in scientific research. In addition, greater efficiency would be made of the funds distributed for that research to benefit the entire community of taxpayers, readers, and users, as well as the researchers themselves." These are important goals for contemporary science and technology.

The Technical Report [4] was prepared within the framework of IUPAC project (https://iupac.org/

project/2019-013-1-100), "Good Reporting Practice for Thermophysical and Thermochemical Property Measurements."

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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 relating to Electronic Photonic and Magnetic Properties of Polymers

These recommendations are specifically for polymers and polymer systems showing a significant response to an electromagnetic field or one of its components (electric field or magnetic field), *i.e.*, for electromagnetic-field-responsive polymer materials. The structures, processes, phenomena and quantities relating to this interdisciplinary field of materials science and technology are herein defined. Definitions are unambiguously explained and harmonized for wide acceptance by the chemistry, physics, polymer and materials science communities. A survey of typical electromagnetic-field responsive polymers is included.

Keywords: electric properties; functional polymers; magnetic properties; molecular electronics; optical properties; organic electronics

Comments by 31 August 2021

Corresponding Author: Jiri Vohlidal <vohlidal@natur.cuni.cz>

Glossary of Physical Organic Chemistry

This Glossary contains definitions, explanatory notes, and sources for terms used in physical organic chemistry. Its aim is to provide guidance on the terminology of physical organic chemistry, with a view to achieving a consensus on the meaning and applicability of useful terms and the abandonment of unsatisfactory ones. Owing to the substantial progress in the field, this 2021 revision of the Glossary is much expanded relative to the previous edition, and it includes terms from cognate fields.

Comments by 30 September 2021

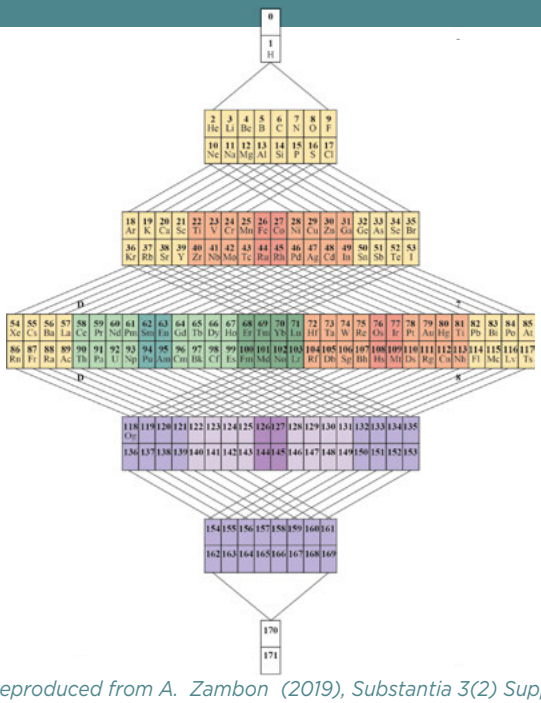
Corresponding Author: Charles L. Perrin <cperrin@ucsd.edu>

The Period System, a history of shaping and sharing

reviewed by Brigitte Van Tiggelen and Annette Lykknes

The International Year of the Periodic Table of the Chemical Elements (IYPT) has witnessed an increase in publications on a topic that was already popular in the literature. As expected, the history of its development, and the discussion about its representation, were the most frequent aspects covered in these publications. To many observers, the fact that 150 years after the Periodic System (PS) proposed by Dmitri Mendeleev and Lothar Meyer is still in use is a testimony to its intrinsic validity. However, the concept of the system as well as of other constitutive notions such as element atom, or matter, have all evolved over a century and a half, and the PS now in use is the result of a continuous reworking in symbiosis with these developments to keep performing as the universal tool it has become. The special issue of *Substantia:* **"The Periodic System, a history of shaping and sharing"** (full online open access) with its introduction https://riviste.fupress.net/index.php/subs/article/view/737/332) edited by Brigitte Van Tiggelen, Annette Lykknes, and Luis Moreno Martinez focuses on that process of reworking which explains several features in the history of the PS that are generally unknown, ignored and under-investigated.

One of these features is the teaching context which was central for the making AND the sharing of the new system of classification. Both Mendeleev and Meyer produced their ordering of chemical elements while they were writing a textbook, and whereas this is often acknowledged, how the new system permeates from their work into the classroom where it is so ubiquitous now, is another question that is usually left aside. It might thus come as a surprise to many contemporary chemists that the introduction of the periodic tables in textbooks and even more their implementation in chemical education only really took off after the beginning of the 20th century. In the special issue these aspects pertaining to the early development of the PS in the pedagogical context are covered by three contributions: one dedicated to the often forgotten work of Lothar Mayer (by Gisela Boeck), another on the early responses in the Portuguese community (by Isabel Malaquias and João A. B. P. Oliveira) and a third one on a precious wall chart acquired in 1888 at St Andrews, UK (by Alan Aitken and M. Pilar Gil). To complement this perspective, two other contributions analyze the way the history of the PS is presented in textbooks in Spain and Norway (by Luis Moreno Martinez and Annette Lykknes) and Ethiopia (by Gebrekidan Mebrahtu Tesfamariam and Mengesha Ayene). They analyze how these occurrences shape not only the central place of the PS in the teaching but also conveys something about the way chemistry developed.



Reproduced from A. Zambon (2019), Substantia 3(2) Suppl. 4: 101-114. doi:10.13128/Substantia-502

The other feature scrutinized in this issue, which is deeply connected with pedagogy, is the plasticity of the PS. The term plasticity refers to the quality of the PS to constantly undergo reform in tune with new understanding of matter and its constitution, but also to be repurposed and adjusted to different needs and level of readings and use. One contribution describes the limited success at standardization by IUPAC (by Ann Robinson). Two other contributions stress new approaches that might help reintroduce chemistry where explanation are usually made in quantum mechanical—and relativistic terms—periodicity trees for secondary school education (by Alfio Zambon) and the computerized reconstruction of groupings of elements by analysis of chemical knowledge in 1869 and now (by Guillermo Restrepo).

All this explains why the discussion on the "best" representation of the PS into a tabular format will probably remain vivid for a long time, and to some extent is an intrinsic part of the process that leads the PS. If indeed the endurance of the Periodic System is due to its ability to be reshaped over time then there is no such thing as the final version, and this is good news for this scientific icon that is will probably stay relevant for another century.

https://riviste.fupress.net/index.php/subs/issue/view/35

IUPAC/CITAC Webinar "Metrology, quality assurance and chemometrics—Correlation of test results and mass balance influence on conformity assessment"

by **Ilya Kuselman**

Since the biannual IUPAC/Cooperation on International Traceability in Analytical Chemistry (CITAC) Workshop on metrology, quality and chemometrics scheduled for January 2021 in conjunction with Isranalytica, Israel, was postponed to Jan 2022 because of COVID-19 a Webinar was organized as a Zoom meeting on 21 January 2021, hosted by NRC, Canada.

The webinar started with the opening remarks and welcoming by Zoltan Mester, NRC, IUPAC ACD President, and CITAC Vice-Chair. Then, participants heard a CITAC update—a foreword given by Bernd Güttler, PTB, Germany, CITAC Chair. Michela Sega, INRIM, Italy, and CITAC Past Chair, spoke about CITAC as a stakeholder of the IUPAC project on mass balance influence on conformity assessment. After her welcoming, Sega continued in the role of the Webinar moderator. Four overview lectures were provided.

Ilyav Kuselman

Ilyav Kuselman, Independent Consultant on Metrology, Israel, (https://orcid.org/0000-0002-5813-9051), gave a lecture on IUPAC/CITAC Guide: *Evaluation of risks of false decisions in conformity assessment of a multicomponent material or object due to measurement uncertainty* and correlation of test results. The Guide was developed by the IUPAC project task group consisting of Francesca R. Pennecchi, INRIM, Italy; Ricardo J.N.B. da Silva, University of Lisbon, Portugal; and D. Brynn Hibbert, UNSW Sidney, Australia; and chaired by Kuselman (https://iupac.org/project/2018-004-1-500). The work was supported by CITAC. In this Guide, risks of a false decision on conformity of the chemical composition of a multicomponent material or object due to measurement uncertainty are defined using the Bayesian approach. Even if the conformity assessment for each particular component of a material is successful, the total probability of a false decision (total consumer's risk or producer's risk) concerning the material as a whole might still be significant. This is related to the specific batch, lot, sample, environmental compartment, or other item of material or object (specific consumer's and producer's risks), or to a population of these items (global consumer's and producer's risks). When the actual values of the components' concentrations or contents, as well as the measured values, are correlated, they are modelled by multivariate distributions. The effect of correlation on the risks is not easily predictable. Examples of the evaluation of risks are provided in the Guide for conformity assessment of denatured alcohols, total suspended particulate matter in ambient air, a cold/flu medication, and a PtRh alloy.

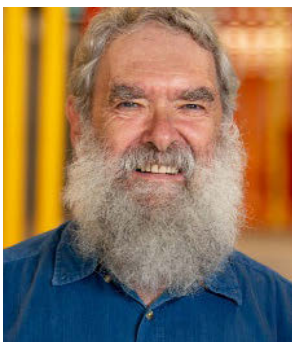
Francesca R. Pennecchi

Francesca R. Pennecchi, INRIM, Italy, (https://orcid.org/0000-0003-1328-3858), discussed in her lecture the influence of a mass balance constraint on risks in conformity assessment of substances and materials. She said that the IUPAC/CITAC Guide *Evaluation of risks of false decisions in conformity assessment of a multicomponent material or object due to measurement uncertainty* offers a general Bayesian approach for evaluating the risks of false decisions in conformity assessment of multicomponent materials or objects. When components of such substances are linked by a mass balance constraint (*i.e.*, the sum of their mass fractions, molar fractions or any other positive quantity ratios is 100 % or 1), test results of the components' contents are named "compositional data." These data are always correlated, because of the constraint. Such correlations, being named "spurious", may influence measurement uncertainty of test results as well as risks of false decisions in conformity assessment of a substance or material. That is important in testing geological and environmental objects, products of metallurgical and food industries, etc. A special case is the evaluation of purity of substances by an indirect method based on a mass balance, and development of corresponding (pure) certified reference materials. IUPAC project 2019-012-1-500 is under development now with the aim of studying how to deal with mass balance constraint in conformity assessment. A Bayesian multivariate approach is applied to different scenarios of the data modelling, based on a Monte Carlo method that includes the mass balance constraint.

Angelique Botha, NMISA, South Africa, (https://orcid.org/0000-0003-3987-359X), gave an overview

Angelique Botha

of development of the ISO/REMCO guidance, and in particular for the production of high purity reference materials. The ISO Committee for Reference Materials (ISO/REMCO) has actively been updating its guidance documents over the past eight years. Since the conversion of the third edition of ISO Guide 34 to the international standard ISO 17034 to address the conformity assessment of reference material producers, the work of the committee has focused on the revision of ISO Guide 35 and the development of up-to-date guidance for the users of reference materials. In 2014, a guidance document, ISO Guide 80, for the in-house preparation of quality control materials was published by the committee. The third edition of ISO Guide 33 *Reference materials—Good practice in using reference materials* was published early in 2015. While the previous edition focused on the use of certified reference materials, the new one relates to all types of reference materials and their uses. The prospects for the future work of the committee include the development of more field specific guidance. At the beginning of 2018 a proposal was approved for the development of a guidance document for the production of qualitative reference materials (ISO Guide 85). Two new proposals (ISO Guide 86 and ISO Guide 87) were also approved for the development of harmonized guidance for the preparation of high purity reference materials for small organic molecules as well as metals and metalloids, respectively.



D. Brynn Hibbert

The lecture of D. Brynn Hibbert, School of Chemistry, UNSW Sydney, Australia, (https://orcid.org/0000-0001-9210-2941), was on metrology and the law: presenting chemical measurements to the courts. In Australia, an expert is bound to help the court no matter who is paying. Expert conferences are encouraged so that complex science can be presented to allow the "trier of fact" to make a properly informed decision. In particular, for example, the issue is often one of conformity assessment—is the driver over the legal limit for alcohol? Three examples from the author's case book will show how reliable measurements have been crucial to providing justice. First, a racing horse is not allowed to have more than 100 ng/mL of cobalt in its urine. In a landmark case the court accepted a statistical distribution of cobalt mass concentrations that allowed calculation of the probability of an 'ordinary horse' having a mass concentration greater than the legal threshold. Second, illegal 'meth labs' are found in most countries. While the identity of the product ('ice' or N-methylamphetamine hydrochloride) is often not in dispute, the amount of drug synthesised determines the length of the custodial sentence. Measurement of purities, and thus mass of drug, requires proof that the sample analysed was representative of the item seized. Estimation of potential yields from seized precursors also has a bearing on indictable amounts. Finally, in a recent cold-case murder, the author successfully argued against the admissibility of lead isotope analysis results that matched bullets in a body to bullets in a box of bullets in the possession of one of the accused. Was the method properly validated? And does the chemical match actually prove the body bullets came from the box?

The number of the participants from different countries and continents varied during the Webinar from about 130 to 200. They had a possibility for questions, and the interaction with the lecturers was interesting. The Zoom event was recorded and published on YouTube, https://www.youtube.com/watch?v=3mZM-v6hwDMY. Corresponding links are available on IUPAC webpage https://iupac.org/event/metrology-quality-and-chemometrics/ and CITAC website www.citac.cc (Conferences & Workshops).

Reprint from CITAC News April 2021, p. 72, https://iupac.org/event/metrology-quality-and-chemometrics/

International Polymer Characterization Conference—POLY-CHAR 2020 (Venice)

by Chin Han Chan, Holger Schönherr, and Valerio Causin

POLY-CHAR 2020 [Venice] is an International Polymer Characterization Conference, under the auspices of the Scientific Committee of POLY-CHAR and IUPAC.

This event, which was originally scheduled for May 2020, but was postponed due to the pandemic, was held, for the first time in virtual format, from 12–14 April 2021. This conference was hosted by the University of Padova, Italy.

Due to the worldwide travel restrictions, it was not possible to meet physically, *i.e.* to experience lectures and discussions in a real conference hall, to exchange ideas over a coffee during the breaks and to discuss together next to the posters. The extra work needed for the scientific research activities coupled with *e*-teaching or even *e*-research was absolutely enormous during the pandemic emergency. The scientific committee as well as the organizing committee of POLY-CHAR were extremely grateful for the participation of many excellent speakers from interdisciplinary fields (*e.g.* physicists, chemists, materials scientists, biologists *etc.*) from all 5 continents, sharing their research findings from theoretical to experimental as well as from fundamental to applied aspects of polymers. The areas of expertise explored in the program spanned from materials science to medicine, from nutrition to forensic science, from nanotechnology to 3D printing, *etc.* Participants were heroic in overcoming the time-zone differences, attendance was always very high and, even if in virtual form, attendees kept this fabulous POLY-CHAR saga active. Of course, everybody's wish was that travel restriction will be lifted soon.

A total of 8 plenary speakers, 27 invited speakers, 57 oral speakers, 8 poster presenters and 100 participants from 27 countries with 75 international participants participated in POLY-CHAR 2020 [Venice].

The conference presentations were organised under the core themes of:

- Polymers and the environment: Recycling and land remediation
- Applications of polymers: food, forensics, adhesives, coatings and preservation of cultural heritage
- Characterisation of polymers
- Mechanics of polymers—Nanoindentation
- 3D printing
- Polymer physics, theory and simulations
- Synthesis of polymers
- Biopolymers, biomedical materials and biotechnology
- Nanomaterials and smart materials

The **POLY-CHAR prizes for the Best Oral Presentations** were awarded to:

- Veronika Gajdosova, Institute of Macromolecular Chemistry, Academy of Sciences of the Czech Republic, for her work on *Antioxidant and pro-oxidant activity of phenolic stabilizers during photooxidation of polyolefins revealed by microscopic methods*
- Anna Liguori, University of Bologna and INSTM, Italy, for her work on *Hybrid composite scaffolds for spinal interbody fusion*
- Zhiqiang Zeng, University of Science and Technology of China, China for his work on *Investigation of multifunctional triphenylamine Schiff-base compounds towards electrochromic applications*

Group photo of the virtual conference

Two **IUPAC Awards for Best Student Posters** were presented to:

- Zrinka Buhin Šturlić, University of Zagreb, Croatia for her work on *PCL/nano-ZnO protective coatings for metals*;
- Yu Jeong Bae, Kyungpook National University, Korea for her work on *Structural characteristics and properties of silk/rayon webs and non-woven fabrics*.

One **POLY-CHAR Prize for the Best Student Poster** was awarded to:

- Laura Dehondt, Tweed Research Center, Onyx Développement SAS, Groupe Nutriset, France for her poster *Optimization of the starch extraction in Cyperus Esculentus to increase the digestibility of a tigernut-based juice*

The next POLY-CHAR conferences were planned as follows: *virtual* POLY-CHAR 2022 [Siegen & Halle], Germany in May 2022 and POLY-CHAR 2023 [Auckland], New Zealand in January 2023.

Chin Han Chan is from the Universiti Teknologi MARA, Malaysia. Holger Schönherr is from the University of Siegen, Germany. Valerio Causin is from the University of Padova, Italy.

Impact of Artificial Intelligence on the Future of Chemistry

Join Us for a Global Discussion on the Impact of Artificial Intelligence on the Future of Chemistry: An Innovative Format for 2021 World Chemistry Leadership Meeting.

The last eighteen months have been a roller coaster ride for all of us. Zoom, Go-to-Meeting, Webex, and other video-teleconferencing tools - perhaps not routinely used in the past have become extensions of our technological skills and for the most part are used on a daily (if not hourly!) basis. As you probably know by now, it has been determined that the 2021 IUPAC World Chemistry Congress (WCC) will be a purely virtual event due to the worldwide pandemic. Rather than consider this to be a negative outcome, it was decided to leverage this as an opportunity to do something unique and innovative that will allow the World Chemistry Leadership Meeting (WCLM) to reach a much larger portion of the global scientific community than is the norm at an in-person meeting. So here is what is currently planned.

First, the WCLM has a very forward-looking topic —*the Impact of Artificial Intelligence on the Future of Chemistry* [1]. Six general topics will be discussed at events around the globe:

- **Discovery:** Processes and Tools of the Future
- **Determination:** Candidates for Process Development and Optimization
- **Development:** Products and services using AI in the Future
- **Impact:** R&D Laboratories and Instrumentation of the Future
- **Information:** Informatics, Datasets and Curation of the Future
- **Insight:** Analysis and Modeling Chemical Research of the Future

One unique aspect of the WCLM will be the format. This event will be a twenty-four hour worldwide discussion, beginning with a live kick-off in Montréal, Canada at 8:00am EDT on **17 August 2021,** with opening remarks and a plenary lecture by Yoshua Bengio, Founder and Scientific Director of Mila – Quebec AI Institute. The WCLM will then be handed-off to Malaysia (the site of the 2025 WCC) where the discussion will continue. This will be followed by a hand-off to The Netherlands (site of the 2023 WCC) for further discussion, and then the WCLM will return to Montréal, Canada for the closing session with a wrap-up panel and a lecture by Jeremy Frey, Head of Computational Systems Chemistry and Principal Investigator for the AI Scientific Discovery Network at the University of Southampton.

Six speakers have been invited. Each will address one of the topics listed earlier via a fifteen-minute video that will be made available to all those registered for the Congress at least one week before the WCLM opens. You will have plenty of time to view the videos in advance if you wish to do so. The will also be live-streamed during the WCLM. During the closing program all six speakers will present a live five-minute summary of their topic and the floor will then be opened for a Q&A session of about forty-five minutes. The WCLM will then close with a plenary lecture.

It is expected that the live sessions in Malaysia and The Netherlands will also be recorded and made available for viewing by registrants. Also, even though there is limited time during the closing session, the goal is to capture and answer all posted questions with the compilation being made available to Congress registrants.

The objective of this topical and innovative program is to shed some light on how the global community of chemical researchers currently perceive as the challenges and opportunities offered by AI and what that might mean for the future of Chemistry... and of IUPAC.

The WCLM Organizing Team

Chris Ober, Chair; Jeremy Frey, Bonnie Lawlor, Leah McEwen, Fabienne Meyers, and Lynn Soby

1. A feature recently published in *Chem Int* echoed the WCLM topic: Lawlor, Bonnie. "Artificial Intelligence and Machine Learning" *Chemistry International,* vol. 43, no. 1, 2021, pp. 8-13. https://doi.org/10.1515/ci-2021-0103

https://iupac.org/event/wclm2021/

Timeline of events in local time:

Event	Montréal (EDT)	Netherlands (CEST)	Malaysia (MYT)
Opening program	8:00am, 17 August 2021	2:00pm, 17 August 2021	8:00pm, 17 August 2021
Malaysia program	9:00pm, 17 August 2021	3:00am, 18 August 2021	9:00am, 18 August 2021
Netherlands program	3:00am, 18 August 2021	9:00am, 18 August 2021	3:00pm, 18 August 2021
Closing program in Montréal	9:00am, 18 August 2021	3:00pm, 18 August 2021	9:00pm, 18 August 2021

IUPAC

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