# CHEMISTRY International

October-December 2021 Volume 43 No. 4

# Putting the A in STEM



INTERNATIONAL UNION OF PURE AND APPLIED CHEMISTRY Restructuring IUPAC

Top Ten Emerging Technologies in Chemistry 🕨



# Chemistry International

#### **CHEMISTRY** International

The News Magazine of the International Union of Pure and Applied Chemistry (IUPAC)

All information regarding notes for contributors, subscriptions, Access, back volumes and orders is available online at www.degruyter.com/ci

#### Managing Editor:

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

Design/Production: Stuart Wilson Printed by: Sheridan Communications

#### Subscriptions

Chemistry International (ISSN 0193-6484) is published 4 times annually in January, April, July, and September by De Gruyter, Inc., 121 High St., 3rd Floor, Boston, MA 02110 on behalf of IUPAC. The 2021 subscription is USD 74.00 for individuals or USD 116.00 for institutional subscription. Special rates for Print and Print + Online are available for IUPAC Members and Affiliates Members; see https://iupac.org/what-we-do/journals/ chemistry-international/ or https://www.degruyter.com/ci for more information.

#### ISSN 0193-6484, eISSN 1365-2192

Periodicals postage paid at Durham, NC 27709-9990 and additional mailing offices. POSTMASTER: Send address changes to Chemistry International, IUPAC Secretariat, PO Box 13757, Research Triangle Park, NC 27709-3757, USA.



M

COOSS 02021 International Union of Pure and Applied Chemistry. This work is licensed under a Creative Commons Attribution-NonCommercial-NoDerivatives 4.0 International License.

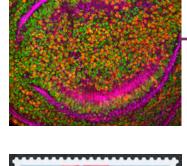
Cover: Putting the A(rt) in STEM has always been a topic of interest for this editor. Therefore, it was a treat to realize this past summer that the IUPAC Congress was no stranger to the scene. See page 46 for more details. This cover of *CI* is the hundred and second in color and the last put "on the press." From 2022 on, CI will be online only. It is the editor's personal satisfaction to close this CI chapter with an A on the cover.

### **Global Women's** Breakfast 2022 February 16, 2022



iupac.org/gwb

#### U S DGS U S







#### CHEMISTRY International October-December 2021 Volume 43 No. 4

#### Features

	Restructuring IUPAC at the Turn of the 20th Century by Edwin D. (Ted) Becker interviewed by Brigitte Van Tiggelen	2
	Systems Thinking and Sustainability by Peter Mahaffy,     Stephen Matlin, Marietjie Potgieter, Bipul Saha, Aurelia Visa, Sarah Cornell,	6
	Felix Ho, Vicente Talanquer, Jane Wissinger and Vania Zuin IOCD turns 40: The future of the chemistry	11
	<ul> <li>for sustainable development by Federico Rosei and Stephen A. Matlin</li> <li>IUPAC Top Ten Emerging Technologies in Chemistry 2021 by Fernando Gomollón-Bel</li> </ul>	13
	IUPAC Wire	
	Chemistry International—Freely-Available Across the World IUPAC Announces the 2021 Top Ten Emerging Technologies in Chemistry	21 21
	Climate Change 2021—The Physical Science Basis	22
	2022 IUPAC-Richter Prize—Call for Nominations	23
	Awardees of the 2021 IUPAC-Zhejiang NHU International Award for Advancements in Green Chemistry	23
	An Interview with Joseph Wang	24
	In Memoriam: Gus Somsen In Memoriam: Aubrey Dennis Jenkins	25 26
	Up for Discussion	
	Combat Ethical Pollution in the Chemical Community by Leiv K. Sydnes	29
	Project Place	
	Safety Training Program e-learning	32
	Green Chemistry in Sub-Saharan Africa	32
	Categorizing Interactions Involving Group 11 Elements Recommendations for terms relating to materials characterization: Latin and other introduced terms	32 32
	IUPAC Provisional Recommendations	33
	Making an imPACt	
	Glossary and tutorial of xenobiotic metabolism terms used during small molecule drug discovery and development	34
	Interpretation and use of standard atomic weights	34
	Glossary of methods and terms used in analytical spectroscopy	34
	The Gender Gap in Science: PAC Special Topics Issue	34
	Reference materials for phase equilibrium studies. 1. Liquid-liquid equilibria	35
	Special CTI on Polymer Sciences	35
,	Stamps International	37
	Conference Call	
	Snow Cover, Atmospheric Precipitation Aerosols: Chemistry and Climate	38
	Educational Workshop in Polymer Sciences 2020+ in conjunction with MACRO2020+, Jeju Island	41
	Where 2B&Y	
	CHEMRAWN in Action—This Time with E-waste in Focus	42
	Poetic Science An Ode to IUPAC by Jeremy G. Frey	45
	From the Cover	46
	Index	47

# Restructuring IUPAC at the Turn of the 20th Century

#### by Edwin D. (Ted) Becker interviewed by Brigitte Van Tiggelen

round the turn of the century IUPAC undertook a major restructuring. Commissions, which had been the heart of IUPAC's scientific work for most of its 80-year history, were virtually eliminated and largely replaced with a system of peer-reviewed projects [1-3]. Brigitte Van Tiggelen asked Ted Becker, Secretary General in that key transition period (1996-2003) and a central figure in the restructuring effort, to reflect on the rationale for this significant change and to describe just what was done.

#### Brigitte: So, what was wrong with commissions?

Ted: In principle, nothing! My experience was that most commissions worked very well, with really dedicated members who worked hard. I was a commission chairman for six years, and I was pleased with what we and other commissions accomplished. The problem was that the entire system of commissions, as it had evolved, was unsustainable in terms of (i) number of commissions; (ii) financial resources devoted to maintaining commissions; and (iii) methods for selecting commission members. In addition, the actual projects

to be undertaken by a commission were chosen by the commission members at each meeting without much real thoughtoften because a single member was enthusiastic and volunteered to do the work. At any given time, there were nearly 500 "active" projects, some of President J. Benard which dragged on for 8 to 10 years.

#### Brigitte: Will you elaborate on these issues.

Ted: First, about the numbers. In 1997 there were 37 commissions, each devoted to a particular aspect of chemistry-e.g., organic nomenclature, spectroscopy, analytical reagents, clinical toxicology-but there were many more emerging areas of chemistry not represented. There was understandably constant pressure to create new commissions, but it was almost impossible to disband an existing commission because that was tantamount to declaring that particular chemistry specialty no longer of any importance-a conclusion that was usually incorrect. IUPAC presidents had long voiced concern about the increasing number of

commissions. As early as 1955 President

Sident A. Tiselius

Arne Tiselius (1951-1955) pointed to the problem of continuing commissions devoted to continuous surveys of a particular field [Fennell, ref. 2, p 142]. In 1973 President Jacques Bénard (1971-1973) said that "it is easy to obtain general approval for the creation of new bodies, but it is difficult to decide to abandon existing ones." [Fennell, ref. 2, p 222] Such comments were echoed almost every year.

Reflecting about the financial resources and the support of members. Each commission was composed of titular members (TMs)-initially 10 per commission, later cut to eight. IUPAC agreed to pay travel expenses for TMs to the biennial General Assembly and often to a commission meeting in intervening years. Commissions also elected associate members and national representatives, who were able to cover travel expenses outside IUPAC, but TMs were at the heart of commissions and the number of TMs became a kind of "currency" within IUPAC because each TM involved a considerable financial commitment.

TMs were selected by each commission to fill vacancies, as they occurred, from experts in the field, with particular concern about geographical distribution and often concern about sub-specialties. This worked well to bring together knowledgeable people to assess issues in a field and to decide how IUPAC could con-

tribute. However, the result was a small number of "insiders" for a given subject. In fact, in 1981 President Heinrich Zollinger (1979-1981) complained about "the involvement of too small a circle of chemists in IUPAC work-a

a dent H. Zollinger

reporter in Davos [30th General Assembly] even called this circle a 'charmed

(19

circle'." [Fennell, p. 293] A reform effort was initiated by President Allen Bard (1991-1993), beginning in 1993. The size of commissions was further reduced, and a "pool" of TMs created that would, it was hoped, be assigned temporarily to a commission to work on specific high-priority projects. Allocation of the pool TMs each year was the responsibility of the IUPAC Officers and Division presidents collectively.

#### Brigitte: How did you become involved?

Ted: As the new Secretary General, my first encounter with the pool TM process was in 1996. I found it frustrating! A dozen officers spent hours debating potential specific projects that most of us knew little

about. In the end,  $e_{A,J,Bard}(199)$  a few TMs were allocated to temporarily

enlarge some commissions. Collectively, the Division Presidents (DPs) recognized the problems of too many commissions and too many projects that were not always well thought out and often dragged on for years. However, each DP understandably defended the commissions within his Division. Most DPs seemed willing to consider changes, and they reacted favorably to my brash suggestion that we use the budget, rather than number of TMs, to set priorities. The result was a special meeting of all DPs, their Division vice-presidents, and the IUPAC officers in Frankfurt in March 1997.

I thought we made some progress in Frankfurt. However, by the time that the concerns of all the Members of Commissions and Division Committees were taken into account, I realized we would have just about as many Commissions and just as many TMs. Moreover, superimposed on this structure would be the need to manage projects, allocate TMs and money, and argue over relatively small changes. We needed to change the focus by starting over—abolishing *all* commissions and establishing new commissions as needed. The Bylaws provide a means to do that: each biennium Council had to authorize the continuation of each commission, but that was almost always done as a routine matter for all commissions as a group.

The problem, of course, is that IUPAC's scientific work would virtually cease unless we could provide a better way of dealing with the actual projects themselves.

### **Brigitte:** How did you find a new approach to break the cycle without endangering IUPAC's productivity?

Ted: The special DP meeting in Frankfurt was held on Monday, March 24, 1997. John Jost and I stayed in Frankfurt on Tuesday to prepare minutes. John had just been named as new Executive Director, and this was his first exposure to the IUPAC bureaucracy and procedures. That evening John and I had dinner with Vice President/President-elect Joshua Jortner and discussed ways to improve IUPAC projects and commission operations. Joshua and I asked John how industry would deal with projects. John had been VP for Research at a large petrochemical corporation. John told us that in response to a serious problem, a project team would be formed from people with relevant expertise in the corporation's various departments-for example, from Chemistry, Geology, Legal, Engineering, etc. When the project team finished its

work, the team would be g disbanded and everyone would continue work in the departments in which they were employed and got

they were employed and got p a y checks. We recognized the analogy to IUPAC, where the expertise was in the Divisions, but everyone was a

volunteer—no pay checks—and no need to continue "employment." Perhaps, we thought, we could form temporary commissions.

Prof A.E. Fischli

Since the IUPAC Executive Committee (EC) was to meet in Jerusalem the weekend of April 5-6

Becker (1996 ranged schedule was to go to Oxford Wednesday aftenoon, spend a long week-end at the Secretariat, rather than returning to the US, then go on to Israel the following Tuesday. This turned out to be Easter weekend,

but I got a key to the offices so I could do email and print documents from my computer. I also was able to consult Roger Fennell's History of IUPAC so I could be sure of facts. I prepared a long Discussion Paper for the EC meeting, proposing that the IUPAC organization would continue to consist of Council, Bureau, EC, Standing Committees, and Divisions (including Division Committees). However, the norm would be that Commissions should not be regarded as part of the "regular" organization but rather as the temporary working groups that carry out specific projects developed by the Division Committees with the help of the Governance and the Secretariat. Divisions should regard the entire worldwide chemical community as the resource for both ideas and for volunteers to carry out projects, not the "charmed circle" of IUPAC insiders. Likewise, ideas for projects should come from the worldwide community.

I proposed that in 1999 we cease the automatic renewal of commissions, effective in 2001. During the two-year "grace" period, Commissions would continue to work on existing projects, but each Commission would have to give thought to what projects, if any, that particular group would propose for the future. Meanwhile, the Division Committees could use whatever means are available to plan projects that would utilize new Commissions.

The EC agreed with all the concepts that I had proposed, and after considerable discussion, President Albert Fischli (1996-1997) immediately appointed a committee to develop proposals [4]. This committee



Secretary General Ted Becker (left) and President Joshua Jortner, during the meeting of the IUPAC Executive Committee held in Tokyo, Japan, 24-25 April 1999.

was very carefully selected to deal with restructuring and also with the development of goals and strategy related to VP Jortner's critical assessment of IUPAC activities. Hence, we chose the name Strategy Development and Implementation Committee (SDIC), and we had specific timelines for completing the work.

### **Brigitte:** So, a new committee, but this time with a specific task!

Ted: Indeed. The SDIC met several times and worked extensively by email as well. It first completed the Strategic Plan, which was approved by the EC and published in January 1998. Then we laid out a complete scenario to convert to a project-driven system but deliberately avoided being too prescriptive, leaving it up to the Divisions to decide on many details [5].

The SDIC report was unanimously approved by the EC in April 1998, but I recognized that the big hurdle would be the Bureau in September. The Bureau had 22 voting members, of which the EC provided only eight. I felt that to make such radical changes, we had to have wider acceptance. I quietly set a goal of positive votes from at least 17 Bureau members, including at least five of seven DPs. To garner more support and to fill in more details, we set up yet another group-Committee on Project Evaluation Criteria, chaired by Bureau member Gus Somsen and comprised of five current, former or future DPs, and one former industry executive, who understood how projects should work. In addition, I took a lot of time while in Europe during the summer of 1998 to meet with almost all DPs individually. In September, after much discussion, the Bureau approved the restructuring proposal from the SDIC and EC by a vote of 20 to 0 with two abstentions [one from a DP. one an elected member of the Bureau]. The new project-driven system went into partial operation in January 1999, in conjunction with all the existing Commissions [6,7].

**Brigitte:** This seems to have moved swiftly by IUPAC standards and without many hurdles...18 months to set up a major restructuring which is unanimously endorsed!

Ted: Well the Council, which is the legal decision-making body of IUPAC, still had to validate the new organization. The final phase was two bylaw changes by Council in August 1999 to confirm and formalize the decision to move from a commission-centered system. This involved a lengthy, contentious, and quite "political" process for Council to endorse, rather than rescind, the entire restructuring. I recall this as very difficult, with daily pronouncements at the General Assembly leading up to the Council meeting and "policy statements" from the Bureau designed to counter specific complaints by opponents. At the Council meeting, President Jortner repeatedly had to publicly "guarantee" that nomenclature activities would be preserved. The key decision came on a UK resolution around which opposition had coalesced, which was treated as an amendment to a Bylaw change. It was defeated 33-74 with 24 abstentions-showing a clear majority basically in favor of the restructuring. A final vote on the restructuring proposal was then overwhelming.

**Brigitte:** You mention "nomenclature" as a core business of IUPAC to be preserved and maintained outside the new project structure. How was this specificity to be reconciled with the new structure?

Ted: Immediately after the Council meeting, we set in

#### Restructuring IUPAC at the turn of the 20th century

motion several actions to avoid what could have been the most serious shortcomings. President Jortner appointed the ad hoc Education Strategy Development Committee, chaired by Peter W. Atkins. The EC developed a budget that carefully reallocated to the Divisions and to a reserve fund the expected significant savings from full support of commission meetings. I undertook the special problems of chemical nomenclature. With the individual Nomenclature Commissions set to be abolished in two years, I thought that we needed outside advice on what IUPAC should do in nomenclature, and I worked with Alan McNaught, who had wide experience within IUPAC in the area of nomenclature and terminology, to hold a "roundtable" strategy meeting in Washington in March 2000. I deliberately did not invite any of the nomenclature experts on the current Commissions because I wanted to focus on what the broader "user community" needed in the future from IUPAC, not review the past accomplishments of the Commissions. We had participants from such organizations as Chemical Abstracts Service, the European Patent Office, the US International Trade Commission and others who really needed internationally agreed terminology in words, not only structural formulas. We also had computer experts, who were dealing with ways to connect the words and formulas by computer algorithms. Overall, I think the meeting was quite successful in assessing needs and defining general directions in which IUPAC might proceed [8]. One very important point was the [then controversial] proposal by Steve Heller (then member of the Committee on Printed and Electronic Publications and past chairman of the Committee on Chemical Databases) for IUPAC taking on a computer process being developed at the National Institute of Standards and Technology, which eventually became known as InChI, the International Chemical Identifier, and is widely regarded as one of IUPAC's recent successes.

Over the next several months, I became convinced that we should try to form a new Division to bring nomenclature activities together. Alan wisely proposed the name "Division of Chemical Nomenclature and Structure Representation" to emphasize future directions and the integrated nature of the subject of nomenclature. The Division was approved by Bureau and Council in 2001, with Alan McNaught as initial division president (2002-2005), thus assuring that Jortner's "guarantee" to protect nomenclature in the restructuring process was clearly fulfilled [9].

### **Brigitte:** What is your assessment of this substantial restructuring of IUPAC?

Ted: I think that all of us advocating for restructuring

were convinced that it had to happen for IUPAC to retain the financial backing from our National Adhering Organizations that is needed to support the ever-expanding scope of "chemistry." Also, it was necessary to counter the perception that IUPAC's scientific work depended on only an elite "charmed circle." Unfortunately we lost some thoughtful discussions without regular Commission meetings—only partially compensated by *ad hoc* advisory groups. I always regretted that some commission members, who had contributed so much to IUPAC over the years, probably felt unappreciated when their commissions were abolished, even though the restructuring was clearly not aimed at any individual commission.

The restructuring actions had exactly the desired effect. Each project would be carried out by a "task group"—a term chosen to emphasize the temporary nature of the group. Anyone in the world could propose a project, with the proposal given peer review via a system that Fabienne Meyers set up at the Secretariat. The proposal and reviewers' recommendations then went to one or [often] more Division or Standing Committees for decision and allocation of funds. With all commissions terminated in 2001, the focus was on what new commissions should be formed [or re-formed] under more stringent guidelines. I was surprised that the Divisions proposed reinstating only two of 37 commissions, and that none have been formed since 2001. Some Divisions used a few subcommittees to carry out specific functions, and others used outside advisory groups to recommend areas for IUPAC work.

**Brigitte:** Thank you so much Ted for having shared your knowledge of these important years from the history of IUPAC and clarified the process and the successive steps that led to a profound reorganizing of IUPAC at the turn of the last century. This successful restructuring in which you were deeply involved demonstrated the ability of a huge international body of chemists composed mainly of volunteers to restructure itself to keep in line with both its duties and challenges.

#### References

- Stanley S. Brown, History of IUPAC 1988-1999, IUPAC 2001, ISBN 0-67-8550-1-2; supplement to Ref. 2.
- 2. Roger Fennell, History of IUPAC, 1991-1987, Blackwell Science, 1994, ISBN 0-86542-8786(94)
- Edwin D. Becker, Think IUPAC Project—Secretary General's Report, *Chem. Int.* 2001, vol. 23, no. 1, pp. 12-13; https://doi.org/10.1515/ci.2001.23.1.12 (alt https://publications.iupac.org/publications/ci/2001/

#### continued on page 10

# Systems Thinking and Sustainability

### Converging on chemistry's role in the 21st Century

by Peter Mahaffy, Stephen Matlin, Marietjie Potgieter, Bipul Saha, Aurelia Visa, Sarah Cornell, Felix Ho, Vicente Talanquer, Jane Wissinger and Vania Zuin

3-year IUPAC project Systems Thinking in Chemistry for Sustainability: Toward 2030 and Beyond (STCS 2030+, IUPAC Project #2020-014-3-050) [1] launched in late 2020 is breaking important new ground in addressing chemistry's orientations, roles, and responsibilities in the 21st Century and helping to map out implications for chemistry education, research, and practice. In taking on this ambitious task, STCS 2030+ draws on expertise available within IUPAC's own structures, as a project co-sponsored by three IUPAC standing committees: the Committee on Chemistry Education (CCE), the Committee on Chemistry and Industry (COCI) and the Interdivisional Committee on Green Chemistry for Sustainable Development (ICGCSD). The project is also working with other organizations, such as the International Organization for Chemical Sciences in Development (IOCD), which is a co-supporter, and involves collaborators with individuals from organizations that include the Stockholm Resilience Centre [2], the American Chemical Society (ACS) Green Chemistry Institute [3], the International Year of Basic Sciences for Sustainable Development (IYBSSD 2022-23) [4], and chemistry educators and chemical industry from around the world.

STCS 2030+ builds on and extends outcomes from the recently completed IUPAC Systems Thinking in Chemistry Education (STICE) project [5], which examined the potential benefits of incorporating systems thinking (ST) into chemistry education and ways to support chemistry educators in using ST. Systems thinking uses a variety of tools and cognitive frameworks to enhance our understanding of complex behaviors and phenomena from a holistic perspective. One of the main drivers behind the STICE project included recognition that, while ST has been has been identified as one of the core competences necessary to achieve sustainability [6] and has been extensively adopted in some other disciplines, including

**Figure 1:** Integrating Sustainability into Learning in Chemistry—the visual representation of Working Group 1 editorial in the Journal of Chemical Education.

biology, engineering, and earth and environmental sciences, virtually no attention has been given to the use of ST in chemistry education. Potential benefits to using ST approaches in chemistry education include (a) enhancing students' knowledge, skills, and values in chemistry through a focus on the interconnections between different chemical phenomena; (b) improving students' knowledge of the influence of chemistry on planetary and societal issues; and (c) preparing students to make informed decisions and to address the complex global challenges of the 21st Century [7]. An important catalyst for the IUPAC ST projects was a proposal by a group at the International Organization for Chemical Sciences in Development (IOCD) that ST should be key to re-imagining chemistry in the 21st Century and optimizing chemistry's contributions to achieving the UN Sustainable Development Goals (SDGs) [8]. The STICE project catalyzed considerable global momentum, with wide dissemination at national and international conferences, publication in Nature journals, 43 contributed papers to the December 2019 special issue of the Journal of Chemical Education [9] and a feature cover story in the February 3, 2020 issue of Chemical & Engineering News [10].

Aims of the *STCS 2030+* project are three-fold: (a) to highlight and strengthen the centrality of chemistry as a sustainability science through chemistry education, engaging with the 2022-2023 IYBSSD to incorporate ST as a fundamentally important approach to support integrating human needs and science in the service of planetary sustainability; (b) to formulate recommendations to guide use of ST in chemistry education; and (c) to seek ways to engage with chemical industry to explore how it can contribute to outcomes of the IYBSSD and how chemical industry views ST and its incorporation into chemistry education, research, and industrial practice.

#### **Progress to Date**

Two working groups have been meeting bi-weekly since the beginning of 2021, focused on the first two STCS 2030+ project aims (sustainability and education), and plans are underway to form a third working group to engage with chemical industry. We report below progress made by the working groups.

Working Group One-Sustainability (WG1) has focused its efforts on Project Aim 1-to articulate the strong contribution that chemistry education and practice will make to achieving sustainability. The group co-authored a guest editorial in the Journal of Chemical Education, titled "Integrating Sustainability into Learning in Chemistry," and Figure 1 [11]. The timing coincided with Earth Day 2021 and ACS celebration of Earth Week in April 2021. The article proposed that chemistry educators have the responsibility to teach the central role chemistry will play in concert with other disciplines, in building a sustainable future for people and the planet. Two frameworks driving global sustainability efforts that can be leveraged to integrate these important concepts into curricula are the UN Sustainable Development Goals (UN SDGs) [12] and the Planetary Boundaries Framework [13].

using the UN Educators are Sustainable Development Goals to provide concrete examples of ways in which green and sustainable chemistry can contribute to achieving the 2030 SDGs and to bring international perspectives into the classroom. The chemistry community is much less familiar with the Planetary Boundaries Framework, which measures the stability and resilience of the Earth system in the midst of rapid global change. The framework's nine earth system processes (climate change, novel entities, stratospheric ozone depletion, atmospheric aerosol loading, ocean acidification, biogeochemical flows of nitrogen and phosphorus, freshwater use, land-system changes, and biosphere integrity) and their dynamic interactions describe the biophysical state, stability, and resilience of our planet. Control variables for each of the earth system processes, many of which are

directly related to the production and measurement of chemical substances in the atmosphere, hydrosphere or lithosphere, have been identified and quantified for seven of the nine earth system processes. As Figure 2 from an interactive electronic version of the framework created by the King's Centre for Visualization in Science (KCVS) [14] shows, the numerical value of the control variable indicates with a green/yellow/ red colour scheme whether that earth system process is still in a safe operating zone (below the planetary boundary), a zone of increasing risk, or a zone of high risk as a result of human activity.

WG1 is exploring ways in which the Planetary Boundaries Framework can be used by chemistry and cross-disciplinary science educators as a ST tool to explore and address the dynamic and complex challenges of sustainability. Chemist Peter Mahaffy, Physicist Rob MacDonald, and the student research team at King's Center for Visualization in Science (kcvs.ca) in Edmonton, Alberta, Canada are collaborating with Sarah Cornell and her colleagues at the Stockholm Resilience Centre to visualize the web of earth system connections in the planetary boundaries framework and to explore how knowledge of chemistry and other STEM science core curriculum concepts can be woven in to approaches to understand and address the complex challenges faced by the Earth

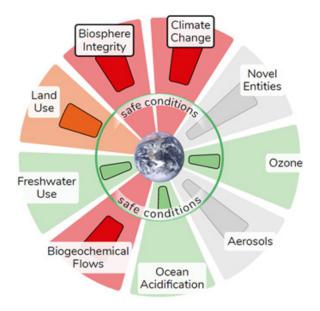


Figure 2: Planetary Boundaries Framework, from the King's Centre for Visualization in Science (KCVS) planetary boundaries interactive learning resource at www.planetaryboundaries.kcvs.ca, building on and adapted from the Stockholm Resilience Centre (Steffen et al., Science 2015 or [13]).

#### Chemistry and systems

system as a whole. The working group is collaborating with the KCVS research team in their development of interactive electronic resources linking STEM curriculum to the planetary boundaries framework. The project is exploring how the outcomes can be disseminated as an IUPAC contribution to the activities and approaches planned for IYBSSD so as to facilitate integrating the teaching and learning of basic science concepts into sustainability considerations [15].

One example of using the web of planetary boundaries connections linking the ocean acidification earth system to other earth system processes is shown in Figure 3. An interactive force-directed graph developed at KCVS [14] highlights the ocean acidification earth system, which then moves to the centre of view for the user, revealing several important chemistry and STEM curriculum topics that are linked to the ocean acidification earth system process. For example, the ocean acidification earth system process is interconnected with the climate change, biosphere integrity, land-system changes, and biogeochemical flows earth system processes, and offers a sustainability context for coverage in foundational chemistry courses of topics such as acid-base chemistry, solubility & precipitation, equilibrium concepts, gas properties, and speciation in aqueous solutions.

Working Group Two–Education (WG2) has focused on developing a common understanding of systems thinking in chemistry education, outlining basic questions that need to be answered to define *what* aspects of ST could be integrated in chemistry education, *why* that integration is important, and *how* that integration could be best accomplished. Initial answers to the following questions have been generated:

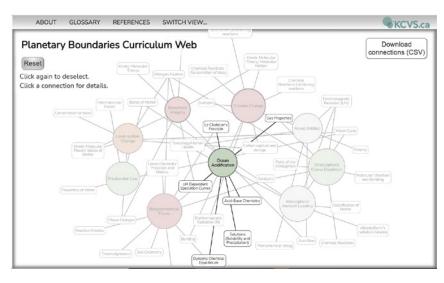
• Why do we think chemistry educators should incorporate systems thinking into their courses?

- Which aspects/characteristics/parts of ST do we anticipate will be the easiest for a typical chemistry instructor to integrate into what they are already doing?
- Which aspects/characteristics/parts of ST do we believe typical chemistry instructors will struggle with the most?
- What are some background terms and concepts that educators might need to know about to understand ST?
- Which general chemistry topics/content do we think will provide the easiest entry points for integrating ST?
- If we were to think about educating educators, what should be our goals for their professional development?

WG2 has agreed to develop guidelines and resources that help chemistry educators incorporate ST into their courses to promote:

- A view of chemistry itself as a system to make the subject more comprehensible and coherent, rather than appearing as a massive list of facts to be learned, so that teaching and learning are facilitated;
- Connections of chemistry with global challenges and sustainability goals that can help to make the discipline more attractive to diverse students;
- Development of skills for thinking at a system scale and seeing how systems interact and influence one another, facilitating understanding and solving complex, multi-dimensional problems.
- Development of thinking skills for tackling the sustainability challenges faced by the world, which involve curricular interactions across disciplines with planetary and societal systems.

Figure 3: Visualization of the web of connections among the ocean acidification earth system and several other connected earth system processes in the Planetary Boundaries Framework. Representative descriptions of the connections are shown for each connection, and a web of curriculum connections to chemistry and STEM disciplines will be developed and disseminated in an interactive resource for educators. (Visualization by Robert MacDonald, King's Centre for Visualization of Science, www.kcvs.ca)



#### Chemistry and systems

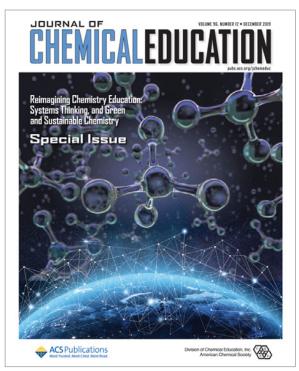


Figure 4: One goal of Working Group Two (Education) is to publish IUPAC recommendations for the use of systems thinking in chemistry education, building on and extending the work of the IUPAC STICE project, the ACS Green Chemistry Institute, and other chemistry educators, published in a special issue of the Journal of Chemical Education, December 2019 [9].

The guidelines and resources to be developed will help educators identify and reflect upon the:

- Big/core/central ideas of ST in chemistry that students should understand;
- Learning objectives (LOs) that should guide instruction and assessment of ST in chemistry;
- Topics and contexts that are most productive in motivating and building student understanding of ST in relation to global challenges and sustainability goals;

as well as to select or design:

- Formative and summative assessment tasks that help evaluate student progress towards and achievement of the targeted LOs;
- In-class activities that help develop student understanding of targeted central ideas and achieve the targeted LOs;
- Ways in which a ST orientation enriches chemistry learning.

The group has reviewed some existing instructional activities to evaluate the extent to which they can help promote ST in chemistry education and propose possible modifications that will enrich their ST components.

### Working Group Three—Chemical Industry (WG3)—proposed

As STCS 2030+ moves ahead, it is engaging in dialogue with people working in chemistry-related industries, which are seen as important to all aspects of the project's aims. In particular, industry perspectives and needs can help to inform what is important to be included in the reforms of chemistry education approaches and curricula; in the focus and cross-disciplinary perspectives of chemistry research; and in the ways that chemistry engages with other basic sciences in channeling efforts in the IYBSSD.

The leadership of *STCS 2030+* invites interested individuals and groups in chemistry-related industries to contact project task group co-chair Stephen Matlin to discuss involvement in the project.

## Future directions for the project and ways for others to get involved

Future directions for the project will include:

- Integrating the activities of the working groups across the entire project;
- Reporting regularly and solicit input from the three IUPAC standing committees and other stakeholders;
- Strengthening and building further interactions with partners and collaborators;
- Developing additional mechanisms for disseminating project outcomes, including the development of a ST web site NS and presentation of outcomes and engage with practitioners through ST workshops at national and international chemistry conferences;
- Articulating IUPAC recommendations and exemplars for the education community;
- Liaising further with leadership of IYBSSD to discuss ways to integrate the interactive resources linking chemistry teaching and learning to sustainability as a contribution to IYBSSD;
- Developing a plan for sustainability of this work beyond the lifetime of the IUPAC project so as to continue to serve chemistry educators and other stakeholders; and
- Working toward building a community of practice among chemistry educators with resources and exemplars.

#### Chemistry and systems

To become involved in the project, please contact any of the task group co-chairs: Peter Mahaffy <Peter.Mahaffy@kingsu.ca>, Stephen Matlin <stephen. matlin@gmail.com>, Marietjie Potgieter <marietjie. potgieter@up.ac.za>, Bipul Saha <drbsaha@rediffmail. com>, or Aurelia Visa <apascariu@yahoo.com>.

#### References

- Systems Thinking in Chemistry for Sustainability: Toward 2030 and Beyond (STCS 2030+) https://iupac. org/project/2020-014-3-050 (accessed 2021-07-13).
- Stockholm Resilience Centre Stockholm Resilience Centre https://www.stockholmresilience.org/ (accessed 2021-07-16).
- ACS Green Chemistry Institute American Chemical Society https://www.acs.org/content/acs/en/ greenchemistry/about.html (accessed 2021-07-16).
- International Year of Basic Sciences for Sustainable Development 2022 https://www.iybssd2022.org (accessed 2021-07-13).
- IUPAC Committee on Chemistry Education. Learning Objectives and Strategies for Infusing Systems Thinking into (Post)-Secondary General Chemistry Education. IUPAC project 2017-010-1-050; https://iupac.org/ project/2017-010-1-050 (accessed 2021-07-13).
- Wiek, A.; Withycombe, L.; Redman, C. L. Key Competencies in Sustainability: A Reference Framework for Academic Program Development. *Sustain. Sci.* 2011, 6 (2), 203; https://doi.org/10.1007/s11625-011-0132-6.
- 7. Flynn, A. B.; Orgill, M.; Ho, F. M.; York, S.; Matlin, S. A.; Constable, D. J. C.; Mahaffy, P. G. Future Directions for

Systems Thinking in Chemistry Education: Putting the Pieces Together. *J. Chem. Educ.* **2019**, *96* (12), 3000-3005; https://doi.org/10.1021/acs.jchemed.9b00637.

- Matlin, S. A.; Mehta, G.; Hopf, H.; Krief, A. One-World Chemistry and Systems Thinking. *Nat. Chem.* 2016, *8* (5), 393–398; https://doi.org/10.1038/nchem.2498.
- Journal of Chemical Education Special Issue– Reimagining Chemistry Education: Systems Thinking, and Green and Sustainable Chemistry https://pubs.acs. org/toc/jceda8/96/12 (accessed 2021-07-13).
- In these classrooms, chemistry is part of a larger whole https://cen.acs.org/content/cen/articles/98/i5/ classrooms-chemistry-part-larger-whole.html (accessed 2021-07-13).
- Wissinger, J. E.; Visa, A.; Saha, B. B.; Matlin, S. A.; Mahaffy, P. G.; Kümmerer, K.; Cornell, S. Integrating Sustainability into Learning in Chemistry. *J. Chem. Educ.* 2021, *98* (4), 1061-1063; https://doi.org/10.1021/acs. jchemed.lc00284.
- 12. THE 17 GOALS | Sustainable Development https://sdgs. un.org/goals (accessed 2021-07-16).
- Steffen, W.; Richardson, K.; Rockström, J.; Cornell, S. E.; Fetzer, I.; Bennett, E. M.; Biggs, R.; Carpenter, S. R.; Vries, W. de; Wit, C. A. de; Folke, C.; Gerten, D.; Heinke, J.; Mace, G. M.; Persson, L. M.; Ramanathan, V.; Reyers, B.; Sörlin, S. Planetary Boundaries: Guiding Human Development on a Changing Planet. *Science* 2015, *347* (6223), 736-747; https://doi.org/10.1126/science.1259855.
- 14. Planetary Boundaries KCVS https:// planetaryboundaries.kcvs.ca/ (accessed 2021-07-16).
- Nugent, C. The Unexpected Ways Climate Change Is Reshaping College Education. *TIME magazine*. April 16, 2021.

#### Restructuring IUPAC at the turn of the 20th century (cont. from page 5)

january/SG-report.html)

- Albert E. Fichli, President's Report, State of the Union, Chem. Int. 1997, vol. 19, no. 5, pp. 152-155; https://doi. org/10.1515/ci.1997.19.5.152 (alt http://publications.iupac. org/ci/1997/september/fischli.pdf) Adapting mission, goals and structures, p. 154
- Report of the Strategy Development and Implementation Committee (posted Apr 1998), https:// old.iupac.org/news/archives/1998/strategy
- Changes in the Organization and Management of the Union's Scientific Work (posted 19 Oct 1998), https:// old.iupac.org/news/archives/1998/october
- 71st Bureau, 26-27 Sep 98, Frankfurt, Germany (posted 11 Nov 98), https://iupac.org/wp-content/ uploads/2020/04/71\_bureau.pdf, or specifically item 6 https://old.iupac.org/news/archives/1998/71st\_ bureau/71b\_p6.html

- IUPAC held a Round Table discussion on "Representations of Molecular Structure: Nomenclature and Its Alternatives"—Summary and Executive Committee Actions (posted 24 Apr 2000), https://old. iupac.org/news/archives/2000/NRT\_Report.html
- Alan McNaught, Chemical Nomenclature and Structure Representation; *Chem. Int.* 2002, Vol 24, No. 2, pp. 12-14; https://doi.org/10.1515/ci.2002.24.2.12b (alt https://publications.iupac.org/publications/ ci/2002/2402/Cl2402.pdf

Edwin D. Becker <tbecker@nih.gov> has been a member of various IUPAC bodies for more than 30 years and ultimately, secretary general from 1996 to 2003. He is a scientist emeritus at the National Institutes of Health, Bethesda, Maryland, USA.

Brigitte Van Tiggelen <br/>bvantiggelen@sciencehistory.org> is Director of International Operations at the Science History Institute, USA.

# IOCD turns 40

### The future of the chemistry for sustainable development

#### by Federico Rosei and Stephen A. Matlin

he International Organization for Chemical Sciences in Development (IOCD) passes an important milestone in 2021, as 1 July marked the 40<sup>th</sup> anniversary of its launch at a meeting hosted by UNESCO in Paris in 1981. Registered in Belgium, IOCD was originally established as the first non-governmental organization to focus on the need to develop opportunities for chemists in low-and middle-income countries (LMICs) to progress professionally and work on projects of relevance to the development of their countries and regions [1].

Driven by the passionate commitment and vision of its founding President, the Nobel Laureate Glenn T. Seaborg [2] and founding Executive Director, organic chemist Pierre Crabbé, IOCD's early years were marked by the creation of Working Groups in areas such as agricultural and medicinal chemistry and chemistry education [3].

While IOCD's governance passed into new hands with the appointment of Robert Maybury [4] as Executive Director following Crabbé's untimely passing in 1987, and with Seaborg being succeeded by the Nobel Laureate Jean-Marie Lehn in 1992, the organization continued to grow and evolve its focus, advancing into areas of institutional and infrastructural capacity-building in fields such as natural products, biotic exploration, and environmental analytical chemistry [5]. On Maybury's retirement in 2009, he was succeeded by the organic chemist Alain Krief, who during the following decade helped steer IOCD's overhaul and transformation into an organization centred on the role of the chemical sciences in sustainable development [6]. A number of activities were phased out and new ones instituted, two notable examples being the creation in 2013 of a Working Group on Materials for Energy Conversion, Saving and Storage (MATECSS), co-led led by Federico Rosei and his colleague Mohamed Chaker based at the Institut National de la Recherche Scientifique (INRS), Montreal and in 2014 the establishment of a group that was subsequently named Chemists for Sustainability (C4S), whose core members are Henning Hopf, Alain Krief, Stephen Matlin, and Goverdhan Mehta. To a large extent, IOCD has evolved and is still evolving towards addressing several UN Sustainable Development Goals (SDGs). In parallel, Rosei and collaborators established at INRS a UNESCO Chair that has the same name as the working group, MATECSS, and is therefore completely aligned with IOCD and its objectives.

Recognising that sustainable development creates a critical need for clean, affordable and environmentally friendly energy to be available across the world, including in LMICs, MATECSS set out with the aims of helping to expedite technology transfer and build capacity through engagement with local scientists, engineers, and students in LMICs; and to foster the development of low cost, adaptive technologies based on materials for energy conversion, saving, and storage that fit within the paradigm of local-scale energy systems and that use local resources. To this end, training courses, workshops, and places for PhD and postdoctoral researchers have been provided. In this sense, MATECSS focuses directly on three SDGs, Goal 4 (quality education), Goal 7 (affordable and clean energy) and Goaly 13 (climate action); and indirectly on others.

The C4S group, which openly invites collaborators to bring additional perspectives to its work, has been serving advocacy and think-tank roles through written articles, lectures at various fora, and web materials related to its mission of promoting the engagement of chemistry in sustainable development [7]. Among notable achievements, a pair of C4S articles [8,9] in 2015-16 highlighted the importance of the chemical sciences in supporting the newly established SDGs and stressed that chemistry would need to make some deep-seated changes in order to optimize its contributions to the SDGs. The nature of these changes was encapsulated in the concept of "oneworld" chemistry, whose defining characteristics included the re-orientation of chemistry as a science for the benefit of society and the adoption of systems thinking and cross-disciplinarity in its approaches. The proposal that chemistry should embrace systems approaches has found particular resonance and led to a project (2017-2019) of the IUPAC Committee on Chemistry Education, also supported by IOCD and co-led by Peter Mahaffy and Stephen Matlin, on infusing systems thinking into chemistry education (STICE) [10]. This initiative was very productive, stimulating a growing body of literature and practice [11]. It has been succeeded by a new project [12], Systems Thinking in Chemistry for Sustainability: Toward 2030 and Beyond (STCS 2030+) in 2020-2023, co-sponsored by the IUPAC Committee on Chemistry

#### IOCD turns 40

Education, Committee on Chemistry and Industry, and Interdivisional Committee on Green Chemistry for Sustainable Development, and also supported by IOCD, described in the accompanying article by Mahaffy *et al* [13].

Besides being the 40<sup>th</sup> anniversary of IOCD's founding, 2021 is marking a further time of pivotal change in both governance and activities for the organization. Alain Krief has been succeeded as Executive Director by Federico Rosei, while Jean-Marie Lehn has announced he will retire as IOCD's President after 30 years of service. The search for his successor is underway. Half of the membership of IOCD's governing body, the General Assembly, has been replaced, with newly elected members being significantly younger that those departing, all female, and bringing experience of green and sustainable chemistry, materials science, physics and industry to complement the expertise of continuing members, resulting in broader capabilities.

The younger, more diverse character of the governance and its leadership attune with evolutionary shifts taking place in IOCD as it redevelops its mission for the 21st century. The changes signpost the intention to be inclusive, mindful of the needs and goals of coming generations and strengthened in focus on efforts to promote the central importance of the chemical sciences in achieving a sustainable future through action in education, research, and practice that unites efforts across disciplinary boundaries.

In pursuing its objectives and ambition to address the SDGs, IOCD is an inclusive organization. We welcome collaborators, volunteers, and sponsors who share our vision and who want to engage with us on common goals, towards a long-term peaceful coexistence of all living species on Planet Earth.

Federico Rosei <ceo@iocd.org> is the Executive Director of IOCD <http:// www.iocd.org/>, holds the Canada Research Chair in Nanostructured Materials and the UNESCO Chair in Materials and Technologies for Energy Conversion at the Centre for Energy, Materials and Telecommunications, Institut National de la Recherche Scientifique, Université du Québec, Canada.

Stephen Matlin <s.matlin@imperial.ac.uk> is the Secretary of IOCD, is a Visiting Professor in the Institute of Global Health Innovation, Imperial College London, UK and a Senior Fellow in the Global Health Centre at the Graduate Institute of International and Development Studies, Geneva, Switzerland.

#### References

 G.T. Seaborg, An international effort in chemical science. Science 1984, 223, 9, https://doi.org/10.1126/ science.223.4631.9



IOCD's action group Chemists for Sustainability (C4S) core members zooming in August 2021; (from left to right) Henning Hopf, Alain Krief, Stephen Matlin, and Goverdhan Mehta.

- S.A. Matlin, A. Krief. Glenn Seaborg, The Periodic Table and a Belgian NGO. *Chimie Nouvelle* 2018, 129, 1-10, http://chimienouvelle.be/CN129/Article%20Krief.pdf
- D.A. O'Sullivan, Group to use chemistry to solve developing countries' ills. *Chem. & Eng. News* 1983, 21-24, https://doi.org/10.1021/cen-v061n001.p021
- S.A. Matlin. Robert Maybury's contributions to IOCD. IOCD, Namur, 2021, http://www.iocd.org/v2\_PDF/ RobertMayburyIOCD-Obit2021-04bp.pdf
- J.-M. Lehn, E.R. Blout, R.H. Maybury. IOCD: 20 Years of Building capacity in chemistry in developing countries. *Chem. Int.* 2002, 24(3), 3-5, https://doi.org/10.1515/ ci.2002.24.3.3
- IOCD: Organization outline and strategy, 2020-2021.
   IOCD, Namur, Brochure, February 2020, published online 7 March 2020, http://www.iocd.org/v2\_ PDF/2020-IOCD-OutlineBrochure-4p.pdf
- H. Hopf, A. Krief, S.A. Matlin, G. Mehta. Chemists for Sustainability: Overview of topics and publications. Brochure. IOCD, Namur, 12 April 2021, http://www.iocd. org/v2\_PDF/C4S-2021-04ap.pdf
- S.A. Matlin, G. Mehta, H. Hopf, A. Krief. The role of chemistry in inventing a sustainable future. *Nature Chem.* 2015, 7, 941-943, http://dx.doi.org/10.1038/nchem.2389
- S. A. Matlin, G. Mehta, H. Hopf, A. Krief. 'One-world' chemistry and systems thinking. *Nature Chem.* 2016, 8, 393-6, https://doi.org/10.1038/nchem.2498
- Learning Objectives and Strategies for Infusing Systems Thinking into (Post)-Secondary General Chemistry Education. https://iupac.org/ project/2017-010-1-050
- P.G. Mahaffy, S.A. Matlin. Next hundred years: Systems thinking to educate about the molecular basis of sustainability. L'Actualité Chimique, December 2019, 446, 47-49. https://www.lactualitechimique.org/Pourles-cent-ans-a-venir-reflexions-sur-l-enseignement-dela-chimie-et-la-durabilite
- Systems Thinking in Chemistry for Sustainability: Toward 2030 and Beyond (STCS 2030+). https://iupac. org/project/2020-014-3-050
- P.G. Mahaffy, S.A. Matlin, M. Potgieter, B. Saha, A. Visa, S. Cornell, F. Ho, V. Talanquer, J. Wissinger, V. Zuin. Systems Thinking in Chemistry for Sustainability: 2030 and Beyond (STCS 2030+). *Chem. Int.* 2021, 43(4) 6-10

### Breakthroughs for a circular, climateneutral future

#### by Fernando Gomollón-Bel

UPAC thrives to boost the impact of chemistry around the world. Recently, it established a new initiative-the Top Ten Emerging Technologies in Chemistry-to showcase the tremendous importance of the chemical sciences by highlighting developments on the verge of becoming game-changing commercial breakthroughs [1]. Some have been truly transformational for our society, such as RNA vaccines and rapid tests, both key technologies to enable a smooth transition to the new normal after the COVID-19 pandemic. This year, the Top Ten efforts continue-featuring a brand-new logo and further actions to disseminate and promote the project beyond this publication. The new selection of emerging technologies gathers both well-established, high-technology readiness level (TRL) applications and ground-breaking opportunities for the chemical industry. Of course, many of them still address the ongoing coronavirus crisis, focusing on new pharmaceutical solutions to prevent the spread of pathogens like SARS-CoV-2. Moreover, many tackle the climate crisis and provide new roadmaps to achieve the United Nations' Sustainable Development Goals (SDGs) [2]. The consequences of global warming are here-heatwaves, floods, and wildfires devastate our planet constantly. Chemistry will provide pivotal tools towards a sustainable future [3], many included in this singular selection. IUPAC experts have selected the Top Ten Emerging Technologies in Chemistry 2021ten ideas to catalyse industrial innovations and transform our world.

### Blockchain technology

#### Digital advances for more reproducible, traceable chemical innovation

Solvay, Evonik, and BASF are some of the world-leading companies that are exploring the uses of blockchain technology in chemistry. Furthermore, many believe that blockchain holds the key to more reproducible science thanks to one of its main built-in features—traceability. Back in 2008, Satoshi Nakamoto conceptualised and designed blockchain—although many other computer scientists had played with similar ideas in the 1980s and 90s. Nakamoto designed the beloved cryptocurrency Bitcoin, a list of digital financial records and monetary transactions linked with encrypted algorithms and managed by a distributed peer-to-peer network of users. Ever since, experts have adapted this technology to develop other applications such as smart contracts, digital stocks,

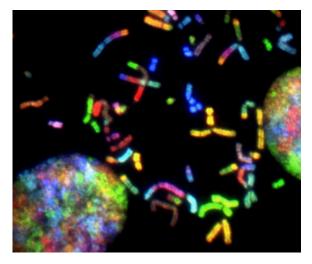


and proofs of authenticity valued in the Arts. By design, blockchains offer an immutable repository to record any kind of transaction, offering great potential all along the scientific process. Since the original record of transactions is safely kept throughout a network of computers under strict cryptographic protection, fraudulent alterations are quickly detected. The U.S. National Institute of Standards and Technology, among other prestigious institutions, believes blockchain could benefit scientists across all fields, as well as solve serious problems such as reproducibility [4]. For instance, chemists in the UK have explored the uses of blockchain to trace a series of simple computational calculations. Their preliminary results suggest that this type of encrypted environment could increase both transparency and accessibility, as every single step of the process is documented and shared within the digital ledger [5]. German researcher Sönke Bartling believes that blockchain can benefit research beyond secure laboratory notebooks and data-collection-enhancing publications, grants, evaluation, and recognition. Indeed, the World Intellectual Property Organization is exploring the potential of blockchain to transform the industry of Intellectual Property (IP)-from evidence of creatorship to the management of royalties [6]. Chemical companies want to stay ahead; many have already created blockchain-based systems to modernise their supply chain. This technology guarantees secure transactions across all parties, boosting traceability to unprecedented levels of detail. "Smart contracts" are fully automated, enabling a continuous tracking of chemical goods from raw materials to the market shelves. European chemical manufacturers also explore the possibilities of blockchain to advance the circular economy-with easier, more reliable life cycle assessment, blockchain will likely increase recyclability, improve the utilisation of resources, and eventually reduce overall costs [7]. Another proof of the possibilities of blockchain in chemistry is the proliferation of start-ups such as ChemChain, supported by the European Commission through different funding programmes. This company ensures that data and information on chemicals is fully-protected

through their decentralised, encrypted ledgers, which has attracted leading industries such as Dow-Dupont. It is expected that Blockchain will generate a business value of over \$3 trillion by 2030 [8], and its applications in chemistry will certainly represent a large share of it.

#### Semi-synthetic life New letters to expand biochemistry and therapeutics

Alchemists dreamt of transforming lead into gold. Nowadays, chemists fantasise with expanding the code of life-a universal system to conceal biological information. In the past few years, this field has become a reality and has already achieved some remarkable milestones. After decades of failed attempts, a team of researchers at Scripps finally succeeded in 2014 in adding two artificial letters to the genetic alphabet-nicknamed X and Y [9]. Since then, scientists have further expanded the alphabet with new bases like B, P, S, and Z [10]. All of these synthetic nucleotides could populate our genomes with new words, new ideas-such as the information needed to create life-saving proteins for diagnostics, treatments, and more. Ultimately, chemists also designed novel biological systems that interpret and exploit these unnatural letters. Genetically-engineered strains of Escherichia coli carry these artificial nucleotide bases in their DNA and transcribe the information they encode into unusual proteins, which also feature non-traditional amino acids such as pyrrolysine and azydo-phenylalanine [11]. Nowadays, chemists study how to perfect these artificial biochemical machinery, developing new systems to minimise the number of transcription and translation errors, which benefit from the swift advances of technologies such as Nobel-winning CRISPR/Cas9. The implications of these discoveries



transcend chemistry-life works with building blocks beyond the ones we bare, sparking new thoughts on what extra-terrestrial life could look like. Aside philosophical questions, unnatural nucleotides and amino acids provide new chemical tools for the design of targeted treatments, including THOR-707, an agent against metastatic solid tumours currently undergoing clinical trials. One of the companies spearheading this technology is Synthorx, established by synthetic life pioneer Floyd Romesberg. It was acquired by French pharma giant Sanofi in late 2019 for \$2.5 billionshowcasing the commercial interest in this emerging technology. In the future, chemists may discover other artificial DNA letters, as well as synthesise novel unnatural amino acids, expanding the limitations of life as we know it and enabling a whole new range of better therapies and medical solutions.

#### Superwettability A centuries-old discovery offers new opportunities

British scientist Thomas Young is mostly known for the double-slit experiment, which supported that light is a wave. However, he pioneered other important fields of science, including the study of wettabilitythe ability of liquids to maintain contact with a solid surface. In 1805, Young proposed the first definition for this concept, based on the contact angle liquid droplets form in the interface. Therefore, something really wetting will adopt rather flat shapes and small angles, whereas non-wetting liquids create almost spherical structures, at angles parallel to the surface [12]. After centuries of studying this phenomenon, scientists acquired a better understanding and even learnt how to tweak wettability at will-designing new materials with exceptional properties. Among these, superwettability emerged as a great promise with applications in energy, health, agriculture, and much more. Some of these advances are heavily inspired by natural microand nanostructures, such as the feet of geckos and frogs, the eyes of mosquitoes, and the surfaces of cacti and roses. Based on many of these examples, scientists have created nanostructured surfaces on metals, polymers, fabrics, and more. Chemistry is, of course, fundamental to these designs, which require carefully controlled manufacturing techniques. Furthermore, superwettable structures have led to surprising reactivities. Such surfaces exhibit unique fluid dynamics, which enhances the efficiency of chemical reactions where interface interactions are key-particularly photo- and electrocatalytic transformations. Examples include high-performance water splitting, epoxidation,

esterification, and condensation. Moreover, this type of nanostructured catalyst usually exhibits enhanced durability, recyclability, and selectivity, paving the way to greener, more efficient chemical processes aligned with the United Nation's Sustainable Development Goals (SDGs) 12 and 13 [13]. The uses of superwettable surfaces beyond chemistry include sensors, printers, energy-storage devices, pollution removal, water harvesting, and others. Several Chinese and Korean companies are exploring its potential in different fields, such as self-cleaning textiles, oil separation, and cooling. Many challenges in fabrication remain, however researchers are confident that this technology will revolutionise materials science. New opportunities keep arising [14].

#### Artificial humic matter

#### Engineering carbon-negative solutions for sustainable and efficient agriculture

Agriculture, livestock, and land use account for almost one-third of all greenhouse emissions. Beyond contributing to the concerning climate crisis, these affect crop yields directly—and reports from the Intergovernmental Panel on Climate Change (IPCC) predict that we will reach a critical situation in 2030. Once again, chemistry could convey a hopeful answer, an artificial alternative to humic matter for a better management of the scarce resources in our soils. Although hidden underneath us, the decomposition of organic matter into humic matter is the second largest process in the carbon cycle,

after photosynthesis. Thus, designing strategies to make it more efficient is currently a priority. Furthermore, artificial humification processes ensure а complete control throughout the reaction, which leads to cleaner, safer, and greener fertilisation solutions. Currently, several approaches exist to accelerate the decomposition of organic matterand hydrothermal humificationisemerging as one of the most attractive among them. Envisioned by Fan Yang and Markus Antonietti, this

technology 'cooks' organic matter in hot water in the presence of basic ashes. The specific conditions of these processes mimic natural geochemical processes and yield a product mixture comparable to natural humic residues [15]. Recent lab experiments suggest that these artificial humic matter improve soil quality and health, as well as agricultural productivity-an attractive alternative to offset the negative effects of climate change. This enhancement comes from the many benefits of artificial humic matter. Research shows it improves water and fertiliser binding-hence improving the utilisation of resources and reducing side-effects such as eutrophication-and stimulates soil microbiology, which benefits the absorption and digestion of minerals. Moreover, unlike natural biochemical decomposition processes that are unavoidably linked to the emission of greenhouse gases such as carbon dioxide and methane, artificial humic matter is essentially carbon negative [16]. Experts believe that these carbon fixation solutions will contribute to the circular economy, aligning with SDG 13 and leading to a carbon-neutral society. Currently, several institutes in Europe are working to develop the first pilot plants to prepare artificial humic matter in large scale. Together with other IUPAC Top Ten Emerging technologies, such as nanopesticides, nanosensors, and artificial intelligence, artificial humic matter will pave the way to more sustainable and efficient agricultural processes.

#### Chemical synthesis of RNA and DNA The future of nucleic acids in medicinal chemistry after COVID vaccines

Last year, IUPAC highlighted the potential of RNA vaccines to put an end to COVID-19 and most likely to many other diseases in the future, including cancer. HIV. and influenza [17]. These vaccines are adaptable and versatile, as well as relatively quick to manufacture. By the end of July 2021. the U.S. had administered over 325 million doses of mRNA vaccines SARS-CoV-2, against according to Our World in

Data. However, none of this would be possible without the breakthroughs in the chemical synthesis of nucleic acids. Now, after more than fifty years of technological developments, the manufacture of RNA and DNA is fully-automated and democratised-to the point that several "benchtop" synthetic devices are commercially available. Amidst the Top Ten selection, this is probably the most established in the market. It has successfully transitioned from basic laboratory reactions, with phosphoramidite chemistry at its core, to an innovation landmark of the past century. Nowadays, the synthesis of nucleic acids has advanced enough to yield results that verge on science fiction. In 2019, Chinese researchers reported a proof-of-concept synthesizer that used the same principles as a conventional inkjet printer. Using this technology, scientists printed different strands of DNA directly and precisely into silicon microreactors-devices with a myriad of applications in chemistry, biotechnology, and medicine [18]. Big IT companies, such as Microsoft and Western Digital, are currently exploring the possibilities of chemically-synthesised DNA for data storage-and the results are very promising. The latest results hint that nucleic acids pack information more durably and densely than conventional magnetic solutions, up to seventeen exabytes per gram, according to recent studies [19]. Beyond these technological advances, the automated chemical synthesis could lead to novel therapies with tremendous potential. As of 2020, the FDA had approved eleven drugs based on oligonucleotides-and several more are currently undergoing medical trials. Leading chemical and pharmaceutical companies-Biogen, Merck, Bausch & Lomb, among others-are studying this technology, which is becoming increasingly popular after the triumph of mRNA-based COVID vaccines. Targets include cancer, infectious diseases, diabetes, and more-all encompassed within SDG 3 [20]. Finally, these decades-old chemical developments yield promising results, proving anew that funding basic scientific research is paramount for progress [21].

#### Sonochemical coatings

### Safer, more durable materials with value-added properties

Physical stimuli regulate IUPAC Top Ten Emerging Technologies such as mechanochemistry, liquid-gating, and high-pressure inorganic chemistry. Under unique conditions, chemicals often behave surprisingly—yielding previously unimagined properties and capabilities. Sonochemistry—the use of (ultra)sonic waves to trigger chemical reactions—stands out among these phenomena, particularly for its huge potential to manufacture

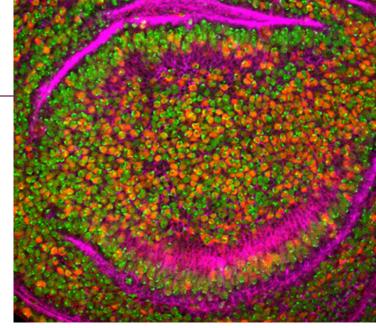


innovative functional materials with value-added properties [22]. This year IUPAC highlights the potential of sonochemistry in surface coating, a technology that directly contributes to several SDGs. This type of treatment conveys all sorts of different properties to a given surface-magnetic, fluorescent, and antimicrobial, among others. The latter has proven especially important during the COVID-19 pandemic, as different surfaces in hospitals, public venues, and others with which we interact in our daily lives required effective antiviral properties to eliminate SARS-CoV-2 residues. Sonochemical coatings cover textiles with antibacterial nanoparticles of metals such as silver, copper, and zinc-all of which reduce the occurrence of hospital infections [23]. Furthermore, several studies show that antibacterial sonochemical coatings withstand many washing cycles without a decrease in performancesomething key in real-life settings in which where garments constantly undergo professional cleaning at high temperatures. Sonovia, an Israeli start-up, uses zinc-nanoparticle sonochemical coatings on reusable masks that kill over 99% of bacteria, virus and fungi, according to their website. Moreover, certain coatings yield 'smart' materials. For example, Spanish researchers covered textiles in Prussian blue nanoparticles, which detect strains of pathogenic bacteria with a simple colour change; they expect that this development could prevent bacterial infections in crowded settings beyond hospitals [24]. Sonochemical coatings provide advantages in the fields of food safety and energy, too, covering strawberries with antibacterial compounds extends their shelf life and the coating of lithium-ion batteries provides high performance and stability. For these reasons, several companies are exploring new possibilities to scale-up this technology to an industrial setting and developing roll-to-roll methods that enable continuous production of coated materials. The European Commission also funded the SONO project with more than €8 million to attain this goal [25]. As an emerging technology, sonochemical coatings now ought to survive the "valley of death" and successfully bridge the gap with industry.

# Chemiluminescence for biological use

### Water-soluble dioxetanes improve the speed and sensitivity of biological tests

Luminescence has always fascinated humans. Admiring the green glow of fireflies and the blue shine of algae is just magical. Scientists have learned to harness the power of these chemical reactions luminol helps crime scene investigators detect blood and the 2008 Nobel prize-winning green fluorescent protein (GFP) lights up biological samples, simplifying microscopy. Yet, scientists thrive to keep improving light-emitting molecules for applications in efficient diodes, safety signalling, biological studies, and more. Recently, researchers discovered highly-efficient chemiluminescent probes with great potential for applications in biology, biotechnology, and medicine. Based on dioxetanes-four-membered, saturated oxygen heterocycles-these molecules sparkle remarkably under physiological conditions, sometimes thousands of times brighter than previous solutions. Most importantly, dioxetanes perfectly perform their duty in water, unlike competitors that need organic solvents. This expedites analyses because chemiluminescent processes happen in vivo, like enzymatic solutions, with a comparable quantum yield [26]. This emerging technology is still in an early stage, yet many interesting applications have already arisen. Among other things, dioxetane probes show great promise detecting certain types of tumours, and even help differentiate between cancer subtypes. They also enable ultra-sensitive detection of pathogenic bacteria such as Salmonella and Listeria, linked to serious foodborne illnesses that cause serious problems even today. Furthermore, dioxetanes bring interesting opportunities to the field of live cell imaging, which could accelerate the understanding of fundamental biochemical processes, as well as provide novel sensitive diagnostic tools. Some molecules even exhibit emission in the near-infrared region, a wavelength with greater penetration than visible light-opening the door to both non-invasive diagnostics and localised treatments [27]. It is remarkable that Biosynth-a company that recently merged with Carbosynth-expressed interest in these novel dioxetane chemiluminescent compounds, and soon started commercialising them. In an official press release, Biosynth's president stated that the potential



of this technology is huge and likely to dramatically improve the speed of biotests [28]. Glowsticks also shine thanks to dioxetanes [29]. Perhaps water-soluble dioxetane probes will become equally popular.

#### Sustainable production of ammonia Green alternatives to the Haber-Bosch process

The Haber-Bosch process for the synthesis of ammonia is one of the most successful chemical reactions of all time. It enables the transformation of atmospheric nitrogen-mostly inert, thanks to the second strongest chemical bond in a diatomic molecule-into ammonia, then nitrates and nitrites, which are used across industries to make fertilisers, plastics, fibres, refrigerants, and more. This single reaction catapulted the demographic boom of the 20<sup>th</sup> century and currently yields over 200 million metric tons of ammonia annually. However, all of this comes at high cost—the production of ammonia emits more carbon dioxide than any other industrial process, without considering all the subsequent transformation into different chemicals [30]. Of course, we need to change that-chemists need a sustainable alternative to make ammonia and remove the strong ties to fossil fuels and greenhouse emissions. To achieve this, they envision two complementary strategies. On one hand, they seek inspiration in Nature-particularly nitrogenases in bacteria and cyanobacteria, which reduce dinitrogen thanks to an iron and molybdenum cofactor. Recent studies only showcase the wisdom of evolution—few metals top the performance of the two that are naturally present in enzymes. Nevertheless, they also favour hydrogen evolution, an unwanted competing reaction, and only the rational design of catalysts will enhance the selectivity of the process towards nitrogen reduction. Some solutions include supporting catalysts onto layered materials or encapsulating them into zeolitic cages. On the other hand, chemists harness the power of electricity to break the triple nitrogen-nitrogen bond and, at the same time,



harvest hydrogen atoms from water. If the energy used comes from renewable sources-wind, hydroelectric, solar-the process becomes doubly sustainable, since it avoids relying on hydrogen obtained from the reforming of fossil fuels. The main challenge here is reducing the electric potential needed, while maximising activity and selectivity. So far, current solutions are far from beating the appeal of Haber-Bosch, hence several companies and funding agencies are supporting research to make hydrogen production greener [31]. Moreover, ammonia technically 'stores' hydrogen, a green fuel that only yields water when burnt, and it could eventually become an alternative to fossil fuels on its own. Unlike hydrogen, ammonia is easily liquified under mild conditions, which will simplify storage and transportation. Australian researchers are optimistic, envisaging a successful ammonia economy by 2040. Before that, we will develop carbon capture technologies to diminish the impact of Haber-Bosch production, then move this process to renewable hydrogen sources. In the latest phase of their roadmap, ammonia will come exclusively from the electrochemical reduction of dinitrogen - eliminating carbon emissions throughout the process [32]. Although many fundamental studies are still ongoing, certain solutions for the manufacture of green ammonia have already reached high TRL, including private endeavours by Yara (Australia), Hiringa Energy (New Zealand), Topsoe (Denmark) and Iberdrola (Spain). Green fertilisers, plastics, and fuels will come alongside sustainable ammonia, contributing to SDGs across the board, from clean energy and efficient agriculture to sustainable cities and responsible production [33].

#### Targeted protein degradation Harnessing our cells' machinery to revolutionise pharma

As previously mentioned, chemists and biochemists often find inspiration in nature. Once again, this is exactly the case of targeted protein degradation (TPD), an innovative chemical tool with great therapeutic potential. The principle is rather simple: harnessing our own cells' degradation pathways to eradicate problematic proteins. This technology has attracted multi-billion in investments, stimulated the creation of start-ups, and even started diverse clinical trials. The key to TPD are small molecules that trigger proteolysis, often known as PROTACs. Their structure is cleverly designed to hijack protein-degrading enzymes and link them to a specific target, which is then eliminated in lieu of the original victim [34]. The potential for medicinal chemistry is tremendous. Before TPD, our strategies to block proteins were mostly limited to inhibitors, which need a specific binding pocket. However, only one in four proteins showcase said functionality-here TPD offers a therapeutic advantage, triggering the elimination of harmful structures. In addition, tracking proteins directly avoids complicated alternatives to knock them out using genetic engineering or small nucleic acids, often instable in vivo [35]. Rationallydesigned PROTACs (as well as other molecules with similar effects) show great promise in the treatment of cancer. Arvinas, a Yale University pioneer spin-off, has entered clinical trials with drug candidates against breast and prostate cancer based on TPD-molecules, providing the first ever in-human data for this technology [36]. Other companies soon followed, including Cullgen, Kymera, Zexin, and Nurix. Big pharmaceutical industries such as Pfizer, Bayer, Novartis, and Amgen, among others, have also seen the potential of TPD and have invested significant amounts to further develop these new drugs. Beyond cancer, researchers explore the possibilities of TPD to treat illnesses related to protein accumulation, including neurodegenerative diseases such as Parkinson's and Alzheimer's. Preliminary studies show that PROTAC-mediated TPD is a good strategy to trigger the elimination of certain protein aggregations-among them pathogenic tau protein, linked to Alzheimer's [37]. TPD expert Craig Crews, co-founder of Arvinas, predicts these results are just the beginning of a new revolution in the pharmaceutical industry. Indeed, a hopeful emerging technology.

#### Single-cell metabolomics Analysing biomolecules, one cell at a time

Last year, the IUPAC Top Ten Emerging Technologies initiative recognised the potential of nanosensors in the detection of single molecules, often called "the ultimate sensitivity." Indeed, the latest advances in chemistry have enabled analyses with unprecedented levels of precision. In this direction, this year's search recognises the progress in single-cell metabolomics. The progress in imaging techniques and technologies such as mass spectrometry have provided new insights into individual cells. Thanks to the enhanced resolution and sensitivity of current mass spectrometers, chemists can analyse several metabolites simultaneously, getting detailed information about cellular pathways, biological mechanisms, as well as unique fingerprints of cells and samples. To optimise the outcome with smaller sample volumes, mass spectrometers extract the entire content of one cell at once. Both electrosprays and lasers offer great alternatives for ionisation. More detailed techniques even enable the analysis of specific cellular parts, using microextractions, capillary samplings, and advanced separations coupling chromatography and electrophoresis. The finest combinations not only provide information about the nature of metabolites, but also provide details on concentration and their special arrangement. The potential to unravel unknown biochemical mechanisms is extraordinary. Nowadays, researchers seek to improve detection limits, as well as develop digital tools. These will serve many purposes: from enriching databases to accelerating the recognition of metabolites to enhancing algorithms to distinguish noise and artifacts from actual biological variability [38]. In the context of the coronavirus pandemic-and future outbreaks-single cell metabolomics will demonstrate their vast possibilities. Several studies harness their power to better understand infection processes and the interactions between the invading virus and our cells [39]. For some experts, the field is still young and full of complex challenges ahead. However, scientists progressively solve these challenges and further validate this emerging technology, which could bring sound answers to fundamental biochemical secrets [40].

#### A bright future ahead Chemistry to tackle prominent societal challenges

The IUPAC Top Ten Emerging Technologies in Chemistry initiative is utterly beautiful. Year after year, it highlights the most exciting developments in a wide variety of fields, from blossoming discoveries



to established techniques already adopted by adventurous start-ups and audacious industries. Experts throughout the world suggest and select the collection-a family that now gathers 30 up-and-coming innovations with huge potential to transform our society. Several tackle environmental challenges, paving the way towards a sustainable world. Others envision novel systems to reduce, reuse, and recycle resources better, headed for a zero-waste, circular-economy. Finally, some of the Top Ten facilitate our transition to the new normal after the terrible coronavirus pandemic. Among these, many prepare us for forthcoming outbreaks and future pathogens-chemistry is crucial to avoid future health crises, key in fields from materials to pharmaceutical sciences. As we announce the 2021 Top Ten Emerging Technologies in Chemistry, we simultaneously begin our search for the 2022 candidates. Every chemist is kindly invited-indeed encouraged-to submit nominations, as IUPAC looks forward to further expanding and establishing this initiative. Please join us on our exciting journey. 📟

#### Acknowledgements

This initiative is only possible thanks to the outstanding group of experts who identified and curated the list of technologies; they are: Michael Droescher (Chair), Jorge Alegre-Cebollada, Sophie Carenco, Javier García Martínez, Ehud Keinan, Rai Kookana, Greg Rusell, Ken Sakai, Natalia P. Tarasova, and Bernard West. Many thanks to Bonnie Lawlor, for all her valuable corrections and contributions that enhanced the quality of this article.

#### References

 IUPAC (2019). "Top Ten Emerging Technologies in Chemistry". https://iupac.org/what-we-do/top-ten/ Accessed on 19/07/2021.

- 2. United Nations (2015). "Sustainable Development Goals". https://sdgs.un.org/goals
- 3. Matlin, S.A., et al. Nature Chem. 2015, 7, 941.
- NIST (2018). "Blockchain Technology Overview". NISTIR 8202, https://doi.org/10.6028/NIST.IR.8202 Accessed on 19/07/2021.
- 5. Hanson-Heine, M.W.D. and Ashmore, *A.P. Chem. Sci.* 2020, 11, 4464.
- Clark, B. "Blockchain and IP Law: A Match made in Crypto Heaven?" WIPO Magazine, February 2018.
- CEFIC (2019). "Molecule managers". https://cefic. org/app/uploads/2019/06/Cefic\_Mid-Century-Vision-Molecule-Managers-Brochure.pdf. Accessed 19/07/2021.
- Gartner.com, 3 June 2019 "Gartner Predicts 90% of Current Enterprise Blockchain Platform Implementations Will Require Replacement by 2021".
- 9. Sefah, K., et al. PNAS 2014, 111, 1449.
- 10. Hoshika, S., et al. Science 2019, 363, 884.
- 11. Zhang, Y., et al. *Nature* 2017, 551, 644.
- 12. Young, T. Philos. Trans. R. Soc. London. 1805, 95, 65.
- 13. Wu, Y., et al. *Adv. Mater.* 2018, 31, 1800718.
- 14. Liu, M., et al. Nat. Rev. Mater. 2017, 2, 17036.
- 15. Yang, F., et al. *Sci. Total Environ.* 2019, 686, 1140.
- (a) Yang, F. and Antonietti, M. *Adv. Sci.* 2020, 7, 1902992. (b) Yang, F., et al. *Chem. Soc. Rev.* 2021, 50, 6221.
- 17. Sousa-Rosa, S. et al. Vaccine 2021, 39, 2190.
- 18. Li, H. et al. Sci. Rep. 2019, 9, 5058.
- 19. Vitak, S. "Technology alliance boosts efforts to store data in DNA". *Nature*, 3 March 2021.
- 20. Roberts, T.C., et al. Nat. Rev. Drug Discov. 2020, 19, 673.
- 21. Berry, D.J. Hist. Technol. 2019, 35, 374.
- 22. Foroughi, F., et al. Catalysts 2021, 11, 284.
- 23. Perelstein, I., et al. Ultrason. Sonochem. 2015, 25, 82.

- 24. Ferrer-Vilanova, A., et al. *Ultrason. Sonochem.* 2021, 70, 105317.
- CORDIS (2013). "A pilot line of antibacterial and antifungal medical textiles based on a sonochemical process". Grant agreement ID: 228730, https:// cordis.europa.eu/project/id/228730/en. Accessed on 02/08/2021.
- 26. Hananya, N. and Shabat, D. *Angew. Chem. Int. Ed.* 2017, 56, 16454.
- 27. Green, O., et al. J. Am. Chem. Soc. 2017, 139, 13243.
- 28. RAMOT Tel Aviv University, News 15 August 2017 "Tel Aviv University announces collaboration with Biosynth on pioneering chemiluminescent molecules".
- Compound Interest (2016). "The Chemistry of Glow Sticks". https://www.compoundchem.com/2014/10/14/ glowsticks/ Accessed 19/07/2021.
- 30. Kriestch-Boerner, L. Chem. Eng. News 2019, 97, 18.
- 31. Yang, B., et al. *Energy Environ. Sci.* 2021, 14, 672.
- 32. MacFarlane, D.R., et al. Joule 2020, 4, 1186.
- 33. Bella, F. ChemSusChem 2020, 13, 3053.
- 34. Alabi, S.B. and Crews, C.M. *J. Biol. Chem.* 2021, 296, 100647.
- 35. Luh, L.M., et al. Angew. Chem. Int. Ed. 2020, 59, 15448.
- 36. Halford, B. Chem. Eng. News 2021, 99, 5.
- 37. Kargbo, R.B. ACS Med. Chem. Lett. 2019, 10, 699.
- 38. Duncan, K.D., et al. *Analyst* 2019, 144, 782.
- 39. Kumar, R., et al. Front. Microbiol. 2020, 11, 1152.
- 40. Fessenden, M. Nature 2016, 540, 153.

Fernando Gomollón-Bel <fer@gomobel.com> is the Graphene Flagship Press Coordinator and a freelance science communicator based in Cambridge, UK. He is also a collaborator of the European Young Chemists' Network, EuChemS.



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

The deadline for nomination is 31 March 2022.

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

#### News and information on IUPAC, its fellows, and member organizations. See also www.iupac.org/news

# IUPAC Wire

# *Chemistry International*—Freely-Available Across the World

rom January 2022 *Chemistry International* will be freely-available to all in electronic form and will no longer be available in print. The objective is to make it readily-available to a much broader audience. It will still be published four times a year and whilst retaining its familiar layout, will be web based in a page-turning format from both the De Gruyter and IUPAC websites.

#### by Colin Humphris

#### Chair of Chemistry International Editorial Board

This is obviously a major change for *Chemistry International* that has been available in print form since 1979, but we want to leverage the opportunities of a digitally-connected world. We want to access a far larger international readership to raise interest in IUPAC and its valuable work. At the same time, we have had to recognise the limitations and costs of international distribution of paper magazines. During the autumn the Secretariat will be contacting all members and current subscribers to advise them of any changes to their membership and entitlements and promoting the new format and access.

This is a step towards a *digital first format* that IUPAC is currently working with DeGruyter to design. The eventual objective is to provide, news, comments, feature articles, project updates and book reviews in real time together with other digital features such as video and webinars. This is work in progress as we explore the capabilities of both the new DeGruyter publishing platform and our own website.

We feel this is an important symbolic, change as IUPAC adapts its data, standards and nomenclature to the digital needs of those who rely on us. Our first century was focussed on the printed form and the availability of reliable, validated chemical information was a key driver for innovation through the twentieth century. The pace of change is accelerating in a digital world and IUPAC will need to evolve to meet these needs. InChI is a good example of the different ways of working and the value of partnerships with users. Expect to see far more of this. These will be exciting times for the Union.

Please enjoy next year's page-turning format, encourage your friends and colleagues to both read *Chemistry International* and to contribute to it as a medium to highlight the pivotal role of chemistry in addressing the challenges the world faces today and tomorrow.

https://iupac.org/what-we-do/journals/chemistry-international/

#### IUPAC Announces the 2021 Top Ten Emerging Technologies in Chemistry

UPAC has released the results of its 2021 search for the Top Ten Emerging Technologies in Chemistry. The goal of this project is to showcase the transformative value of Chemistry and



to inform the general public on the potential of the chemical sciences to foster the well-being of Society and the sustainability of our Planet. Following the same guidance as it did last year, the Jury\*, a selection of international experts, identified different emerging technologies, scientific advances in between a discovery and a fully-commercialized ideas, with outstanding capacity to open new opportunities in chemistry, sustainability, and beyond. The 2021 finalists are (in alphabetical order):

- Artificial humic matter from biomass
- Blockchain technology
- Chemiluminescence for biological use
- Chemical synthesis of RNA and DNA
- Semi-synthetic life
- Single cell metabolomics
- Sonochemical coatings
- Superwettability
- Sustainable production of ammonia
- Targeted protein degradation

IUPAC Vice President, Javier García Martínez, said that "In the last months, we have witnessed how vital chemistry is in facing and overcoming our most pressing challenges. Moving forward, these threats will only be more complex and unpredictable—as the recent IPCC report alerts us to the risk posed by climate change for our survival. With the Top Ten Emerging Technologies in Chemistry, IUPAC provides a fresh look at technologies that are already creating new opportunities and opening new avenues for research and industry. I hope this year's edition arouses the same interest and attention as previous IUPAC Top Ten selections."

The 2021 Top Ten Emerging Technologies in Chemistry are further detailed in a feature article published in this issue of *Chemistry International*, see page 13. The author, Fernando Gomollón-Bel, remarks: "While highlighting breakthroughs for a circular, climate-neutral future, the selected technologies

will change our world for the better, making a more thoughtful use of our resources, favoring more efficient transformations, and providing more sustainable solutions in applications."

The first selection of Top Ten Emerging Technologies in Chemistry was released in 2019 as a special activity honoring IUPAC's 100th anniversary; the results were published in the April 2019 (*Chem Int*, 41(2), pp. 12-17, 2019; https://doi.org/10.1515/ci-2019-0203). The 2020 results were published in October 2020 (*Chem. Int.* 42(4) pp. 3-9, 2020; https://doi.org/10.1515/ci-2020-0402)2019.

The next search for the Top Ten Emerging Technologies in Chemistry has already begun and the deadline for submission is 31 March 2022. It will be led again by Michael Droescher.

For more information on the 2019 and 2020 selections and on the search for the 2022 Top Ten Emerging Technologies in Chemistry go to: https://iupac.org/ what-we-do/top-ten/.

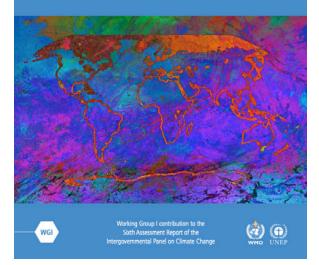
\*The Jury was an international group of objective and unbiased experts who reviewed and discussed a pool of nominations, and ultimately selected the final top ten. The following comprised the panel of judges for the 2021 Top Ten Emerging Technologies in Chemistry: Chair, Michael Droescher, (German Association for the Advancement of Science and Medicine), Jorge Alegre-Cebollada (Centro Nacional de Investigaciones Cardiovasculares, Spain), Sophie Carenco (French National Center for Scientific Research, France), Javier García Martínez (Universidad de Alicante, Spain), Ehud Keinan (Technion, Israel), Rai Kookana (CSIRO Land & Water, Australia), Greg Russell (University of Canterbury, New Zealand), Ken Sakai (Kyushu University, Japan), Natalia P. Tarasova (D. I. Mendeleev University of Chemical Technology, Russia), and Bernard West (Life Sciences Ontario, Canada).

# Climate Change 2021—The Physical Science Basis

he Intergovernmental Panel on Climate Change (IPCC) is the United Nations body responsible for assessing the science related to climate change. The Sixth Report from IPCC Working Group 1 published in August 2021 paints a very sombre picture for the future. This report was commented on in a news item by the International Science Council (ISC) on behalf of its members, of which IUPAC is a founding member.

The report presents the latest advances in modelling and improved historical data to lead to the undeniable INTERGOVERNMENTAL PANEL ON CLIMATE CHARGE

#### Climate Change 2021 The Physical Science Basis



conclusion that the whole world is experiencing the effects of climate change and that this is due to human activities. The extreme weather events which have occurred in 2021 are not taken into account. The goal of the Paris Agreement is that global warming is held to well below 2 °C with respect to pre-industrial values and efforts should be pursued to limit warming to 1.5 °C. All five emission scenarios considered in the IPCC report lead to warming greater than 1.5 °C and three of the five have warming of 2 °C or greater by 2041 to 2060. The curbing of greenhouse gas emissions, mainly carbon dioxide, reducing the carbon footprint, will improve the situation and could potentially reverse the temperature trend later in the century if decisive action is taken urgently now. Ambitious targets are required and implementation is needed immediately.

Chemistry, often referred to as the central science, is crucial in the battle against climate change. Ways of reducing consumption of energy in chemical reactions and processes, renewable fuels produced from sunlight with photocatalysts, reagent recycling and waste reduction, new and more efficient materials are all needed. IUPAC, as a worldwide resource for chemistry with over a thousand volunteer scientists who are experts in their fields of chemistry, from academia and industry, can and must make an important contribution to these questions.

Christopher Brett, IUPAC President commented: "This landmark report on climate shows the current state of the world and the need for decisive and incisive action. We strongly support the statement by the ISC and emphasise the important role that chemistry will

play in addressing the challenges. This is in accordance with a vision for IUPAC to be a global resource for chemistry for the service of humankind and the world. We are already working on many of the topics which will be crucial and we offer our expertise in addressing these issues which must be carried out in collaboration between all scientists and society as a whole."

IUPAC has worked for years in several fields related to the challenges of climate change and the environment, green chemistry for sustainable development and world needs. Before the Covid-19 crisis, it was already implementing an organisational drive to make much greater use of on-line meetings, thus reducing travel and decreasing our carbon footprint.

Examples of IUPAC projects that address the challenges associated with climate change are:

- Evaluated Kinetic Data for Atmospheric Chemistry
- Climate and Global Change: Observed Impacts on Planet Earth
- Multi-scale Biogeochemical Processes in Soil Ecosystems: Critical Reactions and Resilience to Climate Changes
- Assessment of the Contribution of IUPAC Projects to the Achievement of the United Nations Sustainable Development Goals
- Visualizing and Understanding the Science of Climate Change
- Systems Thinking in Chemistry Education
- Systems Thinking in Chemistry for Sustainability: Toward 2030 and Beyond
- Green and Sustainable Chemical Processes

The cover of the IPCC report is *Changing* by Alisa Singer, "As we witness our planet transforming around us we watch, listen, measure...respond." www.environmentalgraphiti.org - 2021 Alisa Singer.

#### https://iupac.org/climate-change-2021-the-physical-science-basis/

# 2022 IUPAC-Richter Prize—Call for Nominations

UPAC and Gedeon Richter, Plc. are pleased to announce the 2022 IUPAC-Richter Prize in Medicinal Chemistry.

The 2022 IUPAC-Richter Prize will be presented during the 37th ACS National Medicinal Chemistry Symposium (26-29 June 2022) in New York (USA) and the recipient will also give a lecture on the subject of their research at the XXVII EFMC International Symposium on Medicinal Chemistry (4-8 September 2022) in Nice (France).

The prize–USD 10,000–is to be awarded to an internationally recognized scientist, preferably a medicinal chemist, whose activities or published accounts have made an outstanding contribution to the practice of medicinal chemistry or to an outstanding example of new drug discovery.

The Prize has been established by a generous gift from the **Chemical Works of Gedeon Richter**, **PIc**. (Budapest, Hungary) to acknowledge the key role that medicinal chemistry plays toward improving human health.

Applicants should be received by nomination only, with just one person needing to serve in that capacity, although a total of five (5) individuals should be listed as referees overall. The package must be submitted electronically and should contain a complete resume, a professional autobiography of not more than two pages, and a one-page summary of what the individual considers to be his/her activities, accomplishments and/or publications that have had the most significant impact upon the field of Medicinal Chemistry. The material will be forwarded confidentially to an independent selection committee appointed by the IUPAC Subcommittee on Medicinal Chemistry and Drug Development.

For further information please contact Janos Fischer, Chair of the Jury and member of the IUPAC Sub-committee on Drug Discovery and Drug Development, by email at <j.fischer@richter.hu>

Nomination materials should be submitted by 15 December 2021

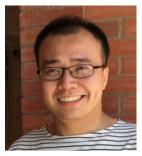
https://iupac.org/2022-iupac-richter-prize-call-for-nominations/

#### Awardees of the 2021 IUPAC-Zhejiang NHU International Award for Advancements in Green Chemistry

e are delighted to announce the 2021 recipients of the established IUPAC-Zhejiang NHU International Award for Advancements in Green Chemistry. We congratulate **Gabriele** Laudadio from the Scripps Research Institute, Lichen Liu from Tsinghua University, and Jingxiang Low from University of Science and Technology of China as the early career award winners, and David Milstein from the Weizmann Institute of Science, Israel for the experienced chemist award.



Gabriele Laudadio



Lichen Liu



Jingxiang Low



David Milstein

These awards were presented during the 2021 Virtual IUPAC Congress in August at a special Symposium scheduled in the Chemistry for Sustainability thematic program in coordination with IUPAC's Interdivisional Committee on Green Chemistry for Sustainable Development (ICGCSD).

The IUPAC-Zhejiang NHU International Award was been established in 2019 to encourage young and experienced chemists alike, and to emphasize the importance of advancements in Green Chemistry, and demonstrating how it adds value to human progress.

The 2021 Winners of the IUPAC-Zhejiang NHU International Award have been invited to prepare a review article for publication in an upcoming issue of *Pure and Applied Chemistry*.

This award, managed by the ICGCSD, is presented every two years. Look for the announcement of the next call in 2022 ahead of the 2023 IUPAC World Chemistry Congress that will take place in the Netherlands. For further information about the IUPAC-Zhejiang NHU International Award, see https:// iupac.org/what-we-do/awards/

See the following page for a brief bio of each awardees: https://iupac.org/awardees-ofthe-2021-iupac-zhejiang-nhuinternational-award-for-advancements-in-green-chemistry/

#### An Interview with Joseph Wang

Professor Joseph Wang of the University of California San Diego (UCSD), USA, is the first to be awarded the IUPAC Analytical Chemistry Medal—an award that recognizes a significant lifetime contribution to analytical chemistry and for researchers who have a substantial record of



Joseph Wang

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.

He spoke with Dr. Vera Koester of *ChemistryViews* about his current research, especially the exciting development of wearables, and giants in chemistry.

What does it mean to you to receive the IUPAC Analytical Chemistry Medal and to be the first to receive it?

It has been a great surprise and is a great honor. I have received numerous international awards, and this is a kind of global recognition. In analytical chemistry we don't have a global award, which makes this very prestigious.

#### What are current trends in the field of sensors?

There is this trend of moving away from the big laboratory to smaller and smaller home testing and towards the body: the lab on the skin or in the mouth. That's true for all techniques. This field began benefitting from nanotechnology 10 to 20 years ago.

I'm glad to be part of this revolution of moving to home testing and towards real-time on-body testing.

### So do you think in 50 years' time we will measure everything that we are doing right away?

Oh, yes, in 50 years for sure. The future will bring increasingly smaller sensors. So at some point you will have a complete lab under your skin. You will swallow a lab in a capsule—namely swallow a small capsule that will then analyze your gut. In fact, you will see that within 10 years. We don't have to wait 40 or 50 years for that.

Sounds amazing but also scary. You have access to so many sensors, what do you monitor on yourself?

Oh, mainly my steps and sometimes my blood pressure.

### What do you like most about IUPAC and what do you think could be different?

IUPAC is responsible for somehow standardizing everything. That is very good. Even in electrochemistry, we have different nomenclatures. Sometimes we use different names for the same techniques or present results in different ways. There was also a lot of confusion in the beginning about what exactly a biosensor is. In my opinion, they did a good job in defining it.

It's also extremely important to take a global perspective. In materials, we have MRS as the global conference for material science; Pittcon is the biggest international conference in analytical chemistry. IUPAC needs to have more visibility. I would like to see IUPAC take a leading role in the top sciences. Merging IUPAC's analytical topics and sessions with Pittcon would mean more visibility for analytical chemistry.

Read full interview in ChemistryViews: https://doi.org/10.1002/chemv.202100077

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

#### In Memoriam

#### Gus Somsen 23 July 1932-12 June 2021

Gus Somsen passed away peacefully in Hoogeveen, Netherlands, while having struggled with Alzheimer's for some time. Gus often said that he enjoyed his work for IUPAC, and his former colleagues on IUPAC Bureau and Executive Committee remember his optimistic outlook on life and his problem solving ability. He was energetic and creative in his thinking and made significant contributions to the IUPAC organization as his records show.

Prof. Somsen graduated in chemistry in 1956 after studying at Vrije Universiteit (VU) in Amsterdam. He received his Ph.D. in physical chemistry after working with Jan Coops. After military service as an officer in the field artillery, in 1958 he joined the faculty of the Department of Chemistry at VU as an instructor and was subsequently promoted to associate professor



Gus Somsen (left) accepts the IUPAC service award from IUPAC President Bryan Henry in 2007 at the General Assembly opening held in the Aula Magna /Rektorat located on the Piazza Castello, in the center of the old city of Torino.

(1964), senior lecturer (1971), and then to professor of physical chemistry in 1980. Somsen served as head of the Department of Chemistry (1980-1983 and 1993-1997), vice rrector of the university (1983-1985), dean of the faculty of Natural Sciences (1985-1987), and member of the University Council (1988-1990) at VU. He became emeritus professor in 1997.

Prof. Somsen's research interests were in experimental chemical thermodynamics, physical chemistry of solutions, and liquids and liquid structures. He authored about 120 publications on thermochemistry and physical chemistry of solutions. He held memberships in the Chemistry Committee of the Royal Netherlands Academy of Arts and Sciences (KNAW), the Royal Dutch Chemical Society (KNCV) and the Royal Society of Chemistry (UK), and served as a member of the editorial advisory boards on several journals.

In IUPAC Prof. Somsen served in numerous positions, starting as a Member (1977-1985) and Chair (1985-1989) of the Commission on Thermodynamics (I.2); Member (1990-1991), Secretary (1992-1993), Vice President (1994-1995), President (1996-1997), Past President (1998-1999), and Associate Member

of the Physical (and Biophysical) Chemistry Division (I) Committee (2000-2001). Following his service in Division I, he was elected on the IUPAC Bureau (1998-2003); in 1998, he chaired the Ad Hoc Committee on Project Evaluation Criteria, and continued as member on the then newly created Project Committee, which he ended up by chairing from 2004 to 2007.

Somsen won numerous awards and in 1995 he was designated an Officer in the Order of Orange Nassau from Her Majesty, the Queen of the Netherlands. He completed his IUPAC tenure in 2007 and was presented his service award by IUPAC President Bryan Henry during the opening ceremony of the General Assembly in Torino.

Wij zijn verdrietig maar dankbaar voor alles wat hij voor IUPAC en anaderen betekend heeft.

He is survived by his wife, Elly, four children, several grandchildren and great-grandchildren.

#### Aubrey Dennis Jenkins

#### 6 September 1927-25 April 2021

#### A tribute by Dick Jones and Claudio dos Santos

Former friends and colleagues were deeply saddened to learn of the death of Emeritus Professor Aubrey Jenkins on 25 April 2021. Aubrey grew to be a distinguished figure within the IUPAC Polymer Division after joining its forerunner, the Macromolecular Division, as a member in 1975. His distinction was equally recognised within both industry and academia by the international polymer community.

Born in London in 1927, he attended Dartford Grammar School from where he matriculated to the University of London in 1943. However, this being at the height of WWII, he needed to take a job, but undeterred he also enrolled as a part-time student at the University's Sir John Cass Technical Institute from where he progressed to King's College, graduating B.Sc. in Special Chemistry with 1st Class Honours in 1948. Awarded the University of London Studentship in Chemistry for 1948, by 1950 he had gained his PhD.

From 1950 to 1964, Aubrey was an industrial chemist, firstly with Courtaulds Ltd. at its Fundamental Research Laboratory at Maidenhead in Berkshire and thereafter with Gillette Industries Ltd at Reading. At Courtaulds he was under the direction of C.H. Bamford. For a year, 'Bam' had him investigate the dimerization of methyl ketene before urging a move into the polymer field as it was clear that this was where the company's future would lie if it was to compete with other chemical giants such as DuPont. His first task was to determine the kinetics of the polymerization of acrylonitrile, the monomer that was predicted to constitute 95 % of a future marketable product. Polyacrylonitrile, however, is one of a very few vinyl addition polymers that are insoluble in their own monomer and this work led to what Aubrey told me whilst holidaying together in the south of France in 2011, that he considered to be the most scientifically significant discovery of his career, kinetic evidence of 'trapped' radicals, the existence of which were later to be indisputably proven by EPR.

Between 1956 and '62, the team of Bamford, Jenkins and Johnston also published about ten papers on the reaction between polymer radicals and transition metal salts and determinations of rates of initiation in vinyl polymerization based on the same chemistry. It is worth pausing to reflect that were it not for a temperature difference of about 80 °C, atom transfer radical polymerization might have hit the billboards many years earlier.

In 1960, the parting of the ways of Bamford and Jenkins was inevitable when Aubrey accepted a long-standing offer to become Head of Chemistry at Gillette Industries. This was a managerial role and although while at Courtaulds he had already travelled widely in Europe, particularly Eastern Europe during the communist era, and in 1959 had accepted an invitation to lecture at a Gordon Conference (his first visit to the USA), he now had to make many transatlantic trips. Typically, these were 'Gillette-focussed' visits to Boston, Chicago and ultimately Washington DC where he was eventually to be seconded for a year. While he was able to recruit excellent scientists of his own choosing he missed the days of open scientific discussion. Secrecy attached to all his team's research but at least it led him into legal work which was to become a source of enjoyment throughout his later career.

To Aubrey, Washington was the most beautiful city in the US and there is no doubting that Gillette hoped that he would resettle there. However, from Colin Eaborn (later Sir Colin) he received an offer he had no wish to refuse: to join the staff of the new University of Sussex as a Senior Lecturer in Chemistry. He took up his new post in 1964 and remained at Sussex throughout the rest of his career, ascending to Reader (1968), Professor of Polymer Science (1971) and serving as Dean of the School of Molecular Science from 1973-78 before eventually retiring in 1992.

At Sussex, again he built a thriving research team and thereby consolidated his already notable international research reputation. Free radical polymerization mechanisms remained a lifelong dominating interest and even after retirement, he picked up on what he and Bam had started, the "Patterns of Reactivity



Aubrey Jenkins

Scheme" for the modelling of radical copolymerization reactions, a development of the Q - e scheme of Alfrey and Price, first presented to the world at the 1959 Gordon Conference. This was the venue that first opened the door to his getting to know a wealth of eminent international polymer scientists and resulted in his receiving many invitations to lecture, each feeding a growing list of lifelong friendships.

In 1975, Aubrey joined the Macromolecular Division of IUPAC (later the Polymer Division) of which he remained an active member until declining health led to his retirement in the early 2010s. From 1977 to 1985 he chaired the Commission on Macromolecular Nomenclature, refusing to refer to it under any other name even after it became the Subcommittee on Polymer Terminology following the millennial structural reorganization of the Union. He was also secretary for the Division from 1985 to 1993. Over the years, his name has featured as co-author or lead author of many of our publications, two of which have notably received over 500 citations.

IUPAC enabled him to travel even more widely but amongst all the countries and continents that he visited during his lifetime; his favourites were Eastern Europe, New Zealand and South America. He could relate tales of adventure and friendship from everywhere he went and it is worthy of note that his last research student, Claudio Gouvea dos Santos from Brazil, is also a present day member of the Subcommittee on Polymer Terminology, and I take pleasure in asking him to write, in a more personal vein, a short finale to this tribute to Aubrey's life and career. However, I cannot end my own contribution without mentioning Aubrey's love of classical music in all its expressions, a love that I share. He frequently attended concerts or operatic/ballet productions wherever he roamed, but particularly in London and Glyndebourne, the world famous opera house just a short distance from his home. There is much of my friendship with Aubrey that I shall personally miss.

Aubrey is survived by his wife Jitka and two sons from his first marriage, nine grandchildren and four great-grandchildren.

#### -Richard (Dick) Jones

Through correspondence, Aubrey had accepted me to study for a PhD under his supervision so, armed with a Brazilian government grant, I arrived at the University of Sussex in 1988. I did not meet him immediately upon my arrival because he had just remarried and was still enjoying a round-the-world honeymoon trip. Two weeks later we met for the first time and I was soon to realize I was in front of a colossal scientist.

Despite his outstanding scientific reputation, Aubrey was to me a very approachable person. During my time at Sussex, apart from delving into the controversies of the various mechanisms proposed for the then newly discovered group transfer polymerisation, about which Aubrey was very passionate, we built a strong relationship and gradually the supervisor turned into a friend. He was a kind and generous man and I was to benefit from his deep knowledge of polymer chemistry, his friendship and wider acquaintance.

Perhaps by my being Brazilian or because he knew I was going to be his last graduate student, I felt a certain affection flowing from him. As Dick has written above, South America was one of his favourite places and, before we met, he had already been to Brazil several times as some kind of "ambassador" for the British



Claudio with Jitka and Aubrey in Rio de Janeiro in 1996

Council. Aubrey loved Brazil and the Brazilian culture. I remember that, at one of the dinners at his home, with great pride and sense of achievement, he surprised me with a glass of *caipirinha* he had prepared himself.

Four years after my return to Brazil at the end of 1992, I was delighted to meet up with Aubrey and Jitka again when they stopped for a few days in Rio on their way to Argentina. I live about 200 miles away and Rio is not a place I go to very often. However, Aubrey knew it like the palm of his hand and gave me several touristic tips that included, not only the best places to visit but also the names and numbers of the buses to take you there! The photo above was taken at the Botanical Garden, one of the not-to-miss spots suggested by Aubrey.

In 2000, I spent a few sabbatical months in UK and had the chance to visit Aubrey and Jitka. Jitka served "duck à *l'orange*" for dinner; even now I can savour the taste when I close my eyes. After that, our contact was mostly by email and through Dick keeping me posted with news about them. In 2006, Dick invited me as an observer to attend the IUPAC Polymer Division Meetings held in conjunction with the IUPAC World Polymer Congress in Rio de Janeiro, and since then I have been a member of the Subcommittee on Polymer Terminology. I was very happy to meet Aubrey in Torino during the IUPAC General Assembly in the following year but it was then that I knew I wouldn't have the chance to welcome them to Brazil again when he told me that his health prevented him from taking long haul flights. However, in Glasgow, during the 2009 General Assembly, I had the pleasure of meeting him for one last time in person.

Aubrey led me along the most important path of my scientific career. I feel privileged to have had him as my supervisor.

-Claudio Gouvea dos Santos



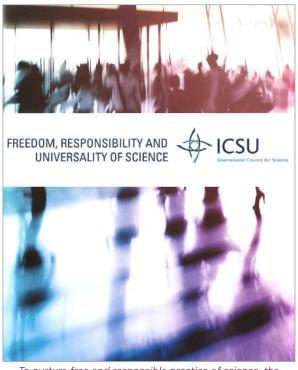
# Up for Discussion

# Combat Ethical Pollution in the Chemical Community

#### by Leiv K. Sydnes

At the IUPAC General Assembly in the middle of August this year, the Council decided to form a new standing committee, the Committee on Ethics, Diversity, Equity, and Inclusion (CEDEI), with the mission to work for the ethical values stated in the Union's strategic plan. This is a significant move because it underlines that international statements and recommendations, outlining ethical guidelines and principles for scientists, are not enough to guarantee that the scientific community "[strives] for diversity and inclusiveness in all forms, [respects] each other and the Union, and [upholds] the highest standards of transparent, responsible and ethical behaviour"[1]. In fact, there are clear indications that the number and nature of violations of the 1979 Vancouver Convention [2], the 2010 Singapore Statement on Research Integrity [3], the 2012 San Francisco Declaration on Research Assessment (DORA) [4], the 2013 Montreal Statement on Research Integrity in Cross-Boundary Research Collaborations [5], and the 2016 ICSU Advisory Note on Science Communication [6], some of the relevant documents to abide to, have increased in recent years.

Unethical research practices and behaviour are nothing new. Publication of "results" based on outright fraud has been known for centuries and increasingly harmed the scientific enterprise in recent decades. But just as worrisome is the growing number of other dubious practises, which include plagiarism, gift authorships, unethical refereeing, improper evaluations, and use of defamatory and insulting language in science-related discussions and debates among scientists. The purpose with all these acts is the same: to improve the likelihood for success in competitions for prestigious positions or appointments, research funding, and all sorts of awards, honours, and prizes. Such activities do indeed contribute to undermine the credibility of science, and this calls for a broadbased action in the scientific community at large. International organizations like the United Nations Educational, Scientific, and Cultural Organization (UNESCO), International Council of Science (ICSU), which in 2018 became International Science Council (ISC) have worked with dedication to strengthen the research integrity globally and nourish science practices based on equity, diversity, and inclusion. However, many of the obstacles to achieve this are

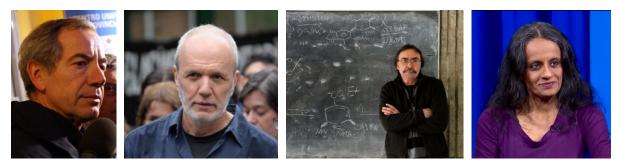


To nurture free and responsible practice of science, the research community must promote equitable opportunities and oppose all sorts of discrimination. How to go about in practice to achieve that is discussed in this booklet, which can be downloaded from the ISC page https://council. science/publications/freedom-responsibility-anduniversality-of-science-2014/ or directly council.science/ wp-content/uploads/2017/04/CFRS-brochure-2014.pdf

discipline specific, and therefore it is significant that IUPAC has formed CEDEI that hopefully aims at becoming clearly visible and contributing to combat and prevent the spreading of ethical pollution in the global chemical community.

I am sure CEDEI will be exposed to all sorts of challenges at many levels when the committee starts its work. At the global level, the first important task will be to raise the awareness of international guidelines and recommendations, both those mentioned above and many others, which is lacking in many countries. But knowledge about their existence is not enough; the documents and their collective spirit must be adopted so that research integrity and professional ethical behaviour become an integrated part of every chemist's professional platform. In order to reach this goal, strong measures have to be taken at institutional levels throughout the world so that staff and, at universities, every student will reflect on research ethics, including diversity, equity, and inclusion, in their work and behave properly.

#### Up for Discussion



From left to right: Guido Bertolaso, Ricardo Villalba, Tomáš Hudlický, and Priyamvada Gopal

Here CEDEI can play a vital role if working with dedication. A great start would be to establish a website at the IUPAC homepage to present relevant documents, such as declarations, recommendations, books, codes of conduct, and case studies, and to put in place a forum for discussion of relevant issues, good practice, and controversial cases. At www.iupac.org the material will be easily available, and if the quality reaches the high level one reasonably can expect, the website should aim at becoming the focal point regarding ethical issues for the chemical community.

Research integrity and research ethics of high standard can only become a reality and subsequently be maintained in open-minded and transparent communities where a free flow of information and a healthy and decent exchange of views based on facts are the norm. A lot of available technology can help us to uphold this level of professionalism: if accurate facts are missing, researchers, journals, libraries, and institutions can easily be contacted; if research results appear strange, dubious, or too good to be true for some reason, documentation can be requested; and if issues are argued based on misunderstanding of facts and opinions, clarification can be obtained by direct contact of people and institutions if there is a will to dialogue. The purpose of all this is to make sure that scientific results are reliable and correct, are understood and presented correctly, and are used correctly when applied to carry out projects in the real world. But this does not guarantee that science is practiced, communicated, and applied in this way. That is why it is so important that scientists are willing to be custodians of their disciplines and speak up when necessary.

But to speak up on scientific matters may indeed be risky. In recent years colleagues in many scientific disciplines, including chemistry, have been persecuted, prosecuted, and imprisoned for doing so to the public and authorities, even when done in an impeccable way following the ICSU Advisory Note on Science Communication [6]. A prominent example is the prosecution of Guido Bertolaso and six other scientists after the disastrous earthquake in L'Aquila, Italy, in 2009; they were put on trial and convicted to years in prison, but eventually acquitted by Italy's Supreme Court at the end of 2016 [7]. Another example is the case against Ricardo Villalba, former director of the national Argentinian Institute of Snow, Ice and Environmental Research, who faced criminal charges because he applied science-based methods in a survey of Argentina's glaciers [8]. To follow up such cases when chemists are the target should also be a task for the new committee, preferably in close collaboration with the ISC Committee for Freedom and Responsibility in Science (CFRS) [9].

Finally, speaking up or arguing among colleagues for an opinion that is not mainstream, can also be a very unpleasant experience and result in violation of recommended ethical guidelines. An infamous example of this sort in the chemical sciences is the Hudlicky case, which erupted in the beginning of June last year when the essay "Organic Synthesis—Where now?" is thirty years old. A reflection on the currents state of affairs" was published on the Angewandte-Chemie website [10,11]. The article resulted immediately in an avalanche of personal attacks, defamatory condemnations, and insults that violated the standards debates among colleagues in science should abide to [11-13]. The reaction from Wiley and Angewandte Chemie has been dealt with previously [14,15], but just as bad in my opinion is the reaction from Thieme Verlag that cancelled the publication of an issue of Synthesis in honour of Hudlicky's outstanding achievements in organic synthesis just a few days after the essay appeared [16]. Such a coupling between research-irrelevant opinions and scientific performance and achievements is indeed objectionable and looks like censorship to me.

This lack of objectivity probably contributed to trigger the Society for Academic Freedom and Scholarship (SAFS) [17] in Canada to look thoroughly into the Hudlicky case at its General Meeting in May

#### Up for Discussion

this year where Professor Hudlicky gave the 3<sup>rd</sup> Annual Chris and John Furedy Lecture entitled "Reflections on Diversity of Opinions, Inequity, and Exclusion-the New DIE Initiative". In the lecture [18], his odyssey since June last year was put in perspective, and the audience was exposed to examples of lack of diversity and inclusiveness, lack of respect of each other, and lack of transparent, responsible and ethical behaviour. How encouraging then to learn about the Gopal case at Cambridge University, UK, where rallies to fire her were met by a strong university defence of its academics' right to express lawful opinions which others might find controversial, followed by her promotion to full Professor Chair [19]. No doubt, therefore, that CEDEI will have an important role to play to combat pollution in the chemical community from the very beginning.

#### References

(All web pages were accessed 4 Sep 2021)

- Item 15.2 on the 51st IUPAC Council Agenda for the virtual IUPAC General Assembly based in Montreal, Canada in August 2021. https://iupac.org/event/ council2021/
- "Recommendations for the Conduct, Reporting, Editing, and Publication of Scholarly Work in Medical Journals" published by the International Committee of Medical Journal Editors www.icmje.org/ icmje-recommendations.pdf; the original known as the Vancouver document was first published in 1979 as "Uniform Requirements for Manuscripts Submitted to Biomedical Journals".
- "Singapore Statement on Research Integrity" wcrif. org/documents/327-singapore-statement-a4size/file or https://wcrif.org/
- San Francisco Declaration on Research Assessment— Putting science into the assessment of research, https://sfdora.org/ or www.ascb.org/files/ SFDeclarationFINAL.pdf
- 5. Montreal Statement on Research Integrity in Cross-Boundary Research Collaborations" https://wcrif.org/ documents/354-montreal-statement-english/file
- Advisory Note on Science Communication, first drafted in 2010 by the Committee on Freedom and Responsibility of ICSU, and last released in 2016: council.science/publications/sciencecommunication-20102016
- "Seven-year legal saga ends as Italian official is cleared of manslaughter in earthquake trial", *Science*, 3 OCT 2016, by E. Cartlidge, https://doi.org/10.1126/science. aah7374 and links therein.

- 8. Nature **2017**, *552* (6 Dec 2017), 159-160; https://doi. org/10.1038/d41586-017-08236-y
- The ISC Committee for Freedom and Responsibility in Science, council.science/about-us/governance/ committees/committee-for-freedom-andresponsibility-in-science
- Dr. Tomas Hudlicky's essay appeared with the DOI:10.1002anie.202006717, but that code does not give access to the article any longer. However, it is found on hudlicky.ca [ref 11 below], but also elsewhere (sites.krieger.jhu.edu/chemdna/files/2020/06/10.1002a nie.202006717.pdf)
- 11. See Tomáš Hudlický website https://www.hudlicky.ca, section "Angewandte essay affair, 2020"
- Hudlicky's Statement on the Angewandte Essay Affair published in July 2020 on hudlicky.ca [ref 11 above]; the 4-page statement documents for the chemical community at large the maelstrom Dr. Hudlicky experienced.
- A Google search for Hudlicky will give many links to sites substantiating this statement. Some relevant links are the following: www.safs.ca/issuescases/case. php?case=brock-chemistry ; www.chemistryworld. com/4011923.article ; cen.acs.org/research-integrity/ ethics/Essay-criticizing-efforts-increase-diversityin-organic-synthesis-deleted-after-backlash-fromchemists/98/web/2020/06
- 14. Leiv K. Sydnes, Chem. Int. 2021, 43(1), 42-44.
- 15. Leiv K. Sydnes, *Kjemi* **2021**, 1, 19-23 (www.kjemidigital.no/dm/1-2021/18)
- Personal communication from Professor Trond V. Hansen, University of Oslo, Norway, one of the editors for the Hudlicky issue, who was relieved from his task in a letter from Thieme Verlag, Stuttgart, Germany.
- 17. A presentation of the Society for Academic Freedom and Scholarship (SAFS) is found on https://safs.ca
- The Society for Academic Freedom Lecture May 2021 is available on Hudlicky's website [ref 11 above] in two parts SAFS-A and SAFS-B under Angewandte essay affair, 2020
- Multiple references about the Gopal case can be found simply searching *Priyamvada Gopal* on Google. Among them are two articles in *Varsity*, *the* independent student newspaper for the University of Cambridge, *e.g.* www.varsity.co.uk/news/19539 published 24 June 2020 and www.varsity.co.uk/news/19542 published 25 June 2020.

Leiv K. Sydnes <leiv.sydnes@uib.no> is Professor emeritus at University of Bergen, Norway. He was president of IUPAC 2004-2005 and chaired the CHEMRAWN committee in 2008-2015. He also chaired the ICSU Committee for Freedom and Responsibility in the Conduct of Science from 2013 to 2018. Project Place See also www.iupac.org/proje

#### Safety Training Program e-learning

The IUPAC Safety Training Program (STP), a global project from the Committee on Chemistry and Industry (COCI), has contributed to Global Chemical Safety for over 20 years. Until now, two main modalities of STP were developed, both face-to-face: STP Fellowship Program and STP Latin America (STP-LA). The scope of both modalities is necessary limited regarding the number of trainees and involves relatively high costs (travels, lodging and meals).

In the last years, it was very difficult get companies willing to host and get partners to financial support for STP Fellowship Program. Considering the current COVID-19 pandemic, this situation does not seem likely to improve. In this context, STP e-learning arises, as alternative of the face-to-face modalities, but with the same spirit and objectives of original STP.

The objective of STP e-learning is revitalize the STP as a whole, broadening the scope regarding the number and countries of origin of the trainees. The STP-learning has four partners: COCI, Organization for the Prohibition of Chemicals Weapons (OPCW), Chemical Industries Association of Uruguay (ASIQUR) and Foreign Affairs Ministry of Uruguay.

For more information and comments, contact Task Group Chair Fabián Benzo Moreira <fbenzo@vera.com.uy> | https://iupac.org/project/2021-003-1-022

#### Green Chemistry in Sub-Saharan Africa

Twenty years ago, when the book Green Chemistry in Africa (IUPAC project 2002-018-1-300) was prepared, green chemistry was just starting in Africa. Now, it has taken off in a number of institutions and countries, it is generally expanding, and sustainability issues are given increasing attention also at policy-making level. The collaborative book titled "Green Chemistry in Sub-Saharan Africa-growth, challenges and perspectives" is the result of this new project. It is meant to offer a panoramic overview of current achievements, recognized challenges and envisaged near-future developments of green chemistry in Sub-Saharan Africa. The information provided by the overview is expected to be useful for anybody engaged in the promotion of green chemistry, both in Africa and beyond, and to favor the recognition of shared interests in view of collaborations and networking aimed at capacity building strengthening.

Another recently-published IUPAC-endorsed book had also focused on Sub-Saharan Africa (L. Mammino, Biomass Burning in Sub-Saharan Africa: Chemical Issues and Action Outreach, IUPAC project 2007-025-1-300), initiating a tradition of projects concerning green chemistry and sustainability with specific focus on Sub-Saharan Africa.

For more information and comments, contact Task Group Chair Liliana Mammino <sasdestria1@gmail.com> https://iupac.org/project/2021-005-1-041

#### Categorizing Interactions Involving Group 11 Elements

The recent focus on supramolecular/nanostructured systems drew major attention on chemical interactions and prompted a flurry of terms indicating specific interaction subclasses. This is particularly true for interactions involving group 11 elements. Group 11 elements afford a wide diversity of chemical interactions which differ for the preferentially involved moieties, the geometric/energetic features, the nature of prevailing attractive forces, etc. Numerous terms are available in the chemical literature to designate specific subclasses of these interactions. For instance, the so-named aurophilic and argentophilic interactions are typically homonuclear short contacts wherein relativistic effects play an important role while coinage (or regium) bonds can be characterized as heteronuclear short contacts wherein the group 11 element is the electrophile. Inconsistent use of these and related terms sometimes occurs, as it is often the case when several terms are employed by different communities to designate phenomena involving analogous moieties.

For more information and comments, contact Task Group Chair Giuseppe Resnati <giuseppe.resnati@polimi.it> https://iupac.org/project/2021-006-2-100

#### Recommendations for terms relating to materials characterization: Latin and other introduced terms

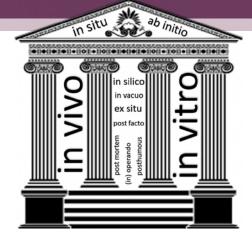
Confused about Latin terms in materials characterisation? Having trouble understanding what the conditions of the sample for a reported characterisation were?

This project has the objective to clarify, as well as resolve discrepancies and conflict, regarding Latin terms

used to describe the characterization of materials made under non-ambient conditions, materials within systems, and of materials during change. These include terms such as *ex situ*, *in situ*, and *(in) operando*. The outcome of the project will be a recommendation for specific Latin terms to the IUPAC. This objective will benefit the materials chemistry community and empower IUPAC to make a decision on recommended terms for these. It is intended that the terminology will comply with the VIM and IUPAC Guidelines for Recommendations.

The task group comprises material characterization experts spanning both diffraction and spectroscopy and three Latin scholars. The project will make a recommendation for specific Latin terms to the IUPAC, compliant with IUPAC guidelines.

- Instrumentation & techniques have advanced faster than terms.
- Consistent language is needed to discuss sample characterization conditions.
- We need to clarify & resolve discrepancies for Latin terms describing materials characterization. Particularly for non-ambient conditions, within systems, and during change.



The task group welcomes input from the broader research communities on further terms to include, particularly those used inconsistently or ambiguously. If you are interested in participating or have an experimental condition or term that you think needs clarification, email to become involved in the project.

For more information and comments, contact Task Group Chair Vanessa Peterson <Vanessa.Peterson@ansto.gov.au> https://iupac.org/project/2021-009-2-500

# **IUPAC** Provisional Recommendations

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

#### Terminology and the naming of conjugates based on polymers or other substrates

A number of human activities require that certain complex molecules, referred to as active species (drugs, dyes, peptides, proteins, genes, radioactive labels, etc.), be combined with substrates, often a macromolecule, to form temporary or permanent conjugates. The existing IUPAC organic, polymer, and inorganic nomenclature principles can be applied to name such conjugates but it is not always appropriate. These nomenclatures have two major shortcomings: 1) the resulting names are often excessively long and 2) identification of the components (substrate, active species, and link) can be difficult. The new IUPAC naming system elaborates rules for unambiguous and facile naming of any conjugate. This naming system is not intended to replace the existing nomenclature but to provide a suitable alternative when dictated by necessity. Although the rules are intended to be primarily applicable to the naming of polymer conjugates, they are also applicable to naming conjugates with other substrates, which include micelles, particles, minerals, surfaces, pores, etc. The naming system should be used when recognition of the substrate and active substance is essential and will also be useful when constraints of name length make the otherwise preferred IUPAC nomenclatures untenable. The proposed rules for the new naming system are complemented by a glossary of relevant terms.

Corresponding Author: Michel Vert <michel.vert@umontpellier.fr>

# Making an imPACt

#### Glossary and tutorial of xenobiotic metabolism terms used during small molecule drug discovery and development (IUPAC Technical Report)

Paul Erhardt, Kenneth Bachmann, et al. Pure and Applied Chemistry, 2021 Volume 93, Issue 3, pp. 273-403 https://doi.org/10.1515/pac-2018-0208

This project originated more than 15 years ago with the intent to produce a glossary of drug metabolism terms having definitions especially applicable for use by practicing medicinal chemists. A first-draft version underwent extensive beta-testing that, fortuitously, engaged international audiences in a wide range of disciplines involved in drug discovery and development. It became clear that the inclusion of information to enhance discussions among this mix of participants would be even more valuable. The present version retains a chemical structure theme while expanding tutorial comments that aim to bridge the various perspectives that may arise during interdisciplinary communications about a given term. This glossary is intended to be educational for early stage researchers, as well as useful for investigators at various levels who participate on today's highly multidisciplinary, collaborative small molecule drug discovery teams.

https://iupac.org/project/2000-009-1-700

# Interpretation and use of standard atomic weights (IUPAC Technical Report)

Adriann M.H. van der Veen, Juris Meija, Antonio Possolo, and David Brynn Hibbert Pure and Applied Chemistry, 2021 Volume 93, Issue 5, pp. 629-646 https://doi.org/10.1515/pac-2017-1002

Many calculations for science or trade require the evaluation and propagation of measurement uncertainty. Although relative atomic masses (standard atomic weights) of elements in normal terrestrial materials and chemicals are widely used in science, the uncertainties associated with these values are not well understood. In this technical report, guidelines for the use of standard atomic weights are given. This use involves the derivation of a value and a standard uncertainty from a standard atomic weight, which is explained in accordance with the requirements of the Guide to the Expression of Uncertainty in Measurement. Both the Recent IUPAC technical reports and recommendations that affect the many fields of pure and applied chemistry. See also www.iupac.org/what-we-do/journals/

use of standard atomic weights with the law of propagation of uncertainty and the Monte Carlo method are described. Furthermore, methods are provided for calculating uncertainties of relative molecular masses of substances and their mixtures. Methods are also outlined to compute material-specific atomic weights whose associated uncertainty may be smaller than the uncertainty associated with the standard atomic weights.

https://iupac.org/project/2013-032-1-200

#### Glossary of methods and terms used in analytical spectroscopy (IUPAC Recommendations 2019)

Heidi Goenaga Infante, John Warren, et al. Pure and Applied Chemistry, 2021 Volume 93, Issue 6, pp. 647-776 https://doi.org/10.1515/pac-2019-0203

Recommendations are given concerning the terminology of concepts and methods used in spectroscopy in analytical chemistry, covering nuclear magnetic resonance spectroscopy, atomic spectroscopy, and vibrational spectroscopy.

https://iupac.org/project/2017-027-1-500

#### The Gender Gap in Science: PAC Special Topics Issue

Mark Cesa and Mei-Hung Chiu, co-editors Pure and Applied Chemistry, 2021 Volume 93, Issue 8, pp. 829-961

In a recent article in *Chemistry International* (Chiu and Cesa, *Chem. Int.* 2020, 42(3), 16-21; https://doi. org/10.1515/ci-2020-0306) we reported on the results of the Gender Gap Project. The project, entitled, "A Global Approach to the Gender Gap in Mathematical, Computing, and Natural Sciences: How to Measure It, How to Reduce It?" (https://gender-gap-in-science. org/), was funded by the International Science Council (ISC, formerly ICSU) and was co-led by IUPAC and the International Mathematical Union, IMU. The results of the project clearly showed that women continue to have less positive experiences than men in education and employment across scientific disciplines, geographic regions, and levels of economic development (https://gender-gap-in-science.org/2020/06/25/ gender-gap-in-science-book/). At the final project conference at the International Center for Theoretical Physics, ICTP, in Trieste, Italy, a series of recommendations for improving gender awareness for scientific unions, local organizations, and instructors and parents was prepared and disseminated (https://gender-gapin-science.org/project-book-booklet/).

The project partners and participants at the final conference contributed a range of approaches to reducing the gender gap in science and improving gender equity in their fields. To raise awareness among chemists about these perspectives, we invited sixteen persons from a range of scientific, mathematical and computing disciplines to prepare articles for a special topics issue of Pure and Applied Chemistry. This issue explores the results of the Global Survey; describes initiatives to reduce the gender gap in astronomy, biology, chemistry, computing machinery, mathematics, ocean science, and physics; includes regional approaches to reducing the gender gap, particularly in the developing world; and proposes new and innovative approaches that include networking initiatives and collections of good practices around the world for encouraging girls and young women to pursue careers in science.

Work in IUPAC on the reducing the gender gap in science continues. In 2020 the Standing Committee for Gender Equality in Science, SCGES (https:// gender-equality-in-science.org/), was instituted, with IUPAC is a founding member along with fifteen other international partners. A current IUPAC project (https://iupac.org/project/2020-016-3-020) includes analysis of the Gender Gap project survey data specific to the chemical science, a compilation of good practices in reducing the gender gap, and participating in an initiative by several scientific publishers to examine gender trends.

### Reference materials for phase equilibrium studies. 1. Liquid-liquid equilibria (IUPAC Technical Report)

Ala Bazyleva, William E. Acree, et al. Pure and Applied Chemistry, 2021 Volume 93, Issue 7, pp. 811-827 https://doi.org/10.1515/pac-2020-0905

This article is the first of three projected IUPAC Technical Reports resulting from IUPAC Project 2011-037-2-100 (Reference Materials for Phase Equilibrium Studies). The goal of this project is to select reference systems with critically evaluated property values for the validation of instruments and techniques used in phase equilibrium studies of mixtures. This report proposes seven systems for liquid-liquid equilibrium studies, covering the four most common categories of binary mixtures: aqueous systems of moderate solubility, non-aqueous systems, systems with low solubility, and systems with ionic liquids. For each system, the available literature sources, accepted data, smoothing equations, and estimated uncertainties are given.

### https://iupac.org/project/2011-037-2-100

### **Special CTI on Polymer Sciences**

A special issue of *Chemistry Teacher International* has been released, resulting of a collaboration project between the Sub-committee on Polymer Education part of the IUPAC Polymer Division, and the IUPAC Committee on Chemistry Education.

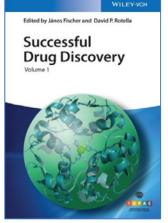
### CTI, Volume 3, Issue 2 June 30, 2021; https://www.degruyter.com/journal/ key/CTI/3/2/html

This special issue, co-edited by Chin Han Chan and Jan Apotheker, contains articles which are intended to bridge the gap between research and education. The idea is to share the good practices for some topics in polymer sciences for educational purposes. We hope that lecturers at the universities may refer to these articles as the references to teach or lecture young researchers. Another purpose is to inform the high-school/pre-university teachers about recent developments in polymer chemistry, so that they may introduce some of the topics in this issue to students.

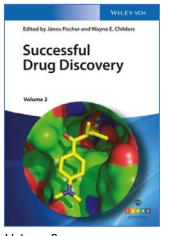
The articles are based on the lecture notes presented at IUPAC Education Workshops in Polymer Sciences (2016, 2017, 2018, and 2020+) and educational materials in polymer sciences covering topics of polymer synthesis (three articles), polymer characterization (five articles), polymer processing (two articles) and polymer applications and others (three articles). The educational materials shared in this special issue have been previously used by researchers with the aim of promoting polymer sciences.

Issue preface published Online April 2; 2021 https://doi.org/10.1515/ cti-2021-0008

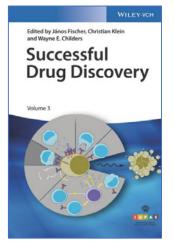
## WILEY-VCH



Volume 1 2015. 256 pages. Hardcover. ISBN: 978-3-527-33685-2



Volume 2 2016. 364 pages. Hardcover. ISBN: 978-3-527-34115-3



Volume 3 2018. 472 pages. Hardcover. ISBN: 978-3-527-34303-4

### **Successful Drug Discovery**

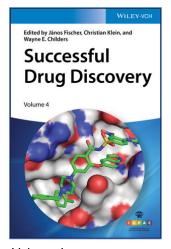
### Series Editors:

J. Fischer, Richter Plc., Budapest, Hungary D. P. Rotella, Montclair State University, USA W. E. Childers, Temple University, Philadelphia, USA C. Klein, Roche Pharma AG, Schlieren, Switzerland

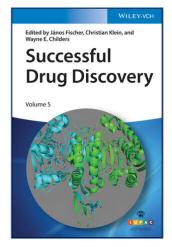
This series highlights the discovery and development of recently introduced drugs of all kinds, including small-molecule-, peptide-, and protein-based drugs.

Inventors and primary developers of successful drugs from both industry and academia tell the story of the drug's discovery and describe the sometimes twisted route from the first drug candidate molecule to the final marketed drug. The five volumes contain almost 40 case histories that describe recent drugs ranging across many therapeutic fields and provide a representative crosssection of present-day drug developments. Backed by plenty of data and chemical information, the insight and experience of today's top drug creators makes this one of the most useful suite of training manuals that a junior medicinal chemist may hope to find.

The International Union of Pure and Applied Chemistry has endorsed and sponsored this project because of its high educational merit.



Volume 4 2019. 256 pages. Hardcover. ISBN: 978-3-527-34468-0



Volume 5 2021. 336 pages. Hardcover. ISBN: 978-3-527-34754-4

### Stamps Internationa

### One Hundred Years of Insulin

he 1923 Nobel Prize in Physiology or Medicine was awarded jointly to Canadian physician Frederick Grant Banting (1891-1941) and Scottish biochemist and physiologist John James Macleod (1876-1935) "for the discovery of insulin". It was a remarkable finding since diabetes mellitus was an untreatable and often lethal disease until then. Much has been written about Banting and Macleod's breakthrough research conducted at the University of Toronto starting in November 1920, including the key roles played by their trustworthy assistants, medical student Charles Best and biochemist James Collip. On the other hand, much less has been written about the pioneering research of Romanian physiologist Nicolae Paulescu (1869-1931), whose work on the metabolic effects of canine pancreatic extracts predates that of Banting and Macleod but was interrupted by World War I. Should Best, Collip, or Paulescu have also shared the Nobel Prize?

Notwithstanding some well-known controversies regarding their Nobel prize, it is remarkable that Banting and Macleod were honored in such a way based on their *first* nomination and less than two years after the first publications describing the hypoglycemic action of purified pancreas extracts on blood sugar appeared early in 1922.

The structural elucidation of insulin is also a fascinating story. The British biochemist Frederick Sanger (1918-2013), the only scientist to have twice won the Nobel Prize in Chemistry (in 1958 and 1980), established the amino acid sequence (i.e., the primary structure) of the two polypeptide chains of bovine insulin in the early 1950's.

Later on, in 1969, the renowned British chemist Dorothy Crowfoot Hodgkin (1910-1984) determined the molecular structure of insulin using X-ray crystallography, five years after receiving the Nobel Prize in Chemistry "for her determinations by X-ray techniques of the structures of important biochemical substances", which included cholesterol, penicillin, and vitamin B<sub>12</sub>.

The centennial of the discovery of insulin has been commemorated so far this year by the postal services of five countries, namely Switzerland, Canada, North Macedonia, Pakistan, and Brazil, and the postage stamps from the first four are illustrated in this note. The Swiss stamp is perhaps the most visually appealing and depicts a ribbon diagram of the A- and



B-chains of amino acids that make up insulin, whereas the one from Pakistan features Banting, Best, and part of the front page of the 22 March 1922 edition of The Toronto Daily Star that announces the discovery of insulin ("Toronto doctors on track of diabetes cure").



While there is no actual cure for diabetes, it is today an easily treatable disease and there are multiple organizations that organize awareness campaigns to promote various diagnostic and therapeutic options. And, since 1991, the International Diabetes Federation and the World Health Organization celebrate World Diabetes Day each year on November 14th, the birthday of Sir Frederick Banting. It is finally worth noting that this past August, a special symposium entitled "Celebrating 100 years of Insulin: Preserving and Sharing the Memory of Chemical Past" was organized by Brigitte Van Tiggelen, Christopher Rutty, and Elizabeth Neswald during the IUPAC Congress, on August 16th.

## **Conference** Call

### Snow Cover, Atmospheric Precipitation, Aerosols: Chemistry and Climate

### by N. lanchenko, A. Sinitskaya, and I. Ognev

The third Baikal International Scientific Conference "Snow Cover, Atmospheric Precipitation, Aerosols: Chemistry and Climate" was organized by the Irkutsk National Research Technical University (INRTU https:// www.istu.edu/news/61545/) and endorsed by IUPAC. The conference was planned to be held on 23-27 March 2020 in Listvyanka, but due to quarantine restrictions, it was postponed a year and took place 11-12 May 2021

The first Baikal International Scientific and Practical Conference, "Snow Cover, Atmospheric Precipitation, Aerosols: Climate and Ecology of Northern Territories and the Baikal Region" was dedicated to the Year of Ecology 2017 in Russia (26-29 June 2017). The second conference, "Snow Cover, Atmospheric Precipitation, Aerosols: Technology, Climate and Ecology" was held 25-30 June 2018. Both were held in the village of Khuzhir, Olkhon Island, Lake Baikal, Irkutsk region.

Since 2018, the Federal State Budgetary Institution Zapovednoye Pribaikalye (Irkutsk) has been providing active sponsorship, as well as scientific and organizational support for the conference. The industrial partner of INRTU and the conference is RUSAL - Bratsk.

The scientific and organizational goal of the conference was the creation of a platform at INRTU for discussing modern knowledge about the chemistry of snow cover, precipitation and aerosols under the influence of climate change; search for ways of cooperation.

It is known that about one-sixth of the world's population depends on snow melt water for agriculture and human consumption, while virtually the entire world's population benefits from maintaining the planet's heat balance, which is provided by the cryosphere. The study of snow cover is relevant for Russia, since for almost half a year, vast territories are covered with snow.

The main scientific directions of the conference were determined as: methods, means, methodology for studying the physical and chemical properties and composition of snow cover, atmospheric precipitation, aerosols; the influence of climate change, physical and chemical processes in the atmosphere and anthropogenic activity on the chemical composition of snow cover, precipitation, aerosols; modeling the study of climate change, chemical composition and physicochemical properties of snow cover, atmospheric precipitation, aerosols; the role of snow cover, atmospheric precipitation, aerosols in biogeochemical cycles and the cryosphere; chemical interaction of the oceans, the earth's surface and the biosphere with snow cover, atmospheric precipitation, aerosols; assessment of the impact of snow cover, atmospheric precipitation, aerosols on natural, socio-economic systems and human health. (http://snow-baikal.tw1.ru)

The chemical composition of the snow cover is determined by the influence of conjugated media, primarily atmospheric air, and the snow cover also affects the composition of the air.

Before the start of the conference, in March 2020, a collection of manuscripts was published. It contained 37 articles submitted by 63 authors. Among the conference participants there are scientists-researchers of the Russian Federation (Moscow, Arkhangelsk, Yekaterinburg, Irkutsk, Obninsk, Tomsk, Barnaul, St. Petersburg) and other countries, including Kazakhstan, China, and Japan.

The majority of articles are devoted to snow cover, followed by publications on precipitation and aerosols (http://snow-baikal.tw1.ru). The study of the chemical composition of the snow cover, atmospheric precipitation and aerosols, allows us to assume the composition of atmospheric air during the year and the factors affecting its composition.

At the opening ceremony on 11 May 2021, the representatives of the administration of INRTU, the sponsor, representatives of the organizing committee and the program committee, participants of the 2017 and 2018 conferences spoke. The conference was opened by the director of the Institute of High Technologies, Ph.D., Evgenii Antsiferov. In his greeting he emphasized the relevance of the topic, the need for cooperation between INRTU and other organizations, and wished the participants fruitful work. Evgenii Antsiferov spoke about the university's mission in the field of winter technologies, because the study of the phenomenon of winter and all accompanying, warning and subsequent events and processes affects the lives of people.

The next speaker was Shuhei Takahashi, Director of the Okhotsk Drifting Ice Museum (Hokkaido, Mombetsu, Japan), retired professor at the Kitami Institute of Technology (Japan), and former president of the Japan Snow and Ice Society. Takahashi thanked the Ministry of Science and Higher Education of the Russian Federation, the administration of INRTU, spoke about meetings with Russian scientists in 2018, announced the upcoming 36th International Symposium on the Okhotsk Sea & Polar Oceans 2022 in Mombetzu (http://okhotsk-mombetsu.jp/okhsympo/ sympo-eng/top-page.html), and also wished good luck to the conference participants.

Head of the Program Committee and leading researcher Natalia lanchenko made a short welcoming



presentation. She said that this conference was held due to the support of the administration of INRTU (rector Mikhail Korniacov https://www.istu.edu/ eng/ob\_irnitu/upravlenie), the work of the program committee, organizing committee and conference participants. The conference is dedicated to the chemistry of atmospheric precipitation, snow cover, aerosols under conditions of changing climate. She noted that the participants of previous conferences gave us a confidence in our interest in subsequent meetings, joint research and publications, in the mutual exchange of experience, knowledge and skills. It is possible that the conferences of INRTU will be relevant, like other long-term conferences of the Russian Federation with similar topics, such as the XVIII MNK "Aerosols of Siberia" (Tomsk), and the III International Symposium "Physics, Chemistry and Mechanics of Snow" (Yuzhno-Sakhalinsk).

Anatolii Baranov spoke on behalf of the program and organizing committees of INRTU. Baranov noted that highly qualified specialists with many years of experience in researching the chemical composition of the snow cover carried out research work on grants for industrial enterprises at INRTU.

Svetlana Babina, Deputy Director for Research of the Federal State Budgetary Institution "Zapovednoye Pribaikalye," as an active participant and co-organizer of the conference and a sponsor, greeted the conference participants.

Alexander Cherednichenko from Kazakhstan (KazNU, Almaty) said that "despite the current situation, the conference still took place, which speaks of our common desire to continue our research and, most importantly, share the results obtained with your colleagues, transfer our knowledge to students and all interested people. The geographical coverage of scientists from different countries shows a great interest in the topic of the conference. The existing challenges faced by humanity at the turn of the millennium cannot be solved without deep and high-quality scientific work that requires competent specialists, equipment and funds. It is not in vain that the conference is held within the walls of the university, allowing symbolic transfer of our knowledge to new researchers who study here. Ecology is inconceivable without the joint participation of all parties and all countries. And events like this conference can provide a worthy platform for communication and exchange of their research. This is one of the most important components of solving a problem, the ability to hear each other, understand and take a step to solve problems."

Greetings and wishes were heard from Kazakhstan scientist Azamat Madibekov (Institute of Geography and Water Safety, Almaty) and from Vladimir Makarov (Nizhny Novgorod State Technical University). Makarov said: "The topic of the work is a continuation of the work carried out in the Nizhny Novgorod Scientific and Practical School of Transport Snow Science. We trace our history since 1929. We recently celebrated our 90th anniversary. During the entire existence of our school, more than 1000 samples of transport and technological machines and complexes for moving on snow have been developed, ice, snow and frozen ground are being researched."

On the same day, eight scientific reports were presented:

- The Role of Green Chemistry in Solving Environmental Problems: Responses to Global Challenges Natalia Tarasova, Russian Academy of Sciences; IPUR RCTU; International Scientific Council (ISC). (The report can be viewed at https://scientificrussia.ru/articles/osnovopolagayushchij-zakon. Starts at 2 hours 56 minutes);
- Contribution of Scientific Results to Societies from a Lecture in the U-Arctic Course in Greenland, 2019. Shuhei Takahashi, Director of the Okhotsk Drifting Ice Museum (Hokkaido, Japan);
- Chemical snow science lanchenko, INRTU, Irkutsk;

### Conference Call

- Process of Snow and Ice Tourism Creation, Takafumi Fukuyama, Center for Advanced Tourism Studies, Hokkaido University, Sapporo, Japan;
- Polycyclic aromatic hydrocarbons in the snow of Tyumen D. Moskovchenko, Tyumen Scientific Center of the SB RAS, Tyumen;
- Characteristics of the snow cover in Moscow, in the second half of the winter season 2020-2021 (on the example of Sokolniki Park) A. Novikov, E. Kuznetsov, V. Litvinenko, Moscow State Pedagogical University, Moscow;
- Experimental study of the physical and mechanical properties of snow-sand mixtures as a track bed for transport and technological machines, V. Makarov, Nizhny Novgorod State Technical University, Nizhny Novgorod.

On the second day of the conference, the moderators were N. lanchenko and I. Ognev. On this day, 11 reports were presented:

- International Union of Pure and Applied Chemistry. IUPAC, Ekaterina Lokteva, IUPAC Representative in the Russian Federation; Moscow State University, Moscow;
- Determination of the dynamics and state of snow cover according to the NDSI and NDVI indices on the example of the Lipetsk region, M. Movchan, V. Litvinenko, Moscow State Pedagogical University, Moscow;
- Monitoring of snow cover and tendencies of changes in its characteristics on the territory of Russia, N. Korshunova, RIHMI-WDC, Obninsk;
- Chemical composition of atmospheric dust in winter as an indicator of the ecological state of urban areas (Western Siberia) A. Talovskaya, Tomsk Polytechnic University, Tomsk;
- Ionic composition of winter atmospheric precipitation in the city of Barnaul T. Noskova, Institute of Water and Environmental Problems SB RAS, Barnaul;
- Results of AAS measurements of atmospheric deposition of copper and lead in the snow cover of the Almaty agglomeration L. Ismukhanova, Institute of Geography and Water Safety, Almaty, Kazakhstan;
- The balance of hydrochemical and biological indicators in the under-ice water of Lake Baikal in the spring Yu. Bukin, Limnological Institute SB RAS, Irkutsk;
- Analysis and modeling of some characteristics of climatic changes in Central Siberial. Ognev, INRTU, Irkutsk;
- Conjugate analysis of the particle size distribution



Working group of the organizing committee of the III conference: (from left to right) Yu Bukin, a university postgrad, A. Sinitskaya, V. Arshinsky, N. lanchenko, E. Antsiferov, and A. Baranov

of aerosol matter in the surface air and snow cover of the Tom-Obsk interfluve (observatory "Fonovaya") in the winter of 2018-19: the effect of air masses on the distribution of aerosol particleD. Simonenkov, Institute of Atmospheric Optics SB RAS, Tomsk;

- The elemental composition of dust aerosols in the vicinity of cement production based on the study of samples of the solid phase of the snow cover in Tomsk D. Volodina, Tomsk Polytechnic University, Tomsk;
- Atmospheric suspensions of the cities of the Far East A. Kholodov, Far East Geological Institute, Far Eastern Branch of the Russian Academy of Sciences, Vladivostok.

Igor Ognev reported brief results of the conference and presented the composition of the working group of the organizing committee.

In total, 19 reports/presentations in Russian and English languages were presented, 23 participated, including 10 women. 41 co-authors contributed reports/presentations. Three countries participated in the 14 hours of live broadcast over two days. 20 organizations took part in face-to-face reports, including universities, research institutes and organizations. The Program Committee included eight men and eight women from three countries.

### Conference Call

The participants presented their results by giving a presentation to other participants, received a participant certificate, diplomas for young researchers, published materials in the collection of 2020, sent papers in English to the IUPAC journal (papers were accepted until March 22, 2021).

The conference adopted a draft resolution containing the main decision: to hold the next IV conference in 2022.

The organizing committee of IRKUTSK NATIONAL RESEARCH TECHNICAL UNIVERSITY invites you and your organization's staff to take part in the preparation and work of the IV conference "Snow Cover, Atmosphetic Precipitation, Aerosols" in 2022.

The third conference was prepared for two years, initially as a visiting face-to-face, and then online, and was held thanks to the creativity of the main working group of the organizing committee: E. Antsiferov, N. lanchenko (project curator, chairman of the program committee), A. Baranov, I. Ognev, A. Sinitskaya, V. Arshinsky, and Yu. Bukin.

The conference site http://snow-baikal.tw1.ru was developed by the Center for Software Engineering of INRTU. The site is maintained and supported by its head—V. Arshinsky.

The conference was held in the videoconference mode on the Zoom platform, with the technical support of the E-Learning Center of INRTU (headed by N. Lukyanov) and A. Podkorytov.

Please address on questions of training, cooperation and participation: snow-baikal@mail.ru; fduecn@bk.ru http://snow-baikal.tw1.ru/index-eng

### Educational Workshop in Polymer Sciences 2020+

### by Melissa Chan Chin Han, Chris Fellows, Holger Schönherr, Per Zetterlund, and Jinhwan Yoon

This interactive educational workshop on **polymers for applications** was organized for the first time using a virtual format in conjunction with MACRO2020+, Jeju Island. It was the fourth in a projected series of four workshops, covering synthesis, characterization, processing, and applications of polymers. All three lectures touched on the understanding of the basic science, terms and concepts that are critical to polymers for applications. Thought-provoking insights into the optimization of molecular structures in relation to the properties and the potential / commercial applications were presented. Since MACRO2020+ was a hybrid conference, the pre-recorded educational workshop was structured. The participants left comments / questions on the workshop webpage and the instructors provided response on the webpage throughout the MACRO2020+ conference.

All lecture notes and videos are accessible from https://iupac.org/project/2019-022-1-400

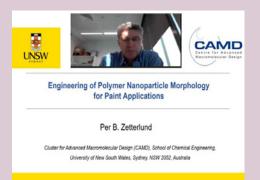
### **Pre-recorded lectures**



Holger Schönherr, University of Siegen, Germany, Polymers for applications—The long way from an idea and work in the academic lab towards a product



Myung-Han Yoon, Gwangju Institute of Science and Technology, Korea, *Polymers for future electronics* 



Per Zetterlund, The University of New South Wales, Australia, *Engineering of polymer nanoparticle morphology for paint applications* 

## Where 2B & Y

### CHEMRAWN in Action—This Time with **E-waste in Focus**

### by Leiv K. Sydnes

For years, electronic waste (e-waste) has been the waste stream growing the fastest globally. Considering the valuable metals this sort of waste contains, it would be natural to think that a bustling modern industry took care of its recycling in a sustainable way, but that is far from the case. In fact, no other waste is so much out of control as e-waste; globally, more than 50% of this waste just disappears and much of it pops up in several African countries, particularly in Nigeria. Here the waste is handled in various ways, but a common feature is that a lot of the handling is primitive and takes place under dubious and substandard working conditions. The result is that the e-waste recycling in these countries has had and continues to have a significant environmental impact. In this way, much fertile land has become useless, and tremendous clean-up operations must be carried out before the land again can be used for pasture and other agricultural purposes.

This inconsolable situation has been caused by many contributing factors, which collectively have generated entangled challenges that have been unsatisfactorily handled. The problems are basically caused by complex chemical processes that many chemists are not familiar with, but they are complicated by the lack of implementation of international conventions regulating transboundary movements of hazardous waste, for instance the Basel Convention from 1989 [1]. Additionaly, many other environmental challenges of global proportions that e-waste issues have not reached proper attention. The resulting situation is very well described in many documents [see for instance 2-5], and what should to be done to solve the problem has been outlined in abundance [see text box]. Time for action is therefore overdue.

### IUPAC on the move

Complex problems of the sort e-waste represents are challenges IUPAC has worked with since the middle of the 1970s, primarily through the CHEMRAWN committee (Chemical Research Applied to World Needs [6]). The committee works with major, multidisciplinary societal problems where chemical aspects are instrumental to understand and study to find a solution. The tool used to address the problems is to organize so-called CHEMRAWN conferences where relevant chemical aspects are presented and discussed, taking into consideration other challenges that have to be resolved to find an integrated way toward a solution [6].

Both lecturers and participants at these conferences have quite a varied background, just like the citizens that suffer from problem(s) under consideration.

The CHEMRAWN committee and an international team of specialists have worked for quite some time to prepare a conference on e-waste. Early on it was suggested that the meeting ought to be held in one of the African countries suffering the most from dubious and illegal dumping of such waste, and after some discussion, Nigeria was proposed. When the Chemical Society of Nigeria (CSN) was approached, the request to host CHEMRAWN XXII E-waste in Africa was very well received. Since then, the CHEMRAWN XXII task group and CSN have worked hard together to develop the conference program, make necessary venue preparations, and secure financial support. The work has been challenging for various reasons, the most important one being the corona pandemic, which spread a fair amount of pessimism and led to several postponements. However, toward the end of last year, the miserable future prospects resulted in an important decision: Instead of running a traditional conference, a hybrid meeting would be held at the end of 2021, November 9-11, in connection with the 44<sup>th</sup> Annual International Conference of the Chemical Society of Nigeria (https://iupac.org/event/chemrawn-xxiie-waste-in-africa/). The physical part will be held in Lagos, Nigeria, while the virtual will be by either Zoom, Teams, or Skype. This removed a lot of the uncertainty related to travel and COVID-related restrictions, lowered the number of participants present in Lagos so that a more economic venue could be used, and made it possible to reduce travel costs significantly by opting for virtual delivery of the invited lectures. This will be the first CHEMRAWN conference in the hybrid format. and if successful, it will open future scientific meetings in countries where IUPAC has been totally absent for more than 100 years.

### CHEMRAWN XXII

If the e-waste problem is going to be solved, coordinated efforts involving scientists from several disciplines, politicians at regional and natioinal levels, and representatives from international organizations have to be put in place and executed in close collaboration with relevant industries, national non-governmental organizations. and media. The conference will include representatives from all these groups, and they will be involved in the lecture program, group discussions, poster sessions, roundtable discussions, and a field trip (physical for the participants in Lagos and by drone for the virtual participants).



E-waste handling under sub-standard conditions near Lagos, Nigeria (photo: Leiv K. Sydnes).

Since the reasons for and the solution of the e-waste problems are chemical in nature, the conference will basically be a chemical congress, but the chemical actions and initiatives will be put in a wider perspective to understand the importance of implementing a number of significant measures at the same time.

Several lectures will focus on the dynamics of the e-waste market and present the environmental and health damages caused by the lack of control of the handling of the waste. Special attention will be paid to the situation in Africa where the impact of e-waste going astray in other parts of the world, particularly in Europe and the Middle East, is appalling.

Other lectures will present new technologies that are continually introduced to obtain purer and more useful products from the e-waste under cleaner, safer, and healthier conditions. Some technologies are applied to remove toxic organic chemicals safely, others to separate precious metals more efficiently, and finally, some to utilize residual waste to make new products. This will generate opportunities to establish new industries, which indeed will be needed to find employment for

### The global impact of e-waste: Addressing the challenge (extract from reference 5)

"Within the informal economy of such countries [China, India, Ghana and Nigeria], it is recycled for its many valuable materials by recyclers using rudimentary techniques. Such globalization of e-waste has adverse environmental and health implications. Furthermore, developing countries are shouldering a disproportionate burden of a global problem without having the technology to deal with it. In addition, developing countries themselves are increasingly generating significant quantities of e-waste.

It is clear that the future of e-waste management depends not only on the effectiveness of local government authorities working with the operators of recycling services but also on community participation, together with national, regional and global initiatives.

The solution to the e-waste problem is not simply the banning of transboundary movements of e-waste, as domestic generation accounts for a significant proportion of e-waste in all countries. Fundamental to a sustainable solution will be tackling the fact that current practices and the illegal trade provide economic stimulus. It is important to recognize local and regional contexts and the social implications of the issue; implementing a high-tech, capital-intensive recycling process will not be appropriate in every country or region. Effective regulation must be combined with incentives for recyclers in the informal sector not to engage in destructive processes. Cheap, safe, and simple processing methods for introduction into the informal sector are currently lacking; hence, it is necessary to create a financial incentive for recyclers operating in the informal sector to deliver recovered parts to central collection sites rather than process them themselves. Multidisciplinary solutions are vital in addition to technical solutions, as is addressing the underlying social inequities inherent in the e-waste business.

Recycling operations in the informal sector of the economy enable employment for hundreds of thousands of people in poverty. A possible entry point to address their negative impacts is to address occupational risks, targeting poverty as the root cause of hazardous work and, in the process, developing decent working conditions. More generally, solutions to the global e-waste problem involve awareness raising among both consumers and e-waste recyclers in the informal economy, integration of the informal sector with the formal, creating green jobs, enforcing legislation and labour standards, and eliminating practices, which are harmful to human health and the environment. It is also imperative to target electrical and electronics manufacturers by introducing Extended Producer Responsibility (EPR) legislation and encouraging initial designs to be green, long lived, upgradeable and built for recycling."

### Where 2B & Y



Typical handling of waste from computers and televisions in Ghana (from https://www.wired.com/story/internationalelectronic-waste-photographs).

all the people that will be out of work when e-waste handling becomes much better controlled. In order to stimulate such a shift, a course in entrepreneurship will be held, mainly for young chemists and experienced students in chemistry and environmental sciences.

In general, the knowledge about chemical problems related to the e-waste recycling is rather low even among well-educated chemists. This is primarily due to the fact that educational programmes in chemistry at university level include little or nothing about the topic. However, in some countries, university chemistry courses cover e-waste handling to some extent, and some of them will be presented and discussed in break-out groups.

If the problems associated with e-waste are going to be reduced and eventually solved, a strong involvement by a well-informed public is required. An active education of the public is therefore necessary, and a strong outreach program, dealing with the impact of e-waste on nature, people, and climate, has therefore to be developed and implemented. A lot of excellent material is already available on the web, and inspired by this, ideas for future IUPAC activities will be discussed planned.

Before closing, a special feature of the CHEMRAWN conferences should be mentioned, *viz*. a working group

named the Future Action Committee. This group connects before the conference to plan its activity, it meets every day during the conference to discuss what has been presented, and after the conference it develops ideas and projects for subsequent implementation. In this way a range of projects have been generated based on CHEMRAWN conferences over the years, and among their outcomes are scientific publications, books, technical reports, educational material, the CHEMRAWN VII Prize for Green Chemistry, and plans for establishing a center for herbal medicine in Dhaka, Bangladesh.

Through the years, I have participated in quite a few CHEMRAWN conferences, and it has always been interesting to experience how chemical problems are understood by audiences that reflect the civil society much better than groups of chemists gathered to discuss chemistry. I therefore recommend CHEMRAWN XXII, which I am sure will give up-to-date knowledge about a tremendous global problem that can only be solved by a strong involvement from the chemical community.

### References

- The name of the convention is the Basel Convention on the Control of Transboundary Movements of Hazardous Wastes and their Disposal, which came into effect 5 May 1992. http://www.basel.int/TheConvention/ Overview/TextoftheConvention/tabid/1275/Default.aspx
- United Nations Environment Management Group (2017), United Nations System-wide Response to Tackling E-waste, https://unemg.org/images/emgdocs/ ewaste/E-Waste-EMG-FINAL.pdf
- A New Circular Vision for Electronics, http://www3. weforum.org/docs/WEF\_A\_New\_Circular\_Vision\_for\_ Electronics.pdf
- 4. https://www.smithsonianmag.com/science-nature/ burning-truth-behind-e-waste-dump-africa-180957597/
- From the abstract of the International Labor Office (ILO) report "The global impact of e-waste; Addressing the challenge", published by Karin Lundgren (2012) ( https:// www.ilo.org/wcmsp5/groups/public/---ed\_dialogue/--sector/documents/publication/wcms\_196105.pdf).
- On an average, there has been a CHEMRAWN conference about central issues every second year since the committee was established in 1974. A thorough presentation of the committee's work and the CHEMRAWN conferences was recently published in the IUPAC chemical magazine *Chemistry International* April 2021, 43(2), pp. 20-26; https://doi. org/10.1515/ci-2021-0205

## Leiv K. Sydnes is professor emeritus at Department of Chemistry, University of Bergen, Norway. He was president of IUPAC 2004-2005 and chaired the CHEMRAWN committee from 2008-2015.

### Poetic Science

### An Ode to IUPAC

by Jeremy G. Frey

Current world conditions Nicely demonstrate the need Start to nurture and grow the seed Lively response to take the lead Supporting chemical collaborations

Enabled by the digital computer age setting, refining, redefining standards help in solving the global hazards energy, water, health and feed, we must not be bystanders

Setting chemists front of stage All invested in Al, not just from the tin basic, fair, unbiased, explainable techniques begin decidedly changing our discipline a new variety for our digital orchard Al - theory, computation and experiments allied to train the next generation, people and facilities, from sciences, arts and humanities—all crucial to inform the digital native of their chemistry

Without continued effort ideas wither dramatic short-term gains from individual drums others balanced by the longer-term outcomes collaboration, academic, industrial hums the whole community come hither

Chemistry, creative science, The future is bright Digital is the novel way to decide what to make and measure Doing all this together

Success? Yes!—and IUPAC has its part to play

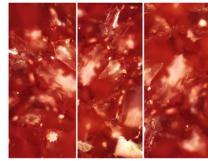
Jeremy Frey is a Professor of Physical Chemistry at the University of Southampton, and is involved in IUPAC activities through Division I, Commission I.1 and CPCDS and several projects for the Green and Gold Books.

This poem represents Jeremy's call to action to modernise the Union of Pure and Applied Chemistry (IUPAC). It was presented at Poetic Science on 11 March 2021; see more details at https://jhg. art/events/poetic-science/ The Poetry Night @JHG is also available at: https:// youtu.be/AcysRMF0bWw

Photo by Luke Richardson (https:// unsplash.com/@lukealrich)

### From the Cover





The Shrike, by Stephanie Gallant



The Temptation of Prostaglandin F Receptor, by Brendan Burkett

### Putting the A(rt) in STEM

by Adam Cook

There has long been a notion that art and science are separated by a vast and impassable gulf. Science is seen as objective and driven by quantitative facts, whereas art is subjective, emotional, and guided by aesthetics. This view reduces both endeavours to caricatures, and leaves little room for dialogue, let alone the possibility for scientists-as-artists or artists-as-scientists.

Practicing chemists have long known that this dichotomy is too simplistic; many are captivated by the tangible and conceptual beauty of the chemical world. While not a carefully guarded secret, until recently, this isn't something we've been shouting from the rooftops.

Organized/curated by Louise Dawe, Brian Wagner, and Vance Williams, ChemiSTEAM – putting the "A" in STEM is an Art of Science competition aims to show the artistic side of chemistry and chemists. The various submissions to "ChemiSTEAM" – the photos, drawings, and even tea towels – showed that in the end it's all about the stories behind the art.

Read/see more in the organizers blogpost @https:// blog.degruyter.com/bridging-chemistry-with-art-howwe-put-the-a-in-stem/ (DeGruyter Conversations, 13.08.2021)

This year 3rd edition was coordinated around the IUPAC World Congress & Canadian Chemistry Conference and Exhibition, organized as a virtual event in August. An online exhibit was on display during the Congress and a special session was organized to meet the artists and learn the stories behind the award winning entries for ChemiSTEAM2021. The celebration of the beauty of chemistry featured the juried exhibition of original chemistry-inspired art from this year's competition, including the following winning entries and honorable mentions:

- *First*—Quinine: the Bite is in the Bark, by Adam Cook
- Second—The Shrike, by Stephanie Gallant
- *Third*—The Temptation of Prostaglandin F Receptor, by Brendan Burkett

Honourable Mentions

- Silver Crystal Fern, by Andres Tretiakov
- A Journey to Obtain Pure Hexagonal Crystals, by Victor Quezada-Novoa
- I'm Picking Up Bad Vibrations, by Ashley Elgersma
- Microscopic Kaleidoscope, by Zvart Ajoyan

While IUPAC publisher DeGruyter offered various book prizes, *Chemistry International* salutes the initiative by presenting a rendition of the three winning entries on this issue cover.

For past and future stories, search 'ChemiSTEAM' on the website of the Chemical Institute of Canada: https://www.cheminst.ca/?s=ChemiSTEAM

## Index 2021

- EuroMedChemTalents reviewed by Gerd Schnorrenber 44(2)
- Glossary of Terms Used in Molecular Toxicology 40(1) The Period System, a history of shaping and sharing
- reviewed by Brigitte Van Tiggelen and Annette Lykknes 44(3) The Periodic System: The (Multiple) Values of an Id
- The Periodic System: The (Multiple) Values of an Icon reviewed by Annette Lykknes and Brigitte Van Tiggelen 42(2)
- The Periodic Table: Past, Present, and Future reviewed by Jan Reedijk 43(2)

### Conference Call

- Bioinspired and Biobased Chemistry & Materials (N.I.C.E. 2020): Hybrid Conference Model by Hernando S. Salapare III, Sonia Amigoni, Thierry Darmanin, and Frédéric Guittard 45(2)
- ChemiSTEAM Putting the A(rt) in STEM 46(4)
- Frontiers in Chemical Technology 45(1)
- Green Chemistry Postgraduate Summer School Online 47(1)
- International Polymer Characterization Conference— POLY-CHAR 2020 (Venice) 46(3)
- IUPAC/CITAC Webinar "Metrology, quality assurance and chemometrics—Correlation of test results and mass balance influence on conformity assessment" 45(3)
- OPCW Convenes International Experts to Develop Strategy 47(1)
- Polymers for applications in conjunction with MACRO2020+ 41(4)
- Research and Innovations in Chemical Science: Paving the Way Forward by Lydia Rhyman, Hanusha Bhakhoa, Nandini Savoo, and Ponnadurai Ramasami 48(2)
- Snow cover, atmospheric precipitation, aerosols: chemistry and climate 38(4)

### Features

- Artificial Intelligence and Machine Learning by Bonnie Lawlor 8(1)
- Challenges for Evaluation of the Safety of Engineered Nanomaterials by Linda J. Johnston, Norma Gonzalez-Rojano, Kevin J. Wilkinson, and Baoshan Xing 4(1)
- COMEST: Ethical Advice across Scientific and Geographic Borders by Leiv K. Sydnes 22(3)
- Diffusion Research with Nanoporous Material by Jörg Kärger, Douglas M. Ruthven, and Rustem Valiullin 25(3)
- Diversity in Science at the Global Women's Breakfast Network by Mary J. Garson, Laura L. McConnell, and Lynn M. Soby 8(3)
- Early Industrial Roots of Green Chemistry by Mark A. Murphy 21(1)
- FAIR and Open Data in Science: The Opportunity for IUPAC by Ian Bruno, Simon Coles, Wolfram Koch, Leah McEwen, Fabienne Meyers, and Shelley Stall 12(3)
- Feeding the World in a Time of Climate Change by Gary W. vanLoon and Atanu Sarkar 14(1)
- IOCD Turns 40: The future of the chemistry for sustain-

- able development by Federico Rosei and Stephen A. Matlin 11(4)
- IUPAC Focus on Digital Health by Helle Møller Johannessen and Ulla Magdal Petersen 17(3)
- IUPAC Top Ten Emerging Technologies in Chemistry 2021 - Breakthroughs for a circular, climate neutral future by Fernando Gomollón-Bel 13(4)
- Macromolecular Science Turns 100 by Christine K. Luscombe and Gregory T. Russell 4(2)
- Malta X Anniversary and COVID-19 by Emma Zajdela and Zafra Lerman 16(2)
- NAO-CNR: The Italian voice at IUPAC by Matteo Guidotti, Augusta Maria Paci, and Maurizio Peruzzini 10(2)
- Polymer Science Language to Public through Arts, by Jan Merna and Jan Prazan 9(2)
- Restructuring IUPAC at the turn of the 20th century by Edwin D. Becker interviewed by Brigitte Van Tiggelen 2(4)
- Strategies for Success as an Industrial Chemist by Carolyn Ribes 4(3)
- Systems Thinking and Sustainability: Converging on chemistry's role in the 21st Century by Peter Mahaffy, Stephen Matlin, Marietjie Potgieter, Bipul Saha, Aurelia, Visa, Sarah Cornell, Felix Ho, Vicente, Talanquer, Jane Wissinger and VaniaZuin 6(4)
- The Continued Need for CHEMRAWN within IUPAC: A Personal Account by Leiv K. Sydnes 20(2)– A Response by Christopher Brett 25(2)

### **IUPAC Provisional Recommendations**

Glossary of Physical Organic Chemistry 43(3) Glossary of terms relating to electronic, photonic and

magnetic properties of polymers 43(3)

Henry's law constants 41(2)

Terminology and the naming of conjugates based on polymers or other substrates 33(4)

### **IUPAC** Wire

2021 Nominees for Election of IUPAC Officers and Bureau Members 35(3)

2022 IUPAC-Richter Prize—Call for Nominations 23(4) An Interview with Joseph Wang 24(4)

Awardees of the 2021 IUPAC-Zhejiang NHU International Award for Advancements in Green Chemistry 23(4)

Awardees of the IUPAC 2021 Distinguished Women in Chemistry or Chemical Engineering 27(2)

Chemistry International—Freely-Available across the World by Colin Humphris 21(4)

Climate Change 2021—The Physical Science Basis 22(4) CPCDS Shorts 29(1)

Election of IUPAC Officers and Bureau Members—Call for Nominations 26(1)

Feed for Thought 29(1)

- Huizhen Liu and Banothile Makhubela have been awarded the 2020 IUPAC-CHEMRAWN VII for Green Chemistry 29(2)
- In Memoriam–Aubrey Dennis Jenkins 26(4)
- In Memoriam—Gus Somsen 25(4)
- In Memoriam—Alexander Lawson 30(1)
- IUPAC Announces the 2021 Top Ten Emerging Technologies in Chemistry21(4)

### Index 2021

- IUPAC Blockchain Technology White Paper—Call for input 29(1)
- IUPAC Congress 2027 27(1)

IUPAC Periodic Table Challenge 2020: Top Schools Announced 31(3)

IYPT 2019—Global Report 28(1)

Not an Epilogue, but a Commencement! 30(2)

- PAC Cheminformatics Special Issue 30(3)
- PAC60 Celebrations 27(1)
- Standard Atomic Weight of Lead Revised 30(3)
- The AsiaChem magazine is born 29(2)

Timothy Noel is awarded the 2020 IUPAC-ThalesNano Prize for Flow Chemistry 27(2)

- UNESCO-Russia Mendeleev International Prize in the Basic Sciences 28(1)
- Winners of the 2021 IUPAC-Solvay International Award For Young Chemists 31(3)
- Winners of the Inaugural 2021 IUPAC Analytical Chemistry Awards 32(3)

### Making an imPACt

Chemical and biochemical thermodynamics reunification (IUPAC Technical Report) 40(2)

Definitions and notations relating to tactic polymers 37(1)

End-of-line hyphenation of chemical names (IUPAC Recommendations 2020) 40(2)

Global occurrence, chemical properties, and ecological impacts of e-wastes 36(1)

Glossary and tutorial of xenobiotic metabolism terms used during small molecule drug discovery and development 34(4)

- Glossary of methods and terms used in analytical spectroscopy 34(4)
- Glossary of methods and terms used in surface chemical analysis 36(1)
- Interpretation and use of standard atomic weights 34(4)

IUPAC/CITAC Guide: Evaluation of risks of false decisions in conformity assessment of a multicomponent material 38(1)

On good reporting practices for property measurements 41(3)

PAC Jubilee—a manuscript from 1967: Dielectric dispersion in solutions of flexible polymers 38(1)

Reference materials for phase equilibrium studies. Liquid-liquid equilibria 35(4)

Special CTI on Polymer Sciences 35(4)

Terminology of polymers in advanced lithography 37(1)

- The Gender Gap in Science—PAC Special Topics Issue 34(4)
- Variation of lead isotopic composition and atomic weight in terrestrial materials 36(1)

Vocabulary of radioanalytical methods 41(2)

### Mark Your Calendar

See https://iupac.org/events/

### **Project Place**

A Database of Chemical Structures and Identifiers Used in the Control of WADA Prohibited Substances 39(2)

- Assessment of Absolute Isotope Ratios for the International Isotope Delta Measurement Standards 34(1)
- Categorizing Interactions Involving Group 11 Elements 32(4)
- Development of a Machine Accessible Kinetic Databank for Radical Polymerizations 34(1)

Development of a Metadata Schema for Critically Evaluated Solubility Measurement Data 35(1)

Examples of the Introduction of Sustainable Development and Green Industrial Processes for Secondary School Chemistry and Introductory Chemistry 39(2)

Green Chemistry in Sub-Saharan Africa 32(4)

Provisional Report on Discussions on Group 3 of The Periodic Table by Eric Scerri 31(1)

- Recommendations for terms relating to materials characterization: Latin and other introduced terms 33(4) Safety Training Program e-learning 32(4)
- Stakeholders' Thoughts on the Future of IUPAC by Lori
- Ferrins, Ito Chao, and Mark Cesa 36(2)

Systems Thinking in Chemistry for Sustainability 37(3)

Your Basic Polymer Sciences with the Subcommittee on Polymer Education: From Synthesis to Application! 36(3)

### **Officer's Columns**

Advancing Chemistry Worldwide by Javier García-Martínez 2(2)

IUPAC2021: IUPAC first Virtual World Chemistry Congress and General Assembly by Neil Burford 2(3) Resilience in Pandemic Time by Christopher Brett 2(1)

### Stamps International

One Hundred Years of Insulin 37(4)

### Up for Discussion

A Path to Entrepreneurial Education by Joseph A. Martino III, James K. Murray, Jr., James Skinner, and Mukund S. Chorghade 33(2)

Combat Ethical Pollution in the Chemical Community by Leiv K. Sydnes 29(4)

Nomenclature vs. Terminology by Bernardo Herold 31(2)

- Poetic Science—An Ode to IUPAC by Jeremy G. Frey 45(4)
- The Challenge to establish a definition by Pavel Karen 38(3)
- The Hudlicky case—A reflection on the current state of affairs by Leiv K. Sydnes 42(1)
- The International Year of Basic Sciences for Sustainable Development 2022: We Need It More Than Ever by Michel Spiro 40(3)

### Where 2B&Y

CHEMRAWN XXII-e-waste in Africa 34(3), 42(4)

Global Women's Breakfast 2022 ifc(4)

WCLM 2021–Impact of Artificial Intelligence on the Future of Chemistry 48(3)



ADVANCING THE WORLDWIDE ROLE OF CHEMISTRY FOR THE BENEFIT OF MANKIND

### The International Union of Pure and Applied Chemistry

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

Vice President Prof. Javier García-Martínez, Spain

Past President Prof. Qi-Feng Zhou, China/Beijing

Secretary General Prof. Richard Hartshorn, New Zealand

Treasurer Mr. Colin Humphris, United Kingdom

### NATIONAL ADHERING ORGANIZATIONS

Australian Academy of Science (Australia) Österreichische Akademie der Wissenschaften (Austria) Bangladesh Chemical Society (Bangladesh) The Royal Academies for the Sciences and Arts of Belgium (Belgium) Bulgarian Academy of Sciences (Bulgaria) National Research Council of Canada (Canada) Sociedad Chilena de Química (Chile) Chinese Chemical Society (China) Chemical Society located in Taipei (China) LANOTEC-CENAT, National Nanotechnology Laboratory (Costa Rica) Croatian Chemical Society (Croatia) Czech National Committee for Chemistry (Czech Republic) Det Kongelige Danske Videnskabernes Selskab (Denmark) National Committee for IUPAC (Egypt) Finnish Chemical Society (Finland) Comité National Français de la Chimie (France) Deutscher Zentralausschuss für Chemie (Germany) Association of Greek Chemists (Greece) Hungarian Academy of Sciences (Hungary) Indian National Science Academy (India) Royal Irish Academy (Ireland) Israel Academy of Sciences and Humanities (Israel) Consiglio Nazionale delle Ricerche (Italy) Caribbean Academy of Sciences—Jamaica (Jamaica)



Korean Chemical Society (Korea) Kuwait Chemical Society (Kuwait) Institut Kimia Malaysia (Malaysia) Nepal Polymer Institute (Nepal) Koninklijke Nederlandse Chemische Vereniging (Netherlands) Royal Society of New Zealand (New Zealand) Chemical Society of Nigeria (Nigeria) Norsk Kjemisk Selskap (Norway) Polska Akademia Nauk (Poland) Sociedade Portuguesa de Química (Portugal) Colegio de Químicos de Puerto Rico (Puerto Rico) Russian Academy of Sciences (Russia) Comité Sénégalais pour la Chimie (Sénégal) Serbian Chemical Society (Serbia) Singapore National Institute of Chemistry (Singapore) Slovak National Committee of Chemistry for IUPAC (Slovakia) Slovenian Chemical Society (Slovenia) National Research Foundation (South Africa) Real Sociedad Española de Quimíca (Spain) Institute of Chemistry, Ceylon (Sri Lanka) Svenska Nationalkommittén för Kemi (Sweden) Swiss Academy of Sciences (Switzerland) Department of Science Service (Thailand) Türkiye Kimya Dernegi (Turkey) Royal Society of Chemistry (United Kingdom) National Academy of Sciences (USA) PEDECIBA Química (Uruguay)

Version 2/2021, last updated 1 June 2021

Science Council of Japan (Japan)

Jordanian Chemical Society (Jordan)

INTERNATIONAL UNION OF PURE AND APPLIED CHEMISTRY





# CONNECTING CHEMICAL WORLDS

## **SAVE THE DATE**

18 – 25 August 2023, General Assembly
20 – 25 August 2023, World Chemistry Congress
World Forum The Hague, The Netherlands

"I look forward to welcoming you to the Netherlands in 2023!"



Ben Feringa, Honorary Chair

**Stay informed** Please visit the website and leave your contact details for updates on IUPAC | CHAINS 2023

www.iupac2023.org



I U P A C

