THEME 8 : SPECIAL SYMPOSIA

Symp. 8.1: A Global Survey on Gender Gap in Mathematical and Natural Sciences

Format : 1 session (3 hours), Invited Lectures and discussion symposium, **no** contribution (CL) from Congress attendees.

The purpose of this symposium is to discuss issues relating to the long term inequities of female scientists and girls in the scientific fields across the world, especially in developing countries. A joint project on global survey on gender gap in mathematical and natural sciences was granted by ICSU and supported by several international scientific unions (e.g., IMU, IUPAC, & IUPAP). Some preliminary data from the global survey on gender gaps in mathematical and natural sciences will be presented to show the most current perceptions of female scientists in their fields and girls in educational systems collected from different countries. Comparisons across regions and cultures, less and more highly developed countries, and across different disciplines will be conducted and reported. Recommendations for practical policies and actions that have the potential of reducing the gender gap will be proposed for policy makers, school administrators and teachers, researchers, and parents to consider as they face the challenges of gender inequality in different science domains and school systems.

Organisers

- *N. Tarasova (IUPAC Past-President, U-Mendeleev, Moscow, RU).*
- *Mei-Hung Chiu (IUPAC CCE, National Taiwan Normal University, TW).*

Keywords

Gender Gap, computing, mathematics, natural sciences

Speakers

- *KN: Mei-Hung CHIU, Dr., IUPAC, Committee on Chemistry Education, NTNU, TW.*
- *IL1: Gillian BUTCHER, Dr., WG5: Women in physics, IUPAP*
- *IL2: Nathalie FOMPROIX, Dr., International Union of Biological Sciences*
- *IL3: Ernesto FERNANDEZ-POLCUCH, Chair, SPP-UNESCO, Paris, FR.*

Moderator

- Nicole MOREAU (IUPAC former President, ICSU, Paris, FR)

Symp. 8.2: Digital Chemistry and the Lab of the Future

Format: A *full day* symposium (2 following sessions), including Invited (IL), Contributed (CL) Lectures, and expert panel discussion.

Scientific research and development worldwide is entering an era of increasing digital communication and data-driven business models. Funding agencies in diverse countries around the globe have mandated public access to research outputs. Machine learning and artificial intelligence are coming into their own in the data economy. What will be the impact of these technologies on the chemistry lab of the future? What types of chemical data will be in demand to support society's grand challenges? What digital workflows make sense for chemists in diverse sectors? What innovations are needed to improve recognition and support of chemistry research? How will chemists want to communicate and share research in the future? This session will aim to bring together perspectives on these issues from across the chemical enterprise and engage discussion on the role of IUPAC in supporting chemistry research of the future.

The mission of IUPAC is to "provide objective scientific expertise and develop the essential tools for the application and communication of chemical knowledge for the benefit of humankind and the world." Key to the success of digital chemistry in the global economy will be "a consistent global framework for Human AND Machine-readable chemical information in collaboration with other science communities, industry, and governments." This framework is already being realized in other scientific disciplines, and the need is becoming clear in chemical databases and other applications that analyze chemical data. In its second century, IUPAC is moving to build a common language of chemistry for machines that will facilitate the management, assessment, sharing, reuse, and global dissemination of digital research information.

Keywords

Artificial Intelligence (AI), Machine Learning (ML), FAIR data principles, knowledge discovery, chemical representation

Organisers

On behalf of the IUPAC Committee on Publications and Cheminformatics Data Standards

- *Ian BRUNO (Cambridge Crystallographic Data Centre, Cambridge, UK)*
- *Kazuhiro HAYASHI (Nat. Inst. Sci. and Techn. Policy NISTEP, Tokyo, JP)*
- *Leah McEWEN (Cornell University, Ithaca NY, USA).*

Session 8.2.1 : Advancing Frontiers in Digital Chemistry

Abstract

The United Nations Sustainable Development Goals present an important yet formidable challenge for society. As a central science, chemistry research and applications are pivotal to global well-being and development. Advances in digital technologies and machine learning are leading to new possibilities for data manipulation and interpretation across disciplines.

Automated workflows are generating unprecedented amounts of chemical data and increasing opportunities for knowledge discovery. Based on a long and robust history of data driven analysis, digital chemistry is in an excellent position to tap this collusion of data availability and scale up solutions for addressing sustainability interests world-wide. This symposium will feature strategies for digital processes in the industrial sector, trends in disruptive technologies such as blockchain distributed legers, targeted solutions for data and knowledge management, and policy efforts to support large scale infrastructure towards advancing the pure and applied chemical sciences.

Keywords

Data analytics, chemical intelligence, data management, blockchain distrubuted leger technology

Speakers

- IL1: Beeta BALALI-MOOD (Lab of the Future Lead, Pistoia Alliance Inc., London, UK)
- IL2: Gilles GEORGES (Chief Scientific Officer, CAS, Cincinnatti, OH, USA)
- IL3: Richard SHUTE (Consultant, Curlew Research, Prestbury, Chesh, UK)

Session 8.2.2 : Quality Data for Quality Chemistry

Abstract

Assuring data integrity is essential for translating chemical research into broader applications. Assessing the validity and utility of data is increasingly important in digital technologies and to promote discovery and interoperability of data globally across the chemical and related sciences. The critical evaluation of chemical data has long been a core IUPAC activity, from its earliest contributions to review and recommend atomic weights in the Periodic Table. This symposium session focuses on three interrelated parts of the evaluation process to generate quality data for the scientific community: accumulated experience and breadth of IUPAC contributions to critically evaluate different classes of chemical data, best practices for creation of evaluated and documented data, and the strategies for disseminating and evaluating data through digital methodologies.

Keywords

Critical evaluation, data integrity, data validation, metrology

Speakers

- IL1: John RUMBLE (President, R&R Data Services, Gaithersburg, MD, USA)
- IL2: David SHAW (Chair, IUPAC Interdivisional Subcommittee on Critical Evaluation of Data, Boston, USA)

Symp 8.3: Hommage to Eduard Hála

Format: A *half-day* symposium including Keynote (KN) and Invited (IL). No contributed lectures (CL)

Prof. Eduard Hála (9. 12. 1919 – 28. 8. 1989) was born in Roudnice nad Labem. After graduating from secondary school that he had attended in Kolín and Chrudim and after an involuntary break caused by WWII he graduated in chemistry in 1947 at the Czech Technical University (CTU). He then became junior lecturer and later on senior lecturer in physical chemistry at first at CTU and later at the independently founded University of Chemistry and Technology (UCT) in Prague. With Arnošt Reiser they wrote a seminal university textbook of physical chemistry the first volume of which was published in 1960. When he was forced to leave UCT for the Czechoslovak Academy of Sciences in 1958, he first worked at the Institute of Physical Chemistry, but was later offered to create his own thermodynamic group at the Institute of Chemical Process Fundamentals. His laboratory very soon became world-renowned not only among physical chemists, but also with chemical engineers. In tribute to prof. Hála, the laboratory was renamed shortly after his death to Eduard Hála Laboratory of Thermodynamics, on suggestion of the international thermodynamic community. When the thermodynamic laboratory became part of the Department of Separation Processes in 2014, Hála's legacy was passed over, in the name of Eduard Hála Laboratory of Separation Processes.

On the occasion of the centenary of Prof. Hála's birth a special session of the IUPAC World Chemistry Congress will commemorate the great scientist and inspiring personality.

Keywords

Eduard Hála, chemical thermodynamics, chemical engineering, phase equilibria, thermodynamic predictive models, data analysis

Organisers

- *Magdalena Bendová* (*Czech Acad. Sci., Inst. Chemical Process Fundamentals, CZ)*
- *Johan Jacquemin (Faculté des Sciences et Techniques, PCM2E, Univ. Tours FR)*

Introductive Honorary Lecture: "*Remembering Eduard Hála"*

- *KN: Karel. AIM (Czech Acad. Sci., Inst. Chemical Process Fundamentals, CZ)*

Invited lectures

- *IL: Emmerich WILHELM (University of Vienna, AU): "Solutions, in particular dilute solutions of non electrolytes: an interpretative review."*
- *IL: Richard C. DARTON (Oxford University, UK): "Chemical engineering thermodnynamics: systems and surfaces"*

Coffee break

Speakers

- *L1: Zdenek WAGNER (Czech Acad. Sci., Inst.. Chemical Process Fundamentals, CZ): "Application of laws of thermodynamics to analysis of experimental data"*
- *L2: Luis M. SANTOS (University of Porto, PT): "Nanostructuration effect on the physical-chemistry properties of ionic liquids"*
- *L3: Jean-Noël JAUBERT (Université de Lorraine, Nancy, FR): "A database for benchmarking and selecting thermodynamic models"*
- *L4: Andreas PFENNIG (Université de Liège, BE): Strong Influence of Molecular Interactions over Large Distances and Its Consequences*
- *L5: Alex DE VISSCHER (Concordia University Montréal, CA): "How well can we predict solubility, Henry constant, and vapor-liquid equilibria?"*
- *L6: Andreas KLAMT (COSMOlogic, Leverkusen,DE): "From Quantum Chemistry to Vapor-Liquid Equilibria"*

Symposium 8.4 : Empowering Women in Chemistry

Format*:* One session *(2 hrs30)*

Abstract:

To be completed

Introduction – 10 minutes

Panel Discussion I – 45 minutes

Panel Discussion II – 45 minutes

Panel Discussion III – 45 minutes

Closing remarks – 5 minutes

Keywords *:*

to be completed

Organisers:

- *Carolyn RIBES (Core Research & Development Group, Dow Benelux, Terneuzen, NL)*
- *Angela WILSON (Michigan State University, East Lansing, USA)*

Symp. 8.5: Chemistry Addressing the UN-17 Sustainable Development Goals

Format: A half-day symposium including Invited lectures (IL) and expert panel discussion (no contributed lectures).

Aim

Development of truly Green and Sustainable Chemistry is key to delivering many of the United Nations Sustainable Development Goals (UN 17 SDGs), but to effectively address the huge challenges faced globally, scientists must understand the wider context of Sustainable Development. In this symposium expert invited speakers will provide perspectives on policy, regulatory, societal and business strategies that could enable more rapid movement towards realizing the "shared blueprint for peace and prosperity for people and the planet, now and into the future" that the SDGs are designed to realize.

In all cases topics will include aspects of science policy or green and sustainable chemical research that support these strategies.

Keywords:
UN Sustainable Development Goals (SDGs), policy, regulation, green chemistry, sustainable development

Organizers: on behalf of IUPAC Interdivisional Committee on Green Chemistry for Sustainable Development, ICGCSD

- *Pietro Tundo (Chair IUPAC ICGCSD, Università Ca' Foscari, Venezia, IT)*
- *Christopher Brett (IUPAC President Elect, Universit of Coimbra, PT)*
- *Janet L. Scott (Secretary of the ICGCSD, University of Bath, UK)*
- *Fabio Aricò (IUPAC Division VIII Representative, Università Ca' Foscari, Venezia, IT)*

The Symposium 8.5 is composed by four sub-sessions :

- Science witnesses
- Industry
- International organisations
- Round table

Science witnesses

- *Michael Graetzel - Ecole polytechnique fédérale de Lausanne (Swtizerland)*
- *Krzysztof Matyiaszewski - Carnegie Mellon University, Pittsburgh (USA)*
- *Recorded videos by other International Sciences Witnesses*

Industry

- Zhejiang NHU Company Ltd (China)
- PhosAgro (Russia)

Winner of the IUPAC-NHU Experienced Chemists Award

International Organisations

- *International Science Council (ISC): Natalia Tarasova - Institute of Chemistry and Problems of Sustainable Development at the D. I. Mendeleev University of Chemical Technology of Russia*
- *ACS Green Chemistry Institute: Mary Kirchhoff, Ph.D., Executive Vice President of Scientific Advancement and Director of ACS GCI*
- *International Sustainable Chemistry Collaborative Centre (ISC3): Prof. Dr. Klaus Kümmerer Director Research & Education Hub ICS3, Lüneburg (Germany)*
- *EuCheMS: Prof Ana Aguiar Ricardo Head of Chemistry Department Universidade NOVA de Lisboa (Portugal)*
- *Centre of National research (CNR): Maurizio Peruzzini - Director of Chemical Sciences and Materials CNR – Rome – Italy*

Round Table

Symp. 8.6: Metal-mediated radical polymerization: a prime example of CNRS-supported French-American partnership

Format: 1 session (4 hours),
Presentation of the CNRS international cooperation scheme, Keynote and Invited lectures, open to oral and poster contributions from Congress attendees.

Abstract:

The French "Centre National de la Recherche Scientifique" (CNRS) has a funding scheme promoting international cooperation between French and Foreign scientists through the creation of international networks ("Groupe de Recherche International" or GDRI) and virtual institutes without walls ("Laboratoire International Associé" or LIA). The purpose of this special symposium is to showcase one example of such a successful international cooperation, an LIA entitled "Laboratory of Coordination Chemistry for Controlled Radical Polymerization" (LCC-CRP). This LIA comprises four teams, two in Toulouse *("Laboratoire de Chimie de Coordination" (LCC, UPR CNRS 8241); "Laboratoire des Interactions Moléculaires et Réactivité Chimique et Photochimique" (IMRCP, UMR CNRS 5623))*, and two in Pittsburgh *(Carnegie Mellon University ; Duquesne University).* The research area for this joint effort deals in broad terms with the contribution of metal complexes and coordination chemistry to the design and development of more performing controlling systems for radical polymerization. All contributions to this topic external to the LIA are very welcome.

Keywords
Coordination chemistry, polymer chemistry, controlled radical polymerization, atom transfer radical polymerization, French-American cooperation

Organizers

- *Rinaldo POLI (Chimie de Coordination, CNRS, INP, Toulouse, FR)*

- *Krzysztof MATYJASZEWSKI (Center for Macromol Eng., U-Carnegie-Mellon, Pittsburgh, USA)*

Speakers

- *Introduction: Eudora BERNIOLLES (DERCI, CNRS, Paris, FR), title: "The CNRS tools for promoting the international scientific cooperation"*
- *KN: Michael P. SHAVER, (Prof., University of Manchester, UK)*
- *IL1: Mathias DESTARAC, (Prof. Université Paul Sabatier, Toulouse, FR)*
- *IL2: Antoine DEBUIGNE, (Dr., CERM and Université de Liège, BE)*