LIST OF THEMES AND SYMPOSIA

GENERAL CONTENTS OF THE SYMPOSIA

A symposium is composed of **1** to **4 half-day sessions**.
On the average, a session will include
- 1 Key-note lecture (KN), 40 min incl. questions
- 2 Invited lectures (IL), 30 min incl. questions
- 8 Contributed lectures (CL), 15 min incl. questions

THEME 1 - CHEMISTRY FOR LIFE

Relevant domains :
Analysis, Synthesis, Modelisation/Simulation, Food/Nutrition, Materials/Hybrids/Biomaterials, Health: diagnosis/drugs/safety, Cosmetics, etc…

Conveners: *Patrick Couvreur* (University Paris Saclay, FR*), Didier Desmaele* (University Paris Saclay, FR), *Dominique Lesuisse* (Sanofi, FR), *Luisa De Cola* (ISIS, University of Strasbourg, FR ; KIT, Karlsruhe, DE)

Symp. 1.1: Chemistry for the generation of artificial biological systems (2 sessions)

Aim:

Cells represent the smallest structural and biological units of all living organisms. However, these entities display an enormous complexity, whose understanding can be approached in different ways. A relevant approach focuses on chemistry and its philosophy of building. Constructing molecules and molecular systems gives the opportunity of exploring the features and the recognition/reactive patterns that characterize molecules, networks and systems of increasing complexity. Moreover, it allows designing and tailoring reaction pathways, modelling specific aspects of living systems, and producing novel biosystems or hybrid bio-chemical systems. Such a vision, fundamentally linked to chemistry, is now emerging as a branch of synthetic biology - often called bottom-up synthetic biology. In this context, two emerging topics are under strong expansion: (1) cell-free systems and (2) expansion of the genetic code. Both heavily rely on chemistry-biology integration.

(1) Cell-free systems have been traditionally used in biochemistry to unveil mechanistic details of biological processes. Chemical synthetic biology uses cell-free systems as powerful alternatives to living cells to engineer systems for specific purposes. Cell-free systems are versatile tools for fundamental and applied studies. They can be realized in the test-tube or can be micro-compartmentalized (e.g., in microfluidic devices or microcompartments) to achieve new promising technologies such as the bio-organic synthesis of drugs, proteins and peptides from non-natural amino acids, biochemical chip based on genetic circuits, biosensors, and ultimately the construction of synthetic cells for nanomedicine or to face the Grand Challenge of life origin on Earth. Cell-free technologies calls for a new blend of chemistry, biochemistry, microfluidics and numerical modelling, and promise applications in the medium-short term. Genetic circuits of increasing sophistication have been reported and characterized in all details. The combination of cell-free systems with micro-compartment aims for the construction of "minimal cells" in the laboratory, with several already-reported important examples. No doubts current efforts on cell-free systems design and construction will impact on next-generation biotechnologies.

(2) Natural biopolymers (nucleic acids, proteins, and peptides) represent the fundamental building blocks of biological structures and functions. Chemical modification of natural biopolymers for the crafting of novel entities with hitherto unknown structures and functions has been a central aim of synthetic biology. Technologies such as amber codon suppression and Darwinian *in vitro* evolution have revolutionized the field

of synthetic biology. Indeed, a vast diversity of unnatural amino acids could be incorporated into mammalian cells and even into model organisms, providing in cell tools for the monitoring and imaging of the progression of diseases. Moreover, engineered polymerases have been developed to accept a broad range of modified nucleotides which enabled the identification of DNA and RNA sequences capable of binding specifically to targets or catalyse reactions such as the replication of their own encoding sequences. Thus, the symposium will also focus on some aspects of the evolution of proteins and peptide with an expanded genetic code and the generation of chemically nucleic acids displaying properties that markedly deviate from their natural functions.

Overall, this symposium will give an overview of the various chemical approaches currently used in cell-free synthetic biology and in the evolution of unnatural biopolymers

Keywords:
Synthetic biology, *in vitro* evolution, modified nucleic acids, modified proteins, cell-free systems.

Organizers:
Marcel Hollenstein, (Institut Pasteur, Paris, FR)
Vincent Noireaux, (University of Minnesota, Minneapolis, USA)
Pasquale Stano, (University of Salento, Lecce, IT)

Symp 1.2: Chemistry for Translational Medicine (3 sessions)

Aim:

The number of new NMEs per year delivered by pharmaceutical R&D has remained constant over the last decades despite exploding investment. This is largely explained by attrition, especially in clinical development and essentially due to efficacy and safety issues; the first being related mainly to poorly validated targets or non-optimal dosing in humans and the second to compounds that are not selective enough. Translational research aims to decrease this attrition through better analysis, validation and prediction of molecular mechanisms and properties that a candidate for development should exhibit to elicit expected efficacy in clinical trials.

Chemical biology, chemo-genomics and chemo-proteomics elaborate selective tools, clickable or activable fluorescent probes for imaging in cells and in healthy and diseased tissues to provide dynamic information about cellular communication, signal transduction pathways, the role of macromolecules and their interactions in order to discover and validate new targets. They design chemical tools to help deconvolution of phenotypic screening hits to identify their targets and off-targets, cellular and in vivo markers to investigate drug efficacy and selectivity/toxicity or label-free techniques to directly analyze small molecule binding to proteins or other macromolecules. They help investigating target engagement and de-risking, or tracking single molecules through cells and tissues.

Synthetic chemistry designs and synthesizes more relevant compound libraries to identify better quality chemical tools and lead compounds, new types of molecules to modulate highly validated but “non druggable” targets (by revisiting macromolecular interactions, stabilizing rather that inhibiting interactions, activating rather than inhibiting enzymes), new types of allosteric modulators to reach higher selectivity or different biological response (by inhibiting protein transport rather than function, or by addressing poorly druggable macromolecular interactions, enzymes like phosphatases, nucleic acid polymers, stem cells, chromatins or the epigenome). This is becoming possible through the discovery of new chemistry, e.g. macrocycles, stabilized peptides and mimetics, irreversible inhibitors, degraders, peptide or nucleic acid based polymers, natural product based scaffolds etc. Specificity and efficacy can be increased by tagging

active small molecules and macromolecules to deliver them into cells, cellular compartments, specific tissues or diseased organs.

Predictive mathematical models are used in systems biology for target identification and validation, druggability assessment and de risking. *In silico* approaches investigate the behavior of molecules on a systems level in cells, organs and whole organisms to predict mechanism of action, selectivity and side effects and potential for drug repurposing. Computational methods help identify targets or off-targets of phenotypic screening results through similarity based target fishing and deconvolution. Statistical and structure based methods are used to generate more efficient and drug-like small and macromolecular target modulators and probes through (i) fragment based design, (ii) new virtual screening strategies including covalent docking, (iii) design of cell penetrable small molecules interfering with nucleic acid polymers from sequence information or by comprehensive analysis of loops at protein-protein interfaces for macrocycle design.

Analytical and biophysical tools are used to identify biomarkers that can translate observations in cells through animal models into humans, understand cellular networks and communications, track molecules to understand and predict polypharmacology and select the right patient population for personalized medicine. Structural biological methods may allow determining macromolecular structures and interactions to help rationally design modulators.

It is becoming clear that many drugs may derive their therapeutic benefit or liability from interactions with multiple proteins rather than a single target. Chemistry needs to meet the challenge of designing compounds for multiple targets but still being selective enough to meet the requirements of polypharmacology i.e. maximizing efficacy while minimizing side effects.

The symposiums will cover new tools, methods and approaches to select more relevant targets and design high quality molecules able to target the "non-druggable" genome together with tools helping a better translation of research findings to clinical success.

Keywords:

Translational medicine, chemical biology, chemo-genomics, chemo-proteomics, target fishing and validation, click chemistry, cellular imaging, macromolecular interactions, virtual screening, structure based drug design, biomarkers, polypharmacology, pathway analysis, site-specific protein labelling, protein engineering, bio-orthogonal reactions, antibody drug conjugates

Organizers:

Stefan Laufer (Eberhard Karls Universität Tübingen, DE)
Laurent Micouin (CNRS, Université Paris Descartes, Paris, FR)
Laurent Schio (Sanofi, Paris, FR)

Symp 1.3: Nanotechnologies for Health, Food and Beauty (3 sessions)

Aim:

Advanced nanoscale systems for drug delivery have recently received tremendous attention, in particular from the field of nanomedicine. The need for drug nanocarriers that efficiently target diseased areas in the body arises because drug efficacy is often altered by nonspecific cell and tissue biodistribution, and because some drugs, in particular promising biological drugs such as miRNA, are rapidly metabolized or excreted from the body. The passage of the drug molecules and drug delivery system across several physiological barriers (i.e. epithelium, endothelium, cell membrane) represents another important challenge in drug targeting. Due to their huge surface area and many possibilities for surface engineering, nanotechnologies may be used for ex vivo analytical detection of disease markers, too. Owing to impressive progress in materials science and pharmaceutics, a broad range of nanocarriers/nanotechnologies with diverse sizes, architectures and surface properties have been designed. These include liposomes, polymer

nanoparticles, micelles, dendrimers, and inorganic nanoparticles as oxides (silica, iron, titanium), quantum dots, gold or metal oxide frameworks. The size of these nanosystems is typically small (from a few tenths to a few hundreds of nanometers) to allow systemic (intravenous) or local (mucosal) administration, to promote drug diffusion within the cell or to perform in vivo or in vitro diagnosis.

In the drug delivery field, current surface functionalization methodologies can impart nanocarriers with the ability to control, at least in part, their pharmacokinetics and biodistribution, whereas delivering drugs to the cells by alternative pathways, allows to overcome certain mechanisms of drug resistance in cancer (incl. multidrug resistance) and infectious diseases which represents an important medical challenge. On-demand drug delivery in spatial-, temporal- and dosage-controlled fashions is also becoming feasible through the design of stimuli responsive systems that recognize their microenvironment and react in a dynamic way, mimicking the responsiveness of living organisms. In this context, synthetic mimics of the Extracellular Matrix (ECM) of different pathological conditions will generate ex vivo human tissue models for pharmacokinetic studies, avoiding the use of animals and moving to a personalized medicine approach. Moreover, the design of « multifunctional » nanomedicines allows combination of various functionalities, by loading in the same nanodevice: (i) two or more drug entities with complementary pharmacological targets or (ii) a chemotherapeutic and an imaging agent for « theranostic » purpose, paving the way for the co-called "personalized" medicine. Apart from drug administration, nanocarriers may also be used for vaccination purposes, in order to elicit a boosted immune response by the delivery of specific antigens. Noteworthy, some nanoformulations have already appeared on the market during the last decade or are in advanced clinical trials (phase III).

Due to the expanding commercialization of products that contain engineered TiO_2 and ZnO nanoparticles in cosmetics and sunscreens for UVR protection, the conditions under which nanoparticles may penetrate the stratum corneum barrier and how their physiochemical properties may influence penetration, systemic translocation and toxicity deserves also to be addressed. It represents an important issue for application in cosmetics and beauty. The symposium will also consider the use of nanodevices for agriculture and food industry.

This symposium will, therefore, contemplate all the aspects related to the use of nanotechnologies for therapy, diagnosis (through in vivo imaging or in vitro detection) and other consumer good applications such as food and cosmetics. The scaling-up and toxicological issues will be discussed, too. Specifically for nanomedicine, special attention will be focused on how to improve the translation from the bench to the clinic.

***Keywords*:**
Nanomedicine, nanocosmetics, nanodevices for food and agriculture, drug delivery, organic and inorganic nanoparticles, theranostic, nanotoxicology

Organizers:
Maria José Blanco-Pietro (Dept of Pharmaceutical Technology and Chemistry, University of Navarra, ES)
Céline Farcet (Advanced Research, L'Oréal Research and Innovation, Aulnay, FR)
Frédéric Lagarce (INSERM, Pharmacy Dpt. - University of Angers, FR)
Francesco Stellacci (Institute of Materials, EPFL, Lausanne, CH)

Symp 1.4: Polymers and soft materials for Life Sciences (3 sessions)

Aim:

Polymers are macromolecules composed of many repeated subunits of different nature leading to a broad range of compositions and properties. Both synthetic and natural polymers play a major role in life sciences.

Natural polymers (nucleic acids, proteins, peptides) are the building blocks of biological structures and functions, and the support of genetic and epigenetic events which are essential for the living processes to occur. Subtle modifications in the sequence of these polymers may lead to either improvements of certain biological processes or, in contrast, to their deregulation with the appearance of physiopathological events and diseases.

Polymerization of monomers through various modern synthetic routes (e.g., controlled radical polymerization, ring-opening polymerization, etc;) enables the design of *synthetic polymers* with unique physico-chemical properties, including robustness, viscoelasticity, and a tendency to form glasses and semicrystalline structures rather than crystals. They may be combined to form tailor-made supramolecular architectures such as colloids, gels, etc. The versatility of the polymer structures and the resulting properties offer many applications in the medical and pharmaceutical fields. Additionally, some polymers, either natural or synthetic, may also act as drugs by themselves or be used in many different bio-related applications such as artificial materials for tissue repair and reconstruction, healing devices, biodegradable vascular substitutes, drug excipients, implants, surgical sutures, etc. « Smart » polymers, designed to undergo reversible physical or chemical changes in response to environmental stimuli (such as temperature, light, magnetic or electric field, pH, ionic strength or enzymes) also hold great promise as drug delivery systems, tissue engineering scaffolds, cell culture supports, bioseparation devices, sensors and even actuators systems.

Polymers also represent an important class of ingredients in cosmetic and food science, as many polymers are employed as film formers, rheology modifiers, emulsifiers, stimuli-responsive agents, or even antimicrobial agents. They can eventually be used for the encapsulation of aromas and flavors or on the contrary, as taste maskers. Data storage using synthetic polymers is another emerging topic to be considered.

The symposium will also focus on some aspects of the synthesis of gels and soft matters for biomedical applications and give perspective on the use of these materials for in vitro and in vivo applications. Gels and hydrogels made by polymers or other soft materials fascinate chemists, material scientists and biomedical researchers since their unique properties will allow also 3D printing of tissues and organs. They can consist of a self-supporting, water/solvent-swollen three-dimensional (3D) viscoelastic network, and can possess self-healing properties, reconfigurable structures and interesting transitions between shapeless to shape persistent structures. Many gels have been designed and used for the diffusion and attachment of molecules and cells since their behavior is reminiscent of the extracellular matrix (ECM) and offers native culture condition that traditional 2D surfaces cannot reproduce.

This symposium will give an overview of the importance of polymers and soft materials in life sciences, from fundamental research to applications.

***Keywords*:**
Natural and synthetic polymers, soft matter, 3D-printing, supramolecular chemistry, pharmaceutics, medical devices, regenerative medicine, cosmetics, food.

Organizers:
Julien Nicolas (Institut Galien, CNRS/University Paris Saclay, FR)
Sebastien Perrier (University of Warwick, UK, and Monash University, AU)
Brent Sumerlin (University of Florida, Gainesville, USA)

THEME 2: CHEMISTRY FOR ENERGY AND RESOURCES

Relevant domains:
Conventional energies, Fossil resources: exploitation and challenges, Renewable energies, Bioresources, Sustainability, Nuclear energy and related, Fusion and relevant challenges, Molecular electronics, Materials and energy, System policies for energy, Energy storage, Energy transport, etc…

Conveners : *Jean-Marie Tarascon* (Collège de France, FR), *Alexis Grimaud* (Collège de France, FR), *Daniel Lincot* (IRDEP, FR), *Yves Bréchet* (CEA, FR), *Robert Guillaumont* (University Paris Saclay, Orsay, FR)

Symp 2.1: Materials for Energy by Computational Design (3 sessions)

Aim:

All governmental institutions throughout the world commonly agree that energy is the most important challenge that our planet will have to face over the next 50 years. We have to double our production without increasing the CO_2 release. Great hopes are placed in the use of renewable energy coming from the sun, wind and biomass. The exploitation of such energies enlists numerous conversion (photovoltaics, thermoelectrics or wind turbines), storage (batteries, supercapacitors or fuel cells) and transport technologies (superconductors). A common denominator to all of them is that their performance is always limited by materials performance.

The materials are essential and technologies are always limited by their availability, cost and stability. Therefore, our challenge is to design newer and better materials and this has to be faster than ever as our time is limited (50 years). Luckily, the chemist has the diversity of elements in the periodic table to design/elaborate new materials. Nevertheless, this richness can rapidly turn into a nightmare when trying to pick the right combination and the finding of the new generation of materials can be tedious and slow if the no external help is given to chemists in their quest. So great hopes are placed on high-throughput theoretical calculations so as to mimic at the material levels what has been done in genomics with DNA and to establish a material genome. Also, the study of the interactions between individual components of a system by computational work is of the highest interest, with special attention paid to how these interactions give rise to the function and performance of the final system.

This symposium will welcome all computational advances aiming towards the design of novel energy related materials with new or improved electronic, ionic and optical properties.

Keywords:

High-throughput calculation, material design, material genome, physical properties of solids, liquids and interfaces

Organizers:

Caroline Mellot-Draznieks (Collège de France, Paris, FR)
Geoffroy Hautier (Université Catholique de Louvain, BE)

Symp 2.2: New Approaches for Electrochemical Energy Storage and Conversion Systems (3 sessions)

Aim:

Energy is the lifeblood of our modern societies and the energy production and renewable energy sources are nowadays major concerns in today's energy conscious society. Due to the intermittency of renewable energy sources such as wind or solar, there will be a far greater need for advanced electrical energy storage/conversion technology. For that, electrochemical energy storage systems enlisting fuel cells, supercapacitors and batteries provide an attractive solution. However, such systems still fall short for large scale mass storage dictated grid application as well as for electrical vehicles that require safe and high energy

batteries at affordable cost. To overcome this limitation, systems with higher energy densities while being sustainable, scalable, reliable and low cost must be developed. This calls for new materials and new concepts. The challenges for materials scientists and electrochemists are enormous, from finding new electrochemical systems, to the development of suitable active materials and electrolytes or the system assembling by mastering the complex processes at the interfaces. So this symposium will welcome research achievements dealing with:

- controlling the electrochemical interfaces by the mastering of coating techniques, grafting methods or wisely designing additive organic molecules
- the harmonious integration of the atomic structure, the elemental composition and the material's microstructure to enable for optimum performance
- the development of 'greener' and more sustainable electrochemical systems based on electrodes having a minimal environmental footprint made via the use of eco-efficient processes enlisting either "soft chemistry" or biomimetic approaches
- high-throughput screening of new electrode materials, electrolyte formulations and additives and their combination in a battery cell
- advances in *in-situ* and *operando* analytical characterization of electrochemical energy storage systems.

Keywords:
Energy storage materials/systems, rechargeable batteries, electrode, post lithium-ion battery chemistry, material design, multi-valent ion batteries, supercapacitors

Organizers:
Kisuk Kang (Seoul National University, KR)
Patrice Simon (CIRIMAT, CNRS Université Paul Sabatier, Toulouse III, FR)

Symp 2.3: Turning Solar Energy to Fuels via Artificial Photosynthesis (3 sessions)

Aim:

Because solar is intermittent and geographically diffuse, solar energy will only meet the worldwide demand in energy and all its promises if stored in a dense and transportable way such as chemical bonds. To do so, natural processes in which sunlight is harvested by photosynthetic organisms such as green plants, algae or cyanobacteria which store this energy by using carbon dioxide and water to produce carbohydrates. The direct pathway of fuels production from solar energy will thus play an important role in balancing the local variations in solar irradiation but currently remains an unachieved dream, despite the concept being 100 years old. Indeed, the field of artificial photosynthesis cannot simply copy the natural processes but must learn from them to design systems meeting the society needs at a much larger scale, the human scale. To produce such amount of energy, the most viable source of electron is water, which oxidized to produce oxygen. The most convenient materials for reduction are protons that form hydrogen, or carbon dioxide that can form hydrocarbons with even higher energy density than hydrogen. Even if carbon dioxide reduction leads to the most attractive photosynthetic fuels, the nature of the multi-electron reactions at play makes it highly challenging and so far no artificial photosynthetic systems succeeded at reducing carbon dioxide with high yields of formation of hydrocarbons. Moreover, while reduction of water or CO_2 can form fuels, the development of these reactions is currently hampered by the lack of cost-effective water oxidation catalysts, for which efforts must be paid.

For a direct solar fuel production, any envisioned systems must possess two functions: a first function capable of adsorbing sunlight and converting it into electrons, and a second one that uses these electrons to reduce either protons or carbon dioxide to produce fuels. For that, both bio-systems and complex systems made of inorganic or organic compounds can be developed, hence covering a large field of expertise that is required

for making those systems efficient and viable at a large scale: bio-chemistry, organic and inorganic chemistry, semiconductors, supramolecular assemblies, charge transfer at interfaces, proton transfer etc… Only the fundamental understanding and the control of such complex processes will eventually lead to the development of new artificial photosynthetic systems for the direct production of solar fuels.
This symposium will therefore focus on the development of each part of the photoelectrochemical devices, from electro-catalysts, to light absorber, membranes and the development of devices, but also to the understanding of processes at interfaces and proton transfer.

Keywords:
Photoelectrocatalysis, electrocatalysts, light absorber, membranes, electron transfer, proton transfer, water splitting, CO_2 reduction

Organizers:
Shane Ardo, (UCal-Irvine, USA)
Vincent Artero (CEA Grenoble, FR)
Peter Strasser (Institut für Chemie, TU-Berlin, DE)

Symp 2.4: Towards multi-Terawatt clean Photovoltaic Energy Conversion – Grand Chemical Challenges (3 sessions)

Aim:

Nature has invented the first molecular quantum photovoltaic system which can be found nearly everywhere on our planet, from tiny leaf of great forests to strands of seaweed in the oceans. These nanochemical factories elegantly transform photo-excited electron-hole pairs into high value chemicals. This extraordinary photosynthesis process using chlorophyll molecules represents hundreds of TW photovoltaic power generation. Humanity had to wait until 1954 for the first practical man-made realization of the direct conversion of sun light into electricity. It was achieved in a photovoltaic device (or solar cell) based on a p-n homojunction in a highly purified silicon wafer. Since 1954 photovoltaics (PV) has moved from a negligible contribution in the energy supply to a significant level (7% of electricity in Germany and Italy in 2014 for example), mostly based on silicon wafer technologies and representing about 300 GW installed in the world.

To reach higher levels in short time, at the multi TW scale, disruptive scientific innovations are needed in addition to incremental improvements of present technologies and concepts. Increasing the conversion efficiencies beyond the Shockley-Queisser-Limit for single junctions (about 33%) toward 50% by innovative concepts or architectures in particular multijunctions (45% limit for double junctions, 50% for triple junctions), reducing the cost of production by innovative technologies and processes, reducing the carbon footprint and grey energy by low cost and abundant materials, to drive down the electricity costs from PV to a few eurocents per kWh, are exciting challenges for all researchers worldwide. Since a few years this gave rise to an impetuous development of new types of solar cells, new processes, like dye sensitized solar cells which mimic natural photosynthesis, organic solar cells, colloidal quantum dot solar cells and more recently organic-inorganic hybrid perovskites solar cells. Plasmonics, hot carriers extraction, photon conversion are emerging disruptive concepts. New multinary materials are also emerging in classical inorganic solar cells like earth abundant kesterite thin film chalcogenides, while new processes like electrodeposition, ink printing, sol gel, solution deposition, are more and more considered. A key point of all this development of disruptive PV is that it involves at an unperceived level chemical sciences and concepts. Developing next generations of photovoltaic devices at the multiTW scale is thus a Grand Chemical Challenge.

The symposium will serve as an active platform for researchers working in different areas mentioned above to share their results and to bring into light the new contributions of chemistry in the field of disruptive photovoltaics that can reach TW of installed power.

Keywords: organic solar cells, Si-based solar cells, inorganic solar cells, hybrid perovskite solar cells, dye sensitized solar cells, quantum dot solar cell, solar energy conversion, thin film solar cells, tandem solar cells, plasmonic, photon conversion, interfacial design, stability, durability, high efficiency,

Organizers:
Negar Naghavi (CNRS, E2P2L, Shanghai, CN)
Moritz Riede (Department of Physics, University of Oxford, UK)
Teodor Torodov (IBM, T. J. Watson Research Center, Yorktown Heights, NY, USA)

Symp 2.5: Management of Renewable Energy Related Materials Resources (3 sessions)

Joint Symposium of the themes *"Chemistry for Environment"* and *"Chemistry for Energy and Resources"*

Aim:

Among the 17 sustainable development goals (SDG), adopted by the UN 70th general assembly in December 2015, SDG 7 "Ensure access to affordable, reliable, sustainable, and modern energy for all", SDG 12 "Ensure sustainable consumption and production patterns" and SDG 13 "Urgent action to combat climate change" can be translated into the problem of an optimal management of natural resources in energy and raw materials.

Our planet faces formidable energy challenges, but great hopes are placed on the use of renewable energies such as wind, wave and sun which can generate huge amounts of electricity. The increasing deployment of photovoltaic/wind farms, of electrochemical energy storage units and of transition lines will call for huge amounts of materials. This triggers severe concerns about materials availabilities and global reserves, and raise questions about recycling. Life Cycle Analysis (LCA) studies will undoubtedly become more important in the next decades. Chemical elements of interest are i) 4d and 5d transition metals of groups 8 to 10 used in catalysis for energy production as well as depollution, ii) rare earths used in electronic components and magnets, and iii) elements used in mobile and stationary batteries. Noble gases, and particularly He are of increasing technological importance, while known sources and reserves are quite limited and geographically scarce.

A special focus will be given on the increasing use of H_2 as a pillar of this global energy challenges, more and more called "the hydrogen economy". Hydrogen will be an energy vector and a starting chemical resource massively produced from renewable and intermittent electricity (sun, wind, tides…) as "power to gas" or "power to chemicals" concepts. Such approaches will allow a better match between a day to day and inter-seasonal offer and demand. Advances in earth abundant materials involved in H_2 production by electro-catalytic, photovoltaic or photo-catalytic water splitting, should therefore be considered. Besides H_2 produced from solar energy, natural hydrogen sources [1] might significantly contribute to the energy landscape. This symposium should also allow review the questions related to origins and reserves, geological contexts, fluxes and exploitation strategies of natural H_2. A fresh geochemical look at this problem is very relevant, all the more as natural H_2 sources have been identified with significant concentrations in He.

This symposium will therefore call for original researches showing i) the multifaceted aspects of chemical recovery processes of energy-related materials so as to revitalize the image of "recycling chemistry", too frequently associated to an old and boring chemistry, ii) the development of models to forecast the worldwide materials reserves under various scenarios, iii) novel LCA models to predict which development scenario is the most sustainable, iv) contributions covering geochemical, extractive and processing aspects of renewable energy-related material resources, v) novel energy storage or catalytic materials involving earth abundant elements, vi) essential rare elements savings, towards the concept of "oligo-elements for energy

conversion", like oligo-elements are involved in biological functions, which is also a solution to manage the resources in a sustainable way.

[1] V. Larin et al., Natural Molecular Hydrogen Seepage Associated with Surficial, Rounded Depressions on the European Craton in Russia, Natural Resources Research, 24(3), 369-383 (2015) [DOI: 10.1007/s11053-014-9257-5, Published online November 15, 2014].

Keywords:
Hydrogen**,** energy, geochemistry, recovery, recycling, substitution of rare elements, life cycle analysis, batteries, fuel cells, electrolysis, oligo-elements for energy conversion

***Organizers*:**
Thierry Lemercier (Solvay, Brussels, BE)
Elsa Olivetti (Dept of Materials Science and Engineering, MIT, Cambridge, USA)
Alain Prinzhofer (GEO4U/BR, IPGP-Paris, FR)

Symp 2.6: Chemistry and Nuclear Energy: new materials and processes for a sustainable nuclear energy (3 sessions)

Aim:

Nuclear energy based on fission of heavy radioelements contributes today to about 10 to 15 % of the worldwide electricity production. Last figure for 2014 is 2410 TWh produced by 390 reactors (the 48 Japanese reactors being momentarily stopped). The nuclear electric productions of each of the 31 countries, which operate civilian power nuclear reactors, are very different: 800 TWh/y for USA, 400 for France and 200 or less for all others (figures for 2014). The production of electricity from nuclear energy will only increase substantially in Asian countries. Hundreds of the Gen II nuclear reactors will come to the end of their lives in the next decennia's. Some will be replaced. Some new countries will access to nuclear energy. New reactors under construction, or intended to be, are or will be post-Fukushima Gen III reactors, with enhanced safety. If nuclear energy increases strongly, depending of many factors but shortage in uranium at low price, the forthcoming reactors should be fast neutrons Gen IV reactors which can self-generate their own MOX fuel. Safety/Security/Safeguard (3S requirements) are mandatory to make nuclear energy sustainable.
Nuclear energy is supported by chemistry at each stage of the Fuel Cycle (FC), which stands from the mining of uranium to the management of the spent fuel unloaded from reactors. The management of this spent fuel depends on the countries policies. If plutonium is recycled (closed FC) more chemistry is needed than if one stores the spent fuel (open FC). For the generation IV fast reactors fuelled with Pu and U (MOX) chemistry will be mandatory to multi-recycle Pu and U from spent fuels, because the front end of the new FC, the reprocessing of the spent fuel, becomes a strategic issue. So chemistry is and will be more and more present in nuclear energy. Anyway even if nuclear energy is decreased, or phased out, the management of radwastes will remain a challenge for chemists. It needs to make waste packages to confine the radioactivity over several thousands of years. Such performance has to be supported by many chemical data to model their behaviour in geological disposals. Specific elements involved in chemistry for nuclear energy are fission products (FP) and actinoids (An) up to Cm. Specific chemistry/radiochemistry occurring inside reactors or dealing with high radioactive materials needs too take into account the effects of all type of nuclear processes and large range of temperature, up to thousands of degrees.
R&D in chemistry for nuclear energy is practically relevant from all chemistry's areas. The challenge is to select materials, which can keep their properties as long as possible, because any replacement -when possible- is highly constraining due to a high radioactivity environment. Processes must be as simple as possible to reduce the dispersion of radioactive matter. In any case, in addition to chemical safety problems,

nuclear safety, as criticality, must be fulfilled. By the side of R&D directed towards reactors and FC, developing nuclear energy implies to take into account the behaviour of radionuclides produced by the fission and nuclear processes in nuclear fuel into the environment and living bodies. It is mandatory in waste management.
The great hope for the end of this century is to master the fusion of hydrogen isotopes of which tritium is highly radioactive. If so, the production of electricity based on thermonuclear reactions could be open. The specific fields of chemistry involved in the present and future experimental installations for nuclear fusion concern new materials for magnet or lithium based materials to produce tritium and the behaviour of tritium in multi phase systems.

As this symposium aims for *chemistry to keep nuclear energy sustainable,* it will welcome, at least, contributions in the following fields:
- advanced materials for nuclear reactors components and nuclear fuels and for conditioning of wastes (metallic, ceramic, hybrid, vitreous, cement based, …)
- chemistry at coolant-material interfaces (water, supercritical water, molten metal, molten salts, molten sodium)
- advanced processes for partitioning of elements (hydrometallurgical and pyrophoric) and nuclear fuels fabrication.
- chemistry of tritium, fission products and actinoids in nuclear multi phase systems (liquids/solids/gas).
- chemistry to improve 3S requirements in nuclear energy

Keywords:
Nuclear fuel cycle, uranium mining, uranium enrichment, nuclear fuel fabrication, nuclear fuel recycling, nuclear waste, long term safety, radioelements chemistry, innovative nuclear systems, thorium fuel cycle, innovative materials for nuclear reactors.

Organizers:
Bernard Boullis (CEA-DEN, Paris, FR)
Mingzhang Lin (Inst. of Nuclear Energy Safety Technology-CAS, Univ. of Science and Technology of China, Hefei, Anhui, CN)
Patricia Paviet (US Dept. of Energy, Systems Engineering and Evaluation, Washington DC, USA)

THEME 3: CHEMISTRY FOR THE ENVIRONMENT

Relevant domains:
Air, Trace analysis and techniques, Biomass, Waste, Depollution, Sustainability, Broader water sector, Ecodesign, Circular economy, Ecotoxicology, Greenhouse gases, Processes and Chemistry intensification, Recycling/Recovery of CO_2, Ocean chemistry, etc…

Conveners: *Michel Che* (Sorbonne Université, Paris, FR), *Hemenegildo Garcia Gómez* (UP-Valencia, ES), *Hervé Toulhoat* (Sorbonne Université, Paris, FR), *Hélène Pernot* (Sorbonne Université Paris, FR), *Hélène Olivier-Bourbigou,* (IFPEN, FR).

Symp 3.1: Monitoring Chemicals for a Safer Environment (3 sessions)

***Topics*:** "Chemistry for Environment" and "Chemistry for Energy and Resources"

Aim:

To meet the sustainable development goals (SDG), adopted by the UN 70th general assembly in, December 2015, advances in analytical and sensing chemical techniques for an objective appraisal of the fate and effects of anthropogenic chemicals in our environment will be more than ever desirable.

This symposium will therefore focus on integrated studies of pollutants or any species disseminated in our

assessment. It should address sampling, preparation and detection strategies for quantification in the laboratory and in industries, as well as developing in situ chemical and biochemical sensing and monitoring techniques.

The compartments of our biosphere to be surveyed are highly diverse and interacting at multiple scales as complex systems: air, fresh and sea waters, soils and underground formations, living organisms including ourselves. The presentation of computer models of pollutants propagation from sources up to metabolic compartments should be helpful but mostly to motivate the significance of chemical analyses and enlight socially responsible decisions.

Species of interest encompass for instance airborne particles, diesel nanoparticles and their precursors, radiogenic compounds, explosives and their residues, hydrocarbons, synthetic organics, metals, acid oxides or inorganics: this list in not exhaustive. Analytical information that is required includes elemental quantification and speciation, but also size distribution, morphologies and surface properties of nanoparticles.

The impact of microfluidic techniques on sampling, preparation and detection in the laboratory is expected. Other emerging techniques akin to bio-sensing like EDA (Effect Directed Analysis) are also fully in the scope of the symposium.

Sensors for in situ monitoring are obviously of growing importance, and also a significant economic sector: this symposium should also help identify breakthroughs in terms of gas-solid, electrochemical and biochemical devices, as well as applications of data science in the field of analytical chemistry.

Communications on remediation engineering will be more welcome by symposium 3.4 "Catalysis, Sorption and Separation for a Cleaner Environment"

Keywords:

Environmental analytical chemistry, sampling, sensors, speciation, pollutants, trace species, modelling of pollutant propagation, atmospheric pollutants, analysis of wastewaters.

Organizers:

Damiá Barceló (ICRA, CSIC, Girona, ES)

Hélène Budzinski (EPOC, CNRS, University of Bordeaux, FR)

Symp 3.2: Addressing Environmental Issues through Biosourced Materials and Green Chemicals (4 sessions)

Topics: "Chemistry for the Environment" and "Chemistry for Energy and Resources"

Aim:

Among the 17 sustainable development goals (SDG) adopted by the UN 70th general assembly in December 2015, SDG7 *"Ensure access to affordable, reliable, sustainable, and modern energy for all"*, SDG12 *"Ensure sustainable consumption and production patterns"* and SDG13 *"Urgent action to combat climate change"* are interrelated and have become a high priority on the research agenda of geochemists and chemists. The reserves of fossil fuels are being increasingly depleted and the current energy scheme is causing enormously high levels of CO_2 emissions at the planetary level that is among the major reasons for climate change through increasing greenhouse effect. In addition, oil and natural gas constitute currently the major

feedstocks for the chemical industry and it is necessary to develop new processes based on renewable resources as alternative to the chemicals and processes that are being used at present.

Biomass can become a source for a certain percentage of transportation fuels and, in addition, can provide novel materials and chemicals that could substitute advantageously industrial processes based on non-renewable resources. The symposium will address various aspects of biomass utilization including application for transportation fuels, but also for new chemicals and materials that can be obtained from cellulose, hemicelluloses, carbohydrates, and lignin. Transformation fuels derived from biomass can serve to reduce CO_2 emissions caused by the use of fossil fuels and thus contribute to reduce the risk of climate changes.

Oil and natural gas are also currently the major feedstocks for the production of solvents, polymers and other bulk chemicals. For the sake of sustainability, there is an interest to develop novel processes based on the use of renewable raw materials. The chemicals thus obtained are expected to play an important role as monomers for the production of new polymers, as solvents, as new molecules for consumer goods production and as starting materials for fine chemicals. The added value of such chemicals should be larger than biofuels and this should be a driving force for the development of new eco-respectful processes. The eco-design of new performance ingredients for industry will also be integrated. This Symposium will cover enzymatic and fermentation processes, as well as, purely chemical reactions to convert renewable resources into useful starting materials. Different platforms such as those derived from furfurals, valerolactone or levulinic acid, are expected to be represented in the Symposium.

Biomass transformation requires the design of novel catalysts, reactors and processes that are capable to convert insoluble materials and produce fast reactions. Combining several steps by using the concepts of cascade reactions can be a solution for process intensification. Engineering and process design should also be represented in this Symposium.

Finally, recycling of bio-sourced chemicals and materials should be considered also following the rules of green chemistry.

***Keywords*:**

Renewable resource conversion, catalysis, biomass, green chemistry, sustainability, biofuels, intensified processes and bioprocesses, production and recycling of bio-sourced materials, green solvents, eco-respectful processes, in silico tools and design

Organizers:

Franck Dumeignil (CNRS, Université de Lille, Villeneuve d'Ascq, FR)
Anne M. Gaffney (Idaho National Laboratory, USA)
Emiel J.M. Hensen (Technische Universiteit Eindhoven, Eindhoven, NL)
Anne-Claude DUBLANCHET (L'Oréal Advanced Research, Aulnay sous Bois, FR)

Symp 3.3: Carbon Dioxide Capture, Storage, and Recycling (3 sessions)

***Topics*:** "Chemistry for Environment" and "Chemistry for Energy and Resources"

Aim:

Among the 17 sustainable development goals (SDG), adopted by the UN 70th General Assembly in December 2015, SDG 13 "Urgent action to combat climate change" is of direct concern for geochemists and chemists. Global CO_2 emissions generated by fossil fuels combustion is a major cause of climate change

through increasing greenhouse effect. Given our dependence on fossil fuels, all scenarios for the "energetic transition" call for carbon capture and storage technologies as one of the few realistic means to reduce CO_2 emissions before renewable energy sources may replace these fossil fuels.
In addition, as 7 % of hydrocarbons are used for chemicals, CO_2 can become an attractive source of carbon for the chemical industry. Moreover, we will have a continuous need for transportation fuels and intermittent renewable energies can in principle be stored as chemicals, optimally as liquid oxygenated hydrocarbons. To that end, at least a fraction of captured CO_2 could be used to react with dihydrogen produced by water splitting. This "power to liquid fuels and chemicals" route appears as the most sensible way to avoid emitting more CO_2, since recycling is an endergonic process. Present or future technologies for carbon capture and recycling rely mostly on chemistry which is also crucial to properly address underground storage safety issues. The general objective of this symposium will be to highlight the most significant advances in chemical research and development on this critical aspect of SDG 13, but also to identify bottlenecks and pitfalls.
Post-combustion carbon capture technologies may be based on reactive absorption from gas into liquid phases (e.g. amine to carbamate processes), or physisorption from gas phase into microporous solids. In both cases, a regeneration step is mandatory to release pure CO_2 from the liquid solvent or solid sorbent, and compression must be applied at some point in order to ensure efficient storage (e.g. injection into underground tight reservoirs) Oxy-combustion processes burn hydrocarbons in pure O_2 and produce an easily separable mixture of CO_2 and H_2O. The penalty of using pure O_2 is to some extent balanced by the avoided dilution in N_2. The so-called "chemical looping" processes achieve hydrocarbons combustion by contact with transition metal oxides as oxygen carriers and carbon scavengers. Re-oxidising the carbides by O_2 in a regeneration step allows recovering pure CO_2 as well as the remaining part of the hydrocarbons heating value. For all cases, the overall energy balance will crucially determine the overall viability: this symposium is expected to help foresee the most competitive processes under this respect.
Along "power to liquid fuels and chemicals" routes, reductive recycling of CO_2 has to be coupled with water splitting as a source of H_2, which involve catalytic (photo-electrolysis, or direct photocatalysis, in separate or combined steps. If separated, the hydrogenation step itself may use either homogeneous or heterogeneous catalysis. This symposium should allow one to compare all options on the basis of process intensity and atoms economy.

Keywords:
CO_2 capture storage and recycling, post-combustion, oxy-combustion, chemical looping, amine processes, sorbents, MOF materials, solar fuels from CO_2, synthesis of chemicals, water splitting, catalysis, electrocatalysis, photocatalysis, reduction.

Organizers:
Thibault Cantat, (CEA / DSM / IRAMIS, Gif-sur-Yvette, FR)
Berend Smit (EPFL-Lausanne, Switzerland and UCAL-Berkeley, USA)
Samuel Saysset (ENGIE, Paris, FR)

Symp 3.4: Catalysis, Sorption and Separation for a Cleaner Environment (3 sessions)

Topic: "Chemistry for the Environment"

Aim:

Among the 17 sustainable development goals (SDG) adopted by the UN 70th general assembly in December 2015, SDG 6 "Ensure availability and sustainable management of water and sanitation for all", SDG 7 "Ensure access to affordable, reliable, sustainable, and modern energy for all" and SDG 11 "Make cities and human settlements inclusive, safe, resilient and sustainable" will more than ever rely on innovative and

intensified catalytic processes and separation operations. Indeed, these technologies rooted in chemical sciences are key for efficient and economical cleaning of fuels, exhaust gases, and water, with main goals of minimizing air and water pollution caused by human activities.
This symposium will then focus on advances in catalysis, sorption and separation for a cleaner environment. It should address design from first principles, preparation, characterization, and performances screening of catalysts, sorbents and functionalized membranes, theoretical studies of reaction pathways at the microscopic scale, and multiscale modelling of processes.
Catalytic processes may encompass reductive or oxidative ways to selectively remove contaminants, with thermal, as well as electrochemical and photochemical activation. Heterogeneous, homogeneous and enzymatic catalysts can be considered. Bioremediation processes are included in the scope, as special cases of *in vivo* biocatalysis.
The disclosure of innovative catalysts, sorbents and membranes preparation methods allowing control of structures, textures and morphologies of solids at the nanoscale will be of major interest but should be supported by demonstration of performance improvements. Advanced architectures of molecular catalysts will be considered in the same spirit. *Operando* characterization studies of the working catalysts, sorbents and membranes are expected to provide insightful results, all the more as they are combined with first-principles atomistic modelling studies.
Examples of topics of great global significance are the deep hydrodesulfurization of fossil fuels (and more broadly deep hydrorefining), catalytic converters and particle filters for car exhausts, industrial exhausts gases cleaning, volatile organic compounds reduction in workshops, confined public spaces and homes, water pollution by nitrates and pesticides dissemination generated by intensive agricultural activities, processing of waste waters such as oxidative Fenton or photo-Fenton processes, decontamination of nuclear sites. This list is not exhaustive.

Keywords:
Catalysis, sorption, clean fuels, biocatalysis, photocatalysis, electrocatalysis, catalysis by nanoparticles, computational design, multiscale modelling, in-silico screening, multifunctional membranes, process efficiency, carbon efficiency, processing of waste waters.

Organizers:
Christophe Copéret (ETH, Zürich, CH)
Gerhardt Mestl (MuniCat, TU-Munich – Clariant, Münich, DE)
Pascal Raybaud (IFP Energies Nouvelles, Solaize, FR)

Symp. 3.5: Innovative Chemistry for Environmental Enhancement (3 sessions)

Topic: "Chemistry for the Environment"

Aim:

Increasing global economic competitiveness, social inequalities and the dimension of environmental problems have raised awareness of the need to change the technological paradigm and challenge the technological *status quo*. Environmental innovations are essential in reducing environmental impacts and resolving the environment *vs*. economy dilemma, and chemistry has a significant role underpinning these innovations.
Environmental innovations can be achieved via a combination of inputs, such as raw materials, energy and labour. These innovations may be specifically developed to targeted environmental damage, for instance, in response to regulations; or their benefit is the result of the environmental components of other types of innovations. In this symposium, we explore the role of innovative chemistry in: a) end-of-pipe solutions in

which a technology is applied to a preexisting production system; b) technologies for pollution and wastes reduction and control; and c) approaches to tackle global environmental challenges.
Innovative industrial solutions – this session presents the chemistry behind cutting-edge process-integrated changes in production technology that reduce the quantities of pollutants and waste generated during production. For instance, pre-composite polymers to create higher performing and greener architectural house paints; efficient and precision conversions of renewable raw materials into innovative polymeric products; process chemical that that optimize costs and increase machine efficiency, functional chemicals that lend specific properties and coating chemicals that improve the appearance and performance of finished paper and board. Life cycle analysis (LCA) is an important tool for environmental policy and for industry taking into account environmental impacts of the production process, and associated wastes and emissions, but also the future (downstream) fate of a product. Understanding the close interplay between LCA and chemistry will contribute to the forecasting of future material and energy fluxes on regional and global scales, provide a 'green' solution as a function of various economic growth and regulatory scenarios.
Pollution and waste reduction – this session showcases the chemical technologies that minimize the release or presence of substances harmful to the environment as well as reduce waste by reutilization of materials recovered. Nano- and microparticles-based remediation methods represent a significant advance in the *in situ* decontamination of soil and groundwater pollution. Green jet fuel from a new feedstock which can reduce the greenhouse gas emissions by 65 to 85% when compared to petroleum-based fuels. Low-energy process that uses chemical ligands to selectively recover noble metals can be recovered from secondary sources such as automotive scrap and waste electrical and electronic equipment (WEEE). Microbial fuel cells hold great potential in utilizing electrochemical and biological process to treat wastewater and also generate electricity from organic matter present in wastewater.
Tackling global environmental challenges – Innovative chemistry can have a global reach to help tackling environmental issues in emerging economic countries. For example, an innovative but low-cost chemical process has been applied to improve the access *to safe drinking water and sanitation worldwide*. Bioinspired materials and devices that are fabricated artificially have been used to capture atmospheric water. Nanofertilisers and nanopesticides can be integrated into the science of formulation to facilitate more sophisticated products that may help to reduce the impact that modern agriculture has on environment and human health, and contribute to global food security. Using biomimetic strategy bioinspired materials have been designed and fabricated of for efficient atmospheric water collection to provide potential solution to global water crisis.

***Keywords*:**
Biomimetic materials, carbon reduction, chemical processes, circular economy, corporate responsibility, green chemistry, nanomaterials, life cycle analysis, low carbon innovations, microbial fuel cells, molecular design, next generation polymers, pollution reduction and remediation, resource and material efficiency, smart materials, sustainability, waste recycling, waste valorisation, water recycling and purifications.

Organizers:
Diane Purchase (Faculty of Science & Technology, Middlesex University, UK)
Rai Kookana (CSIRO, AU)
Roberto Terzano (University of Bari "Aldo Moro", IT)
Hemda Garelick (Faculty of Science & Technology, Middlesex University, UK)
Bradley W. Miller (US Environmental Protection Agency, Denver, USA)
Naida Kandile (Chemistry Dept., Ain Shams University, Cairo, EG)
Wenlin Chen (Syngenta Crop Protection LLC, USA)

CHEMISTRY ACROSS THE THEMES

Conveners: *Clément Sanchez* (Collège de France, FR)
Bernadette Charleux (Saint-Gobain, FR)

Symp CT.1: Advanced Methodologies for Matter Characterization and better Knowledge (3 sessions)

Target*:* Academia + Industry

Aim:

Sydney Brenner (Nobel Prize in Physiology or Medicine 2002) formulated the interesting remark or question that *« Progress in science depends on new techniques, new discoveries, and new ideas, probably in that order».* This could be considered as a way to point out the ability of characterization methods to promote the development of new branches of basic sciences or applications. The availability of atomic scale to macroscopic scale spatial or temporal resolution from spectroscopy or imaging techniques or spectroscopies has provided new insights to the structure of matter in its overall complexity and changed our ways of understanding its properties by departing from the study of idealized structures and considering the multi-scale structure and dynamics including surfaces and interfaces. The challenges and driving force for progresses in characterization methodologies can be viewed in complementary angles that associate to bring at the same time answers and new questions.

Sensitivity is probably the first major aim of characterization a method. It potentially turns details from inaccessible to visible, or experimental time from lengthy to straightforward, changing hypothesis to evidences. Sensitivity is a key driving force for the development of brighter light-sources of X-Ray or neutrons, higher voltages microscopes or higher magnetic fields for NMR for example. Sensitivity also comes with a variety of enhancement and edition techniques that allows focusing on chemical or structural specificities: atomic selective images, functional edition, surface enhancement, specific enhancement are found in all the variety of method developments and application.

Resolution can be viewed in space, time, chemical composition, structure or dynamics and benefits from sensitivity enhancements and edition capabilities. Localized spectroscopy, spectroscopic edition of images or tomography, surface characterization, are examples of these developments which are further enriched by considering the time resolved evolution of systems in a constantly increasing range of time-scales.

Sample environment with in-situ, in-vivo, operando or environmental capabilities open possibilities to examine realistically real systems in their working conditions: reactivity, catalytic processes, dynamics… under high or low pressures, high or very high temperature, or irradiation to cite a few. They cover a variety of specific challenges and allow making the bridge from idealized to real systems.

By combining these different aspects that encompass developments of new concepts, new technologies, or new experimental settings we observe a constantly increasing field of application of characterization methods that provide new data for better understand matter in combination with *in silico* modeling and simulation approaches with equal benefit to basic and applied science.

***Keywords*:**
Resolution, sensitivity, enhancement, selectivity, in situ, operando, environmental, tomography, spectroscopy, microscopy, multi-scale, time resolution

Organizers:
Heinz W. Amenitsch (Elettra SincrotoneTrieste, Graz University of Technology – AT)
Valérie Briois (Synchrotron Soleil, CNRS, Saclay, FR)

Marco Daturi (Infra Red Operando, LCS-ENSICaen, FR)
Dominique Massiot (CEMHTI-CNRS UPR3079, Orléans, FR)
Gustaaf Van Tendeloo (Microscopy, EMAT, U-Antwerp, BE)

Symp CT.2: Sustainable Chemistry, Materials and Resources for the City of the 2050s
(3 sessions)

Target: Academia + Industry

Aim:

According to the United Nations, Department of Economic and Social Affairs [1], the world population is projected to be between 9.4 and 10 billion in 2050 with 80% of that in Asia and in Africa. At the same time the percentage of the population residing in urban areas is predicted to grow from 54 % in 2014 to 66% in 2050, and the number of megacities of more than 10 million inhabitants will also increase [2]. Asian and African cities will show the highest growth rates, with 90% of the projected 2.5 billion global increase in population by 2050 being localized in those cities. Furthermore, the overall number of people above 80 will grow globally to half a billion by 2050; meaning that the current population will be multiplied by a factor of three.

The world is thus undergoing a huge transformation and everywhere the industries now have an added obligation of reducing their environmental impact. In light of that, the construction and transportation sectors must address several challenges. They have to simultaneously maximise energy and resource efficiency and maintain the life and environment quality for the inhabitants in the city. The chemists have to play a role in this objective of achieving sustainable solutions for cities. This is indeed the major aim of this symposium to present and discuss the most important developments in this field.

Regarding the **construction sector**, the main goals are to develop new materials with low impact on the environment and on the resources, to decrease the carbon footprint of the manufacturing processes, to improve the energy efficiency (high performance insulation) of the buildings (renovation and new construction), and to address both the quality of indoor environment and the safety. Achieving lightweight materials, using renewable resources and recycling construction materials are therefore important challenges to tackle. For everyone, comfortable indoor environment with healthy air, thermal comfort, acoustic comfort and daylight has to be taken into account in all places (homes, offices). Finally, safety is a main issue, including for instance fire resistance of the materials and reduction of toxic fumes, structural resistance toward seismic events and extreme climatic events.

In the case of the **automotive industry**, the primary goal will always be to produce vehicles that are affordable and accessible to the general population. Thus, in a connected world, where autonomous cars play an important role, where the pressure of environmental regulations is high, and where there is a strong emphasis on safer vehicles, material science and chemistry will play a major role.

In fact, the solutions to some of the challenges are already available with the technology we have today. However, the difficulties lie in scaling up the solutions for a mass production market. As a result, the problem still remains to be addressed and is an opportunity for the future.

There are many areas where advances in chemistry will be necessary. Breakthroughs in lightweight material technologies will help to reduce vehicle mass; improvements in high performance biomaterials can reduce the lifecycle print of cars; electrochemical systems can be developed to replace the existing lithium technologies and etc. This short description directly elucidates La Palice's expression: "a vehicle of 1 ton is 1 000 kgs of materials" and chemistry provides the buildings blocks for any new material.

In parallel, both the **aircraft and train transport industries** face similar challenges in reducing their environmental footprint. For example, light weighting continues to be an active area of research as the industry tries to reduce mass while simultaneously improving comfort for the user. Furthermore, as the

availability of fossil fuel based energy is decreasing, a lot of work is ongoing on diversifying electricity production. In all these areas, the common theme is that research in chemistry and material sciences will play a central role in developing the solutions.

[1] United Nations, Department of Economic and Social Affairs, Population Division (2015). *World Population Prospects: The 2015 Revision, Key Findings and Advance Tables*. Working Paper No. ESA/P/WP.241.

[2] United Nations, Department of Economic and Social Affairs, Population Division (2014). *World Urbanization Prospects: The 2014 Revision, Highlights (ST/ESA/SER.A/352).*

Keywords:
Construction materials, resource efficiency, recycling, indoor and outdoor air quality, acoustic, energy efficiency, daylighting, smart cities, transportation, aeronautics, automotive chemistry, material science, environmental, energy.

Organizers:
Bernadette Charleux (Saint-Gobain, Paris, FR)
Stéphane Delalande (Groupe PSA, Paris, FR)
Josef R. Wünsch (Structural Materials & Systems, BASF, Ludwigshafen-am-Rhein, DE)

Symp CT.3: Hot Topics in Chemistry: a better world through Chemistry (4 sessions)

Target*:* Frontier research

Aim:

Chemistry is the science of the assembly of atoms, molecules and construction of the most complex components of building matter. All disciplines, from organic, inorganic and macromolecular chemistry to solid state chemistry, biochemistry, physical-chemistry, *via* the chemistry of soft or hard matter and polymers, today express a variety of strategies and ever more advanced ways to understand construction and development of novel assemblies. The structures and properties of molecules, clusters, aggregates, macromolecules, and organic, inorganic, or hybrid solid materials can be deeply analyzed and characterized *via* physical methods that are becoming increasingly efficient. Structure-property relationships of chemical structures are becoming better understood thanks to the intense development of many modelling techniques. Chemistry has thus a dual vocation. It raises many fundamental questions to help our understanding of the construction of matter, be it organic or mineral, living or inert, but it also offers important applications for industry and society (health, environment, energy, science and technology of communication and information) and opens original pathways for the construction of future societies, seeking to meet current great challenges of our century (energy transition, scarcity of resources, new contributions to medical research, etc..). In this context, chemistry is essentially a multidisciplinary science that we must continue to enrich and develop. Many societal problems will be solved *via* smart chemical approaches.
However, the chemical palette is extremely diverse, and thus may lead to excessive specialization causing the ignorance of other subdomains. The purpose of this symposium is precisely to present the richness of chemistry by providing to speakers a selective forum to present their most significant recent results to a broad and diverse audience. The different communities of chemists will be well brewed and may express themselves at best. This call concerns all chemists offering them the opportunity to participate in this symposium unifying chemistry in all its facets.

Keywords: All topics in chemistry

Organizers:
Mir Wais Hosseini (UNISTRA, Strasbourg, FR)
Carsten Bolm (University of Aachen, DE)
Joao Rocha (University of Aveiro, PT)
Clément Sanchez (Collège de France, Paris, FR)

Symp CT.4: Chemistry and Waves: an ocean for interdisciplinarity (4 sessions)

***Target**:* Academia + Industry

Aim:

According to the intricate light-particle duality highlighted by A. Einstein in 1905, all matter can exhibit wave-like behavior and waves are particles. Along these lines, the symposium "Chemistry and Waves" focuses on how this duality nurtures today's research on frontiers in the interdisciplinary role of chemistry through the interfaces with physics, biology and material science. Five interdisciplinary topics are suggested that cover large aspects of such research subject.

Innovation in materials synthesis. Innovative synthesis of nanoparticles and functional hybrid materials requires the control of interface interactions that are the source of growth control and / or organization of material. A new impulse is expected with the use of microwaves giving spectacular results. Quick reactions and energy efficiency induced by microwave absorption dramatically increase the kinetics of reactions, shift the chemical equilibria of species in solution and modify the adsorption selectivity at interfaces. For example, the fast heating rates triggered by microwave increase the different cation reactivity and facilitate the synthesis of binary oxides. It can also create hot spots using components having high dielectric constant that can induce heterogeneous nucleation. This technique that is rarely used in the development of nano- and hybrid materials as well as nanoparticle functionalization opens new perspectives to tune chemical and surface composition, structures, morphologies and unusual organization.

New concepts and material characterization methods using EM waves. The development of high-end materials is not only a challenge from the synthesis point-of-view, but would not be possible without state-of-the-art photochemical characterization procedures (e.g. XPS, time-resolved spectroscopies, THz imaging etc.). These are rapidly evolving, since new concepts and techniques are emerging as to how waves interact with nanomaterials. In addition, the latter are now an integral part of material chemistry. As an example, time-resolved spectroscopy establishes a fertile interdisciplinary feedback loop between scientists active in modern photochemistry and opto-electronics or nanomaterials for health.

Optoelectronics, Information and communications technology. Flat panel displays play an essential role in our everyday life. Promising new comers like blue phase liquid crystals have demonstrated the possibility to reproduce images at 240Hz frame rate without any alignment layer. Organic light emitting diodes (OLEDs) displays which lead to thinner screen and improved color rendering are now implemented in some commercially devices. Micro inorganic light emitting diodes (µ-ILEDs) could also be the technology for true flexible displays with improved lifetime. For telecommunications of the future operating at frequency higher than 110GHz, electro-optic polymers with improved thermal stability remain very promising for making Mach-Zehnder interferometers with driving voltage less than 1V at the telecom wavelength of 1.55µm. Amplification of telecommunication signals required for a variety of loss compensated components is currently achieved using well-established planar integrated optics technology based on erbium doped glass or silica-on silicon. The strong demand for increased bandwidth has generated a lot of interest for Er complexes which are compatible with polymers processing to achieve low cost components.

New materials for Medical imaging. Improvement in medical applications is expected to be of major benefit to society within the next years, especially for patients suffering from cancer, cardiovascular diseases,

neurological disorders, inflammatory or infectious diseases. The development of new imaging tools that refers to a broad class of technologies used to look inside of the body in order to diagnose various pathologies is a challenging task to obtain more reliable and early diagnosis. These technologies using ultrasonic, magnetic or electromagnetic waves are becoming routine procedures in hospitals. Development of new materials for the improvement of such techniques and emergence of original contract agents are of the utmost importance in diagnostic imaging as they can greatly increase the sensitivity of an imaging technique allowing for the diagnosis of previously undetectable pathologies.

This symposium aims at bringing together leading chemists, physicists, engineers to share recent breakthroughs in these topics and to address the grand challenges in a forward-looking perspective.

***Keywords*:**

microwave-assisted synthesis and functionalization, high-temperature chemistry, non-thermal microwave effects, ultrafast spectroscopy, XPS, THz imaging, OLEDs, ILEDs, blue phase, luminescence, optical amplification, electro-optic materials & modulators, imaging nanoprobes, MRI, optical and ultrasonic imaging.

Organizers:

Pierre Le Barny (ASA, Université de Lille, FR)
Corinne Chaneac (Sorbonne Université, CNRS, Collège de France, Paris, FR)
Stefan Haacke (IPCMS, CNRS, UNISTRA, FR)
Mario Leclerc (Université Laval, Québec, CA)

Symp CT.5: New Challenges for Chemistry, Materials and Processes in Extreme Conditions (3 sessions)

***Target**:* Academia + Industry

Extreme conditions of temperature, pressure, physical and chemical environment are generally considered in the society as generating more problems than solutions, even if they are extremely useful in many aspects of our common life, in metallurgy for instance. This symposium aims to focus on the solution's axis with the objective to address some aspects which make working under extreme conditions highly desirable and unique in the future, both on fundamental issues and on applicative issues. Plasmas, high temperature chemistries and physics, high pressure transformations, cryogenic conditions, material's behavior are examples where new impetus could be given in the next period. Out of this, useful applications can be foreseen like synthesis processes in plasmas, extremely high thermal solar chemistries, high temperature & pressure catalysis, space applications (e.g. atomic oxygen effect, contamination and space debris, re-entry problematics…), new metallurgies.

Keywords:

High temperature, cryogenics, solar energy, space, ceramics, composites, metallic alloys

Organisers

Marianne Balat-Pichelin (PROMES-CNRS laboratory, Font-Romeu Odeillo, FR)
Hélène Combes (CNES, Toulouse, FR)
Elizabeth Opila (University of Virginia, Charlottesville, USA)

Symp CT.6: Hot Topics for the Industrial Chemistry of the 2050s (3 sessions)

***Target**:* Industry + Academia

Format: *Half-day symposium with an introductive joint session, followed by 3 parallel sessions with lectures and debate with the audience, and then by a joint closing session.*

Aim:

In 2050 the global population will grow to 10 billion people. Consequently, the demand for fundamental resources and the need for global preservation are rising. Access to food and water, need for infrastructure -particularly housing-, healthcare availability and an evolving approach to transport and communication are some of the challenges that face our societies. Minimizing the impact of human activities on climate change, effectively managing natural resources and biodiversity conservation are necessary constraints to insure the future of mankind.
The community of chemists confronting these imperative challenges over the next 30 years will provide responsible solutions toward the 17 Sustainable Development Goals* set by the United Nations. The science of chemistry and the Chemical Industry (start-ups, SME, and large companies) are the heart of these objectives. The shifting mindset toward digitalization and sustainability will lead to substantial and continuous gains in productivity by improving safety, energy availability, and advanced manufacturing including reducing the industrial environmental footprint. This 4th Industrial revolution will support the design of new chemicals or materials for the 2050's.

(*) https://sustainabledevelopment.un.org/post2015/transformingourworld
http://www.undp.org/content/undp/en/home/sustainable-development-goals.html

Keywords:
Industrial chemistry, scientific challenges, digitization, resources, mobility, well being.

Organizers:
Gérard Guilpain (Scientific Director, ARKEMA, Colombes, FR)
Patrick Maestro (Scientific Director, SOLVAY, Brussels, BE)
Thomas Weber (Senior Vice-President, Innovation Management, BASF-SE, Ludwigshafen–am-Rhein, DE)

THEME 4: CHEMISTRY AND SOCIETY

Conveners: *Lydie Valade* (CNRS-LCC Toulouse, Chimie et Société / Fondation de la Maison de la Chimie, FR*), Michel Claessens* (European Commission, Directorate-General for Energy, ITER, Brussels, BE)

Symposium 4: Chemistry and Society **(3 sessions)**

Aim:

The 2019 international congress celebrating the centenary of IUPAC provides for the first time an opportunity to chemists to debate about the perception of their discipline by the citizens. The sessions will show in particular existing differences across countries in public attitudes as well as good practices to improve the dialogue with society.
Chemistry, both as a scientific discipline and an industrial activity, achieved an impressive record of new knowledge and knowhow over the last years, in both understanding and transforming matter, and in their applications in analysis and production. Chemistry covers areas as diverse as food, health, welfare, water management, energy, transport, materials, electronics, to name a few.

However, many problems arise from these activities, often associated with mass production: resource depletion, pollution, and impact on human, animal and environmental health. This objective situation is nonetheless perceived by social groups in quite diverse and sometimes subjective ways. On one side, chemists are proud of their contribution to the well-being of humanity. On the other side, parts of the population express a diffuse fear, due to the presence in their environment of a lot of manufactured products, of which the long term environmental and health effects are largely unknown. The distance and misunderstandings between the two worlds are obvious. However, many members of the chemists' community and environmental NGOs are successfully interacting without ideological *a priori* on these issues. Unfortunately, these debates are often lacking visibility. As a result, the public opinion is left aside and therefore highly formatted through media reports, a problem largely amplified by the wide circulation of uncontrolled data and fake news on internet.
This Symposium 4 will first feature the current situation of relations between chemistry and citizens, taking in account the evolution that has taken place in recent years (Session 1). The point of view of academic and industrial representatives will be presented. Participants are invited to submit abstracts for contributions addressing this theme. Perception of chemistry is highly influenced by education, which is not just about teaching at school or through lectures, but also includes science outreach and information provided and disseminated by the media. Their respective impacts will be compared (Session 2): here, teachers, mediators and journalists are most welcome to submit abstracts of possible contributions. Lastly, the public must be listened to establish a constructive dialogue in favor of a better perception of chemistry: Session 3, which will be opened to the public, will allow to express and confront different opinions. A large amount of time will be devoted to a panel discussion including participation of the audience.

Keywords:
Public surveys, regulations, public understanding of science, risk perception, content analysis, experience sampling, doxastic attitudes, scientific outreach, education, communication, media, social networking, science in society, public debate, dialogue, academic and industrial chemists, ethics, whistle-blowers, precautionary principle, …

Sessions organizers:

Session 4.1: Chemistry and Society: current knowledge

Marie-Claude Vitorge (Chimie et Société/Fond. Maison de la Chimie, Paris, FR)
Patrick Bauchat (Univ. Rennes, Chimie et Société/Fond. Maison de la Chimie, FR)
Fabienne Crettaz Von Roten (Faculté Sciences Soc. et Politiques, Lausanne, CH)
Hélène Mejean (Consultante, Paris, FR)

Session 4.2: Scientific outreach vs Teaching, Perception and communication in chemistry

Arnaud Tessier (CNRS-CEISAM, U-Nantes, Chimie et Société/Fondation Maison de la Chimie, FR)
Séverine Martrenchard (CNRS-ISMO, U-Paris Saclay, Chimie et Société/Fondation Maison de la Chimie, FR)
Marie-Blanche Mauhourat (Inspection générale, Ministère de l'Éducation Nationale, Paris, FR)

Session 4.3: Chemistry and Society: intensifying the dialogue

Andrée Marquet (Sorbonne Université, Chimie et Société/Fond. Maison de la Chimie, Paris, FR)
Jean-Michel Lefour (Chimie et Société/Fondation Maison de la Chimie, Paris, FR)
André Cicollela (Réseau Environnement Santé, Paris, FR)
Esther Gaudreault (Association Francophone pour le Savoir-Acfas, Montréal, CA)

THEME 5: CHEMISTRY EDUCATION

***Convener/Organizers**: Jérôme Randon (Université Claude Bernard-Lyon 1, FR),*
Jan Apotheker, (Dept of Chemistry, RUG, Groningen, NL)

Symposium 5: Chemistry Education **(3 sessions)**

Aim:

Science Education is one of the 17 UN-Development goals. Chemistry Education plays a vital role in achieving quite a view of these UN-development goals. In the Chemistry Education Symposium, we bring together three key issues together needed for the further development of chemistry education. Leading chemistry educators will join together discuss a chemistry education that will appeal to young students, linking concrete knowledge to society and societal needs. This type of chemistry education is needed to induce more students to choose for a science career. In the near future scientists, able to use novel design methodology, for example cradle to cradle, are needed to solve many of the problems we and future society are facing.

In three different sessions several aspects will be presented and results will be shared:

Session 5.1: Relation between education and society
Session 5.2: Tools in chemistry education
Session 5.3: The development of education

THEME 6: IUPAC AND CHEMISTRY: A CENTURY OF INTERTWINED HISTORY, A COMMON HERITAGE FOR THE FUTURE (1919-2019)

***Conveners/Organizers**: Danielle Fauque* (GHDSO, Université Paris Saclay, FR),
Brigitte Van Tiggelen (UCL, Louvain-la-Neuve, BE, and Director for European Operations, Science History Institute, Philadelphia, USA)

Symposium 6: IUPAC and Chemistry: A Century of intertwined History, a common Heritage for the Future (1919-2019) **(3 sessions)**

Aim:

Less than a century ago, IUPAC was born, with the main purpose of enabling communication between chemists worldwide. Emphasis was thus put on calibration, normalization and nomenclature to facilitate comparison and discussions inside the community, as different regions of the world were sometimes using different standards or terminologies, which made collective progress cumbersome and difficult. Furthermore, as chemical instrumentation continuously evolved towards more precision and more tools were created to assess the chemical and physical properties of any given substance, the need for negotiating and building consensus on these new techniques and the related processes of calibration kept growing. Last but not least, conceived as an international organization, IUPAC was born in the aftermath of the First World War that deeply shook the belief in the universalism of science in general and chemistry in particular, and the peaceful use thereof for the benefit of the whole of mankind. By holding regular meetings all over the world,

IUPAC contributed to create and sustain an international community that dealt with all aspects of chemistry, pure as well as applied.

A hundred years later, IUPAC and chemistry are jointly facing world challenges such as globalization, energy crisis, climate change and environmental issues. The 2019 IUPAC congress is thus a suitable time to commemorate the centennial organization, but also evaluate the impact of IUPAC on the shaping of the chemical sciences, broadly construed. It is timely to have a critical and thorough look back with the purpose of equipping the community for the future.

The legacy is a very rich one indeed; over a century of activity and growth, IUPAC has influenced a very reactive field of knowledge, since chemistry has reinvented itself several times since 1919, reorganizing its structure through the creation of new sub-disciplines, fostering new topics at the crossroads of well rooted specialties, and forging multidisciplinary communities tackling contemporary problems, like the creation of new materials, or the environmental studies. Along with its constant effort to regulate and adjust the language of chemistry to the new developments, IUPAC has also been instrumental in supporting teaching, and the growth of chemistry in less wealthy countries.

2019 is also the 150th anniversary of Mendeleev's successful attempt to arrange the chemical elements according to their atomic weights, into what we call the Periodic Table (PT) and the UN has proclaimed 2019 as the International Year of the Periodic Table of Chemical Elements. While IUPAC is not concerned with the development of the PT, the organization plays a decisive role in filling it. Indeed, since 1919, IUPAC is the place where claims for new elements are made, controversies and priorities are resolved, where the naming is decided as well as the different characteristics established.

Because this topic is of wide interest to the IUPAC community at large, and could even be open to a wider and general public, the sessions do not aim at being specialized in history of chemistry. On the contrary, it is our wish to bring together historians of chemistry, and chemists, to tackle the interwoven evolution of IUPAC and chemistry, and we intend to build a network prior to the meeting itself, in particular connecting to those chemists or groups of chemists who have a "long history" within IUPAC and can contribute with their testimony and experience. According to this aim, sessions will include both invited and submitted papers.

Keywords:
IUPAC centenary, history of IUPAC, history of chemistry, periodic table, standardization, heritage, archives, oral history, sites of chemistry, chemical landmarks, universal language of chemistry

Session 6.1: IUPAC's legacy to Chemistry
Session 6.2: IUPAC and the heritage of Chemistry
Session 6.3: The Periodic Table at 150 (4 hours)

THEME 7: YOUNG SCIENTISTS PROGRAMME

***Conveners/Organizers**: Camille Oger,* (IBMM, U-Montpellier, FR).
Bradley W. Miller, (National Enforcement Investigations Center-EPA, USA).
Sophie Carenco, (CNRS, Sorbonne Université, Paris, FR)
Stéphanie Halbert, (Sorbonne Université, Paris, FR)
Victor Mougel, (ETH, Zurich, CH)
International Young Chemists' Network (IYCN)

Symp 7: Young Scientists, their needs, interests and issues (6 sessions)

Format: *Sessions (variable duration) dealing with topics listed below will be spread over the 4 days of the Congress.*

Aim:

Theme 7 will focus on Young Scientists and on their needs but will be designed to be of interest for a broad community of chemists, not only below 35 years old. The program will cover multiple aspects related to early carrier chemists' interests and issues, among which proposal and article writing skills, research and project management, scientific outreach and communication but also networking with academic and industrial partners. A series of talks and round table talks on these topics will be organized during the conference, in parallel with other symposia. These sessions are independent (they can be attended separately) and are intended to target a broad audience of chemists interested to these topics. Invited speakers in this theme will not only originate from the academic chemistry community, but will also be selected from a broader audience, as experts in project management, scientific writing, scientific outreach and politicians will be also invited to participate to these sessions. In addition to this scientific program, a meeting space at the congress location will be available for Young Scientists to meet each other and for networking activities, a special focus being given in catalyzing interaction with potential employers, from industry and 31 academies. CV clinics and soft skills tutorials will be organized in that room to strengthen these interactions. Last, the early career scientists taking part to the congress will be invited to an "early career researcher" celebration of the 100th anniversary of IUPAC organized on the evening of Wednesday July 10, 2019 in Paris (Maison de la Chimie). This event, involving a broader community of young scientists from Paris area, will be organized around a talk from a world known scientist and followed by a dinner and networking night.

Keywords:
Young scientists, industrial and academic careers, networking, social skills, future leaders, leadership development, early-career, graduate student, post-doc, post-doctorate, work life balance, scientific outreach.

Session 7.1: Scientific writing
Session 7.2: New channels and challenges of scientific outreach
Session 7.3: From Bench to the Market
Session 7.4: Teaching
Session 7.5: Recruiting and Networking
Session 7.6: IYCN Symposium

Suggested collaborations:
European and International Young Chemist's Networks (EYCN and IYCN), American Chemical Society Younger Chemists Committee, EuChemS, IUPAC and their network, Young Chemist Network of the French Chemical Society (RJ-SCF).

Associated Events:
Monday evening: Networking reception (co-organized with IYCN), to meet and discuss with colleagues and friends.
Thursday evening: A **historical visit** of Paris that will be the opportunity to be in the footsteps of Marie-Curie.
Wednesday evening: As part of the Celebration of the 100th anniversary of IUPAC an evening of exchanges in a convivial atmosphere with personalities from the world of research and politics. This event will take place at the in Maison de la Chimie.

THEME 8: SPECIAL SYMPOSIA

Convener: *Jean-Pierre Vairon* (Sorbonne Université, CNC, Paris, FR)

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.

Aim:

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.

Keywords:

Gender gap, computing, mathematics, natural sciences

Organizers:

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

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

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

Aim :

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, sharing, reuse, and global dissemination of digital research information.

Keywords :

To be completed

Organizers :

Ian Bruno (IUPAC SCDS, Cambridge Crystallographic Data Centre, Cambridge, UK)
Kazuhiro Hayashi (IUPAC CPCDS, National Institute of Science and Technology Policy, Tokyo, JP)
Leah McEwen (IUPAC CPCDS, Cornell University, Ithaca NY, USA)

Symp. 8.3: Hommage to Eduard Hála

Format: One session (half day), Invited Lectures and discussion symposium, no contribution (CL) from Congress attendees.

Aim:

Prof. Eduard Hála was one of the most prominent Czechoslovak thermodynamicists whose scientific erudition and foresight earned him renown far beyond his country. With Arnošt Reiser he was a co-founder of the so-called Prague school of physical chemistry, ensuring top education in this field to many generations of scientists and chemical engineers. On the occasion of the centenary of Prof. Hála's birth a special session of the IUPAC World Chemistry Congress will be organized, to commemorate the great scientist and inspiring personality.

Keywords:

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

Organizers:

Magdalena Bendova (Institute of Chemical Process Fundamentals, CAS, Prague, CZ).
Johan Jacquemin (Chemistry Department, U-François Rabelais, Tours, FR).

Symp. 8.4: Empowering Women in Chemistry

Format: One session *(2 hrs30)*

Aim:

short abstract to be added

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

Organizers:

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 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, University 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)

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