THEME 3: CHEMISTRY FOR THE ENVIRONMENT

Symposium 3.1: Monitoring Chemicals for a Safer Environment

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 environment as a result of human activities combining advances in analytical chemistry and toxicity risks 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, ecotoxicology, sampling, sensors, data science for analytical chemistry, speciation, pollutants, detection of explosives and their residues, trace species, modelling of pollutant propagation, diesel nanoparticles, microfluidics for analysis.

Organizers:

- *Damiá BARCELÓ (ICRA, Girona, ES)*
- *Hélène BUDZINSKI (EPOC, Bordeaux University, FR)*

Symposium Honorary Contribution (short video):

- **THL: Avelino CORMA** (ITQ, U-Valencia, ES)

Session 3.1.1: New insights in mass spectrometry and effect directed analysis

Abstract:
Adverse effects observed in the wildlife are most often caused by mixtures of known and unknown pollutants. However, environmental risk assessment is currently based on targeted chemical analyses. Such analyses focus on the detection of a selection of known pollutants, which do not often explain the observed toxic effects in complex environmental samples (e.g. unknown compounds, transformation product, cocktail effect...). One of the key challenges in environmental chemistry and ecotoxicology is to characterize and identify those toxicants. To achieve this, in view to extend the range of environmentally relevant pollutants to be monitored and to decrease detection limits, new tools have been recently developed. This session intends to present recent developments in the field of new analytical methodologies such as non-target screening, in vitro bioassays and Effect-Directed Analysis approach (EDA).

Keywords:

Contaminants of emerging concern, High Resolution Mass Spectrometry, Effect Directed Analysis

Speakers

- KN: Emma SCHYMANSKI (Luxembourg University, LU)
- IL1: Thomas TERNES (Federal Institute of Hydrology, Koblenz, DE)
- IL2: Nicolas CREUSOT (EWAG, SW)

Session 3.1.2: New challenges in environmental complex sample analyses (e.g. waster waters and sludges)

Abstract:

Wastewaters and sludges (including their derived biosolids and/or biochards) accumulate emerging contaminants [human and veterinary pharmaceuticals, personal care products (PCPs), artificial sweeteners, polybrominated diphenyl ethers (PBDEs), perfluoroalkyl substances (PFASs), pesticides, PAH-derivatives, benzotriazoles, benzothiazoles, plasticizers, surfactants, disinfection by products, engineered nanomaterials (ENMs), etc.] that are, sooner or latter, released to the environment. Within the present-day context of global change, increased water scarcity and population growth, wastewater for irrigation and application of biosolids in soils have already became important and, in the near future, will become a pivotal source of nutrients and water all over the world as already are in arid regions, i.e, Mediterranean countries, California, Australia, Saudi Arabia, etc. However, there is still a lack of knowledge on the presence and accumulation of these emerging contaminants from wastewater and sludges into soil and the subsequent uptake by plants that posses some inherent risks when applied to agricultural crops for food production. Specifically, this session puts emphasis on the different sources of emerging contaminants, their incorporation into vegetables through irrigation and their metabolization, accumulation and translocation and linking with the ecological effects they produced by reacting in the environment during various applications of wastewater and biosolids in soils under the ongoing risk of water scarcity. We particular welcome contributions within the following areas: i) development of new rapid

analytical methods covering the widest possible range of emerging contaminants and their transformation products and/or metabolites, ii) application of high resolution mass spectrometry to address significant challenges associated with the transformation and metabolism of emerging contaminants within the plant. ii) deep understanding on their inherent properties (partitioning behavior, degradation pathways, bioaccumulation behavior), accumulation mechanism (environmental and tissue transfer and distribution) and toxic effects, iii) improved understanding of their sources and occurrence, fate and transport processes, and associated risks and v) risk management. Ultimately, the session aims at center attention on the understanding of the current approaches, identify existing knowledge gaps, outlining new doors open for continued research and providing prospects for future scrutiny to ensure sustainability of these practices that will palliated severe water scarcity.

Keywords:

Sample preparation, on-line techniques, passive sampling, hyphenated techniques, complex samples, matrix effects

Speakers :

- KN: Yolanda PICO (Valencia University, ES)
- IL1: Serge CHIRON (IRD, Montpellier University, FR)
- IL2: Thomas KNEPPER (Univ. of Applied Sciences-Fresenius, Idstein, DE)

Session 3.1.3: New insights in occurrence and reactivity of pollutants in environmental compartments

Abstract:
Understanding the fate of pollutants in water or in air compartments is essential especially when they are not stable. This is the case for the majority of organic compounds whose interactions with their environment are still not well understood, particularly their mechanisms of formation, transformation and transfer at all scales, spatial and temporal. It is therefore important to develop works studying their occurrence but also their transfer, dispersion and transformation. For example, with regard to the aquatic compartment, the oxidation and photo-oxidation processes are important to elucidate as they condition the presence of these compounds and of their transformation products. Homogeneous and heterogeneous phase reactivity studies of the major classes of atmospheric pollutants are also essential and make it possible, in particular, to propose new relations of structure-reactivity type and thus to improve the quality of models of atmospheric chemistry; this in the interest of a better understanding of air quality, or a better knowledge of the impacts on climate change (aging organic aerosol). The study of new formation tracers of secondary organic aerosols, directly related to the evolution of future legislation on air quality and climate, requires a better knowledge of the sources of pollutants, and also a better understanding of the reactivity of various compounds, of the fate of their oxidation products and also of their role in the formation of secondary aerosols. This session intends to present recent developments in water and in air quality assessment.

Keywords:

Reactivity, transformation products, secondary aerosol, oxidation, water quality, air quality

Speakers :

- KN: Marja Liisa RIEKKOLA (Helsinki University, FI)
- IL1: Wahid MELLOUKI (ICARE, CNRS Orléans, FR)
- IL2: Davide VIONE (UNITO, Torino, IT)

Symposium 3.2: Addressing Environmental Issues through Biosourced Materials and Green Chemicals

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, Lille University, Villeneuve d'Ascq, FR)*
- *Anne M. GAFFNEY (Idaho National Laboratory, USA)*
- *Emiel J.M. HENSEN (Eindhoven Technology University, Eindhoven, NL)*
- *Anne-Claude DUBLANCHET (L'Oréal Advanced Research, Aulnay sous Bois, FR)*

Symposium Honorary Contribution (short video):

- **THL: Avelino CORMA** (ITQ, U-Valencia, ES)

Session 3.2.1: Novel technologies for biomass valorization

Abstract:

Novel technologies will cover enzymatic and fermentation processes as well as purely chemical reactions via homogeneous or heterogeneous catalysis and hybrid catalysis (direct combination of biocatalysis and chemocatalysis) that make possible the conversion of renewable resources into "drop-in" chemicals/fuels or new intermediates or materials. Engineering and process design will be considered, including feedstock pretreatment and product separation steps.

Keywords:

Biotechnology, bioprocess, homogeneous, heterogeneous and biocatalysis, hybrid catalysis, process engineering, biorefinery, separation technology, intensified Processes, sustainability

Speakers

- KN: Liane M. ROSSI (Sao Paulo University, BR)
- IL1: Sergei VARFOLOMEEV (Emanuel Inst. Biochem. Phys., RAS, Moscow, RU)
- IL2: Bala SUBRAMANIAN (Kansas University, Lawrence, USA)
- IL3: Joachim VENUS (Leibniz Institute, Potsdam, DE)

Session 3.2.2: Valorization of biobased compounds & coproducts into sustainable chemicals

Abstract:

All aspects of biomass and bioproducts valorization will be considered including applications for transportation fuels, new chemical and materials, or "drop-in" materials/chemicals. Different platforms molecules such as those derived from furfurals, valerolactone, levullinic acid, polyols are expected to be represented. Concerning biobased compounds, they can be issued from first generation renewable resources (such as vegetable oil and co-products) as well as from second generation resources (non-edible nature, from agriculture or forestry) such as lignocellulose derivatives (cellulose, hemicellulose, saccharide…) including waste wood forest residues (coppice surplus), agriculture residues, organic wastes…. Recycling of bio-sourced chemicals and materials should be considered as well.

Keywords:

biofuels, biochemicals, lignocellulose, agriculture and forest residual and waste valorization, recycling of bio-sourced materials, oleochemical platform

Speakers :

- KN: Pieter C.A. BRUYJNINCX (Utrecht University, NL)
- IL1: Haichao LIU (Peking University, Beijing, CN)
- IL2: Agnieszka M. RUPPERT (IGEC, Lodz Technology University, PL)
- IL3: Julie ZIMMERMAN (Yale University, New Haven, USA)

Session 3.2.3: Synthesis of biobased polymers

Abstract:
This session concerns the development of new bio-based polymers from renewable resources (vegetable oils, terpenes, lignocellulosic derivatives, …) through green pathways (catalysis and processes), which includes:
Naturally derived biomass polymers: direct use of biomass as starting polymeric material, either in the native form or chemically upgraded, including cellulose, cellulose acetate, starches, chitin, modified starch, etc… should we include that class ?
Bio-engineered polymers: bio-synthesized by using microorganisms and plants such as poly(hydroxy alkanoates (PHAs), poly(glutamic acid), etc…
Synthetic polymers such as polylactide (PLA), poly(butylene succinate) (PBS), bio-polyolefins, bio-poly(ethylene terephtalic acid) (bio-PET) or poly(ethylene 2,5-furandicarboxylate)(PEF).

Keywords:

Biopolymers & bio-sourced Polymers, lignin, biodegradable polymers, polylactides, biobased polyamides; succinate polymers; polyterpenes; modified lactide, poly(hydroxylalkanoates) (PHAs); bio-poly(ethylene terephthalate) (bio-PET); poly(ethylene 2,5-furandicarboxylate) (PEF), etc..

Speakers :

- KN: Henri CRAMAIL (ENSCBP, U-Bordeaux, FR)
- IL1: Luigi CAPUZZI (Novamont, Novara, IT)
- IL2: Tadahisa IWATA (Agricultural and Life Sciences, Tokyo University, JP)

Session 3.2.4: How sustainable chemistry can contribute as a source of sustainable innovation: design of high performance products with low environmental impact

Abstract:

Chemistry faces a huge challenge: the need to find renewable starting materials to develop new ingredients that, when formulated, should strictly fulfill the consumer needs and regulatory constraints. The three conditions - use of renewable raw materials, development

of eco-respectful processes and innovation based on ingredients that present a favorable impact on the environment - are inseparable for sustainable innovation.
Several industrial groups have integrated the principles of sustainable development into all stages of a product's life cycle, from its design to consumer with a key-objective of sustainable innovation.
Some highly efficient strategies were developed to identify new performance ingredients, through sustainable chemistry, aiming at operating beyond green chemistry rules:

- In silico tools to better predict human and environmental safety profiles of molecules
- In silico tools to better design "consumer-friendly" molecules
- Using sustainable co-products to valorize useless wastes from other industries.
- Use of new methodologies and processes for a cost effective industrial production

Keywords:

Eco-designed ingredients, new performance molecules, cosmetics, consumer goods, product life cycle analysis, biomass and co-product valorization, new methodologies and processes for cost effective and sustainable production

Speakers:

- KN: Paul ANASTAS (Yale School of Forestry & Environmental Studies. Yale University - New Haven- US)
- IL1: Silvia VIGNOLINI (Department of Chemistry, Cambridge University, Cambridge, UK)
- IL2: Carlo ADAMO (Institut de Recherche de Chimie ENSCP-Chimie ParisTech, Paris, FR)
- IL3 : Maude BROSSAT (L'Oréal Research & Innovation (R&I), Aulnay-sous-Bois, FR)

Symposium 3.3: Carbon Dioxide Capture, Storage, and Recycling

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) Oxycombustion processes burn hydrocarbons in pure O2 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. 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, oxycombustion, 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 ; UCAL-Berkeley, USA)*
- *Samuel SAYSSET (ENGIE, Paris, FR)*

Symposium Honorary Contribution (short video):

- **THL: Avelino CORMA** (ITQ, U-Valencia, ES)

Session 3.3.1: Carbon Capture

Abstract:

The capture of CO_2, either directly from air or from industrial fumes, is a key technology to enable future storage or utilization of this gas. This session will cover the latest developments in the field and focus on the different sources of CO_2, their availability, the technical separation solutions and their cost and energy consumption.

Keywords:

CO_2 capture – amine processes – sorbents – oxy-combustion – post-combustion – MOF materials

Speakers :

- KN: Niall MAC DOWELL (Imperial College, London, UK)
- IL1: Abhoyjit BHOWN (Electric Power Research Institute, Palo Alto, USA)
- IL2: Mohammed EDDAOUDI (KAUST, King Abdullah University of Science and Technology, Thuwal, SA)

Session 3.3.2: CO_2 Utilization/Recycling through Chemical Conversion

Abstract:

The utilization of CO_2 and its recycling through chemical conversion offers opportunities to re-introduce CO_2 in value chains. A myriad of solutions is currently explored at the fundamental and more technological levels, to convert CO_2 to useful chemicals and fuels. The session will foster discussions on the use of CO_2 as a carbon feedstock for the production of commodities or as part as an energy system for the storage of renewable energy.

Keywords:

CO_2 utilization – chemical looping – solar fuels from CO_2 – synthesis of chemicals – water splitting – catalysis – electrocatalysis – photocatalysis – reduction

Speakers :

- KN: Xinbin MA (Tianjin University, CN)
- IL1: Etsuko FUJIT (Brookhaven National Laboratory, USA)
- IL2: Alessandra QUADRELLI (CPE Lyon, FR)

Session 3.3.3: CO_2 Storage and Comparison of Overall Efficiencies of CO_2 Removal Technologies

Abstract:

CO_2 capture, storage and conversion technologies should be analyzed as systems in order to explore efficiently their possible outcomes and impacts. The aim of session III is to present and stimulate discussions on various systems where CO_2 is either captured, stored and/or converted based on volumes, time scales, energy and materials intensity and cost.

Keywords:

CO_2 storage – mineralization – efficiencies

Speakers :

- KN: Alissa PARK (Columbia University, NY, USA) "In situ remediation of metal-contaminated soil and sediments"
- IL1: Susana GARCIA (Heriot-Watt University, Edinburgh, UK) "Urban Mines: innovative sustainable methods for critical elements recovery"
- IL2: David NEVICATO (TOTAL S.A., Paris La Défense, FR) "Nanoscale engineering strategies for developing high performance functional eco-friendly polymer nanocomposites for water purification"

Symposium 3.4: Catalysis, Sorption and Separation for a Cleaner Environment

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 modeling 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 modeling 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 modeling, 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)*

Symposium Honorary Contribution (short video):

- **THL: Avelino CORMA** (ITQ, U-Valencia, ES)

Session 3.4.1: Advanced preparation and in situ/operando characterization of catalysts

Abstract:

Current industrial catalytic processes have been very highly developed during the last 40 to 100 years of continuous efforts in academic and industrial research and development. Further advancements hence can only be achieved if and when all aspects of the catalytic processes ranging from surface chemistry to process engineering are studied at most fundamental levels. To achieve this goal high-end operando and in situ characterization techniques are being developed allowing the in depth investigation of chemical processes occurring during catalyst precursor synthesis, catalyst activation, operation, and with time on stream, deactivation. Fundamental knowledge generated in such studies leads on one hand to advanced preparation methods of novel, improved catalytic materials as well as catalytic process design and control on the other.

Keywords:
Operando spectroscopy ; in situ spectroscopy ; advanced catalyst synthesis ; novel catalytic processes.

Speakers :

- KN: Ulrike DIEBOLD (Vienna University, AT)
- IL1: Kenichi SHIMIZU (Institute for Catalysis, Hokkaido University, Sapporo, JP)
- IL2: Stig HELVEG (Haldor Topsøe, Lingby, DK)

Session 3.4.2: Atomic scale simulation of the active site, in silico screening of catalysts and multi-scale modelling of processes

Abstract:
This session aims at illustrating the strong impact of theoretical chemistry methods in catalysis and separation and how these methods may help for the design of the catalytically active site architecture . Thus, this session is devoted to computational studies of catalytic reaction mechanisms by using various theoretical levels: quantum, (reactive) force fields, static and dynamic approaches... It addresses the rational design of catalysts by means of in silico screening, quantitative structure-activity relationships, machine learning... Multi-scale modelling (mean field microkinetics, kinetic Monte-Carlo…) is also encouraged to bridge the gap with realistic catalytic process conditions.

Keywords:
Computational design, in silico screening, multiscale modelling

Speakers :

- KN: William SCHNEIDER (Notre Dame University, Indiana, USA)
- IL1: Karsten REUTER (TU-München, DE)
- IL2: Véronique VAN SPEYBROEK (U-Ghent, BE)

Session 3.4.3: Bio-inspired catalysts, bio-catalysis, photo-/electro-catalysis

Abstract:

This section is devoted to learning how nature operates to transform efficiently small molecules into fuels (H_2, CH_3OH, CO, NH_3) and how we as chemists can do it by cascading processes involving photons, electrons and protons to activate and convert selectively small molecules.

Keywords:

Enzymatic catalysis; Photo- and Electro-catalysis; electrochemistry; Proton and Electron Transfers, CO_2, O_2, and H_2

Speakers:

- KN: Marc FONTECAVE (Collège de France, Paris, FR)
- IL1: Markus RIBBE (California University, Irvine, USA)
- IL2: Marcella BONCHIO (Padova University, IT)

Symposium 3.5: Innovative Chemistry for Environmental Enhancement

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, is critically important. 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)*
- *Nadia KANDILE (Chemistry Dept., Ain Shams University, Cairo, EG)*
- *Wenlin CHEN (Syngenta Crop Protection LLC, USA)*

Symposium Honorary Contribution *(short video):*

- **THL: Avelino CORMA** (ITQ, U-Valencia, ES)

Session 3.5.1: Innovative chemistry in industrial solutions

Abstract:

This session celebrates the key role of chemistry in providing innovative solutions to a number of industrial processes to overcome pre-existing challenges, including regulation compliance, carbon footprint reduction, waste and energy consumption minimisation, performance enhancement and sustainability attainment. Life Cycle Analysis (LCA) has already been applied to support different decision-making procedures in product lifecycle management, such as eco-design, process optimizations, supply-chain management, and marketing or strategic decisions. In this session, how LCA provides a driver for innovative chemistry to provide more sustainable solutions for industries.

Keywords:

Biomimetic materials, green energy, nanomaterials, low carbon innovations, microbial fuel cells, molecular design, next generation polymers, smart materials, sustainability, water recycling and purification.

Speakers:

- KN: Anne M. GAFFNEY (Idaho National Laboratory, USA)
- IL1: Simone LIGI (CEO of Graphene-XT, Bologna, IT)
- IL2: Willie PEIJNENBURG (RIVM, Bilthoven, NL)

Life Cycle Assessment and Risk Assessmnet of Emerging Technologies

Session 3.5.2: Advanced techniques for pollution and waste reduction

Abstract:

This session focuses on the contributions of chemistry in advanced treatment of pollution and the alternative solutions to minimise the release of pollutants into the environment. The development of circular economy is particularly important in overcome the challenges related to our finite resource and waste production. Innovative chemical process and techniques in recycling and valorising wastes will be particularly welcomed.

Key Words*:*

Circular economy, green chemistry, nanomaterials, microbial fuel cells, next generation polymers, pollution reduction and remediation, smart materials, waste recycling, waste valorisation, water recycling and purifications.

Speakers:

- KN: Sabu THOMAS (*Mahatma Gandhi University, Kottayam, IN)*

Nanoscale engineering strategies for developing high performance functional eco-friendly polymer nanocomposites for water purification

- IL1: Angela SERPE (Cagliari University, IT)

"Urban Mines": innovative sustainable methods for critical elements recovery

- IL2: Petr FEDOTOV (Russian Academy of Science, Moscow, RU)

Session 3.5.3: Novel approaches to tackle global environmental challenges

Abstract:

This section highlights how novel chemical approaches are helping to meet some of the UN Sustainable Development Goals e.g. providing clean water and sanitation, affordable and clean energy. We particularly welcome contributions that provide solutions to environmental challenges in the developing world.

Keywords:

Biomimetic materials, carbon reduction, chemical processes, circular economy, corporate responsibility, green chemistry, nanomaterials, 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.

Speakers:

- KN: Melanie KAH (Environmental Geosciences, Auckland University, NZ)

Applications of nanotechnology in agriculture and implications for environmental and human health

- IL1: Volker ABETZ (Chemistry Dpt., Hamburg University, DE)

Development of polymer membranes with controlled pore size in flat sheet and hollow fiber geometry: a new generation of membranes for clean water

- IL2: Maria ZANONI (Institute of Chemistry, Sao Paulo State University, BR)

Photoelectrocatalysis as alternative technology to tackle safe drinking water, sanitation and carbon reduction challenges