1st EuCheMS European Chemistry Congress

Special Topics Symposia

A New Developments in Theoretical and Computational Chemistry (David Clary, Jerzy Konarsky)

Keynote Lecture: David Clary (Oxford, UK): "New Developments in Theoretical and Computational Chemistry"

Invited Lectures by Michael Klein (Philadelphia,USA); Michele Parrinello (Lugano, CH); Mike Robb (London, UK); Joachim Werner (Stuttgart, D); Wilfred van Gunsteren (Zurich, CH).

Computations have become a central tool in understanding chemical problems. This symposium will describe the most recent developments in this field. Quantum chemistry underlies all such advances and new theories that have particularly promising applications will be a major topic. New theories for describing the dynamics of chemical systems have also been the subject of much recent research and an emphasis will be on dynamical methods that interface with the quantum chemistry approaches. Computational chemistry now influences a remarkable range of scientific areas, going all the way from materials science to molecular biology, and ambitious applications that directly link with experiment will be a significant feature of the symposium

B Cutting Edge Spectroscopy (Helen Fielding)

Invited Lectures by Bertrand Girard (Toulouse, F); Marsha Lester (Philadelphia, USA); Gerhard Meijer (Berlin,D); John Simons (Oxford, UK).

Modern laser spectroscopy has become a truly interdisciplinary field with applications across the whole of chemistry. Traditional spectroscopy techniques are exploited to investigate problems ranging from fundamental photoionisation and photodissociation dynamics of small molecules, to structure determination of large biomolecules. Modern femtosecond experiments not only employ traditional pump-probe techniques but are now capable of employing specially shaped laser fields to control molecular dynamics. The quest to control molecular systems also extends to the new field of cold molecules which seeks to achieve sub-microKelvin temperatures where interesting new phenomena should emerge. Short oral communications and a poster session form an integral part of this symposium.

C New Concepts and Methods in Catalysis

(Manfred Reetz, Pablo Espinet)

Keynote Lecture: Manfred Reetz (Mülheim, D): " A New Approach to Asymmetric Catalysis: Directed Evolution of Enantioselective Enzymes"

Invited Lectures by Jan-Erling Bäckvall (Stockholm, S); Irina Beletskaya (Moscow, RUS); Matthias Beller (Rostock, D); Donna G. Blackmond (London, UK); Peter Chen (Zurich, CH); Antonio Echavarren (Tarragona, ESP); Karl-Anker Jorgensen (Aarhus, DEN); Benjamin List (Mülheim, D); Nicholas J. Turner (Edinburgh, UK); Robert Schlögl (Berlin, D).

Traditional optimization of known catalysts based on years of experimental effort is important, but the implementation of new concepts and in-depth knowledge of mechanisms in the area of catalysis is crucial to fundamental progress in the area. The Symposium "New Concepts and Methods in Catalysis" brings 10 renowned chemists together, who cover such innovations as organocatalysis, combinatorial catalysis, en-

zymes, kinetics, novel ligands and solid materials. The programme is completed by short oral communications and a poster session.

D Frontiers in Supramolecular Chemistry (François Diederich)

Keynote Lecture: François Diederich (Zurich, CH): "Principles of Supramolecular Chemistry In Drug Discovery Research"

Invited Lectures by Thomas Carell (Munich, D); Makoto Fujita (Tokyo, J); Christopher Hunter (Sheffield, UK); David Leigh (Edinburgh, UK); Roland Nolte (Nijmegen, NL); Julius Rebek (La Jolla, USA).

This symposium, comprising a keynote Lecture, six invited Lectures and a series of short oral presentations, gathers both today's and the future's leaders in the field of supramolecular chemistry to discuss major accomplishments from ongoing research as well as the perspectives for future fundamental study and technological innovation. Topics covered in the keynote and invited Lectures are:

- molecular recognition studies to quantify intermolecular interactions in chemical and biological systems
- recognition and catalysis in molecular capsules
- electron transfer processes in biological macromolecules and model systems
- moleculer devices on the way to molecular machines
- creation of functional supramolecular architectures by self-assembly.

E New Frontiers in Medicinal Chemistry (Pierre Potier)

Keynote Lecture: Pierre Potier (Paris, F): "New vistas on Diabetes type II"

Invited Lectures by: Daniel Bur (Actelion, CH); Ian Hughes (Glaxo-Smith-Kline, UK); Rainer Metternich (Schering, D); Klaus Müller (Hoffmann-La Roche, CH); Hans Ulrich Stilz (Sanofi-Aventis, D); Constant A. A. Van Boeckel (N.V. Organon, NL).

Blending synthetic chemistry, molecular modeling, structural biology, and pharmacology, this one-day symposium deals with the discovery and design of new drugs, and their interaction at the molecular and cellular level. The Lectures will highlight key issues in drug discovery and development. They will also focus on the latest research in important topics including thrombin inhibitors, diabetes, and malaria. A series of short oral presentations on other aspects of medicinal chemistry will complement these topics.

F 3D Chemical Imaging in Analysis (Reiner Salzer)

Invited Lectures by Krijn P. deJong (Utrecht, NL); Maya Kiskinova (Trieste, I); Jean-Michel Ortega (Orsay, F); Monika Ritsch-Marte (Innsbruck, A); Gunther Wittstock (Oldenburg, D).

Transition state missed? Functional protein misfolded? Nano-material inactive? Chemical potential, molecular structure or trace impurity profile may change across a sample. Minimal variations can impact upon the scientific and economic success of ambitious projects. Variations of chemical properties in three dimensions across a sample need to be known in all branches of chemical and molecular sciences. Remarkable progress has already been made and frontiers for 3D analysis of all types of materials have been pushed significantly. The symposium "3D Chemical Imaging in Analysis" shall present promising techniques and review successful applications from leading laboratories, beginning immediately after the Plenary Lecture by Nobel Laureate Ahmed H. Zewail.

G | Materials and Nano-Materials for Devices (Malcolm Green)

Keynote Lecture: Malcolm Green (Oxford, UK): "The Unique Structures of Nanocrystals inside Filled Carbon Nanotubes"

Invited Lecturers include: Evgeny V. Antipov (Moscow, RU); Bob Denning (Oxford, UK); Marcel Mayor (Karlsruhe, D); Kenneth R. Poeppelmeier (Evanston, USA); Lauri Niinstö (Helsinki, FIN); Maria Vallet-Regi (Madrid, ESP).

This Symopsium reflects the intense interest and research activity in the field of nanomaterials and their potential applications. Topics to be covered include nano oxide materials for physical properties such as superconductivity, for devices in molecular electronics or for bioceramics and drug delivery. Other topics include developments of composite materials for 3-D holographic lithography of photonic crystals and the unique structures found for ionic and covalent nanocrystals formed inside the holow interiors of single- and double wall carbon nanotubes.

H | Environmental Chemistry (Philippe Garrigues)

Invited Lectures by Pim DeVoogt (Amsterdam, NL); Kevin Jones (Lancaster, UK); Akos Rédey (Veszprem, H); Maria Teresa Vasconcelos (Porto, POR).

Environmental Chemistry has overcome many difficulties in establishing a distinct identity residing as it does between Chemistry, its parent discipline, on the one and and the natural sciences Biology and Geology, with which it shares the same biotope, on the other; between studies of the fate and effects of chemicals in the environmental compartments and risk assessments supporting numerous regulations and directives. The European Water Framework Directive (WFD) and the Registration, Evaluation, Authorisation of Chemicals (REACH) system are the major issues of current concern in the protection of people and the environment.

It is of importance to develop not only analytical methodologies to track pollutants and their routes in the environment, but also toxicity assessment methods to estimate biological effects at low dose in very complex matrices. This symposium will be dedicated to all aspects of Environmental Chemistry, in conjunction with an additional one-day satellite symposium taking place at the EuCheMS congress.

I Chemistry, Food and Health (Reto Battaglia, Roger Fenwick)

Invited Lectures by: Elke Anklam (Geel, B); Konrad Grob (Zurich, CH); Naresh Magan (Bedford, UK); Ben van Ommen (AJ Zeist, NL); Gary Williamson (Nestle, Lausanne CH).

Food chemistry is perhaps the branch of molecular sciences with the widest range of interdisciplinary interaction. Based on analytical methods, food chemistry makes the connection of food composition - from macronutrients to trace constituents, from macromolecules to simple gases - with human health, spanning the bridge from agrigenomics through toxicology to bioavailability and nutritional science. The present symposium intends to illustrate in an exemplary way some of these aspects. Topics covered include mycotoxins: their formation and strategies for prevention, current analytical know-how in food authentication, diet - gene interactions, nutrigenomics and the food/food packaging interface. Short oral communications and poster contributions will further elaborate these topics as well as cover other aspects of food chemistry. Scientists from industry, regulatory bodies and academia are cordially invited to join the discussions.

J Chemistry Meets Biomolecules (Annette Beck Sickinger)

Keynote Lecture: Annette Beck-Sickinger (Leipzig, D): "Selective Protein-Engineering and —Labelling by Chemical Ligation Strategies"

Invited Lecturs by: Sabine Flitsch (Edinburgh, UK); Ernest Giralt (Barcelona, E); Kai Johnsson (Lausanne, CH); Herbert Waldmann (Dortmund, D).

Biomolecules, like carbohydrates and proteins play an important role in all physiological processes. However, techniques that are most suitable to modify small ligands cannot easily be applied because of their size, the number of functional group and the sensitivity of bonds. Within the last years significant progress however has been made to obtain chemically modified proteins, glykoproteins, lipoproteins or carbohydrates. Recent techniques and examples will be shown in this symposium and demonstrate the impact of chemistry to understand the structure and function of biomolecules.

K Teaching Chemistry - Past, Present, and Future (Ernst Homburg, Paul Yates)

Invited Lectures by: Bernadette Bensaude-Vincent (Paris, F); William H. Brock (Canterbury, UK); Ilka Parchmann (Oldenburg, D); Tony Smith (Lyon, F).

The talks in this symposium will examine how the teaching of chemistry has developed through the nineteenth and twentieth century at various levels. There will then be an opportunity to consider the current status of chemical education, and consider what developments may be important in this subject in future years.

L Green and Sustainable Chemistry and Processes (Walter Leitner)

Keynote Lecture: Walter Leitner (Aachen, D): "Green Solvents for Multiphase Catalysis"

Invited Lectures by Keith W. Hutchenson (DuPont Inc., USA); Shu Kobayashi (To-kyo, J); Ronny Neumann (Rehovot, ISR); Peter Saling (BASF AG, D); Roger Sheldon (Delft, NL).

Fundamental chemical science is of key importance for a sustainable development. For the chemical supply chain itself, it is now widely recognized that the development of inherently clean synthetic methodologies can offer new avenues to benign *and* cost effective processes. The EuCheMS session on "Green and Sustainable Chemistry" will focus on novel synthetic methods, materials, and catalytic processes which can contribute to more sustainable routes to chemical products. Invited Lectures on selected topics presented by an international group of outstanding academic and industrial researchers will set the scene for discussion of science and innovation in this mini-symposium.

M Polymer Architecture - From Structure to Functional Control (Klaus Müllen)

Keynote Lecture: Klaus Müllen (Mainz, D): "Organic Functional Nanoparticles"

Invited Lectures by Krzysztof Matyjaszewski (Pittsburgh, USA); Bela Ivan (Budapest, H); Shiro Kobayashi (Kyoto, J); Bert Meijer (Eindhoven, NL); Martin Möller (Aachen, D).

Polymer synthesis must meet strict requirements such as structural perfection (even of high molecular weights), variation of molecular topology and dimensionality or selec-

tive chemical functionalisation. This needs sophisticated methods for both, synthetic and bio-inspired target structures and often implies metal-catalysis and reactions in confining geometries. The next, equally important, step toward designed materials' properties is processing, i.e. creating a well-defined macroscopic state of matter, which often possesses supramolecular order at different length scales. This architectural control leads to superior performance of polymers in complex functional systems for which examples from chemistry, biology and physics will be presented.

N | New Frontiers in Organic Synthesis (Steven V. Ley)

Keynote Lecture: Steven V. Key (Cambridge, UK): "The Changing Face of Organic Synthesis"

Invited Lectures by: Tohru Fukuyama (Tokyo, J); Andreas Kirschning (Hannover, D); Johann Mulzer (Vienna, A); Ian Paterson (Cambridge, UK); Richard Taylor (York, UK); John Wood (Yale U, New Haven, USA); Sam Zard (Palaiseau, F).

Chemists' skills of synthesizing complex organic molecules advance at a tremendous rate. With the global emphasis shifting towards more eco-efficient and sustainable practices new challenges are posed for chemistry. Cleaner reaction processes with significantly improved atom efficiencies require the discovery of many more strategically important reactions and the generation of many more new catalytic processes than those available at present. We need much greater diversity in not just the molecules we make but in the chemistry and reagents used to create them. This symposium, consisting of a keynote lecture, seven invited lectures, short oral presentations and an extensive poster session will highlight the state of the art of the field and outline future directions of organic synthesis.

O Novel Multifunctional Ligands in Coordination Chemistry (Jan Reedijk)

Keynote Lecture: Jan Reedijk (Leiden, NL): "Ligand design for supramolecular applications in coordination chemistry"

Invited Lectures by: Ronald Hage (Unilever Inc., NL); Bernhard Meunier (Toulouse, F); Isabel Moura (Lisbon, POR); Peter J. Sadler (Edinburgh, UK); D. P. Stack (Stanford, USA); Peter Tasker (Edinburgh, UK); Lydie Valade (Toulouse, F).

In the symposium the inorganic coordination chemistry approach for newly designed ligands will be a central issue. Inspiration for newly designed ligands often comes from other, applied areas such as drugs, materials, catalysts, biomimetic reaction, protein engineering, and sustainable chemistry. In the symposium a strong focus will be on the multifunctionality of the ligands.

P Structure and Function of Biomolecules (Ivano Bertini, Bengt Norden)

Invited Lectures by: Lucia Banci (Florence, I); Wim DeGrip (Nijmegen, NL); Torleif Haerd (Göteborg, S); Dinshaw Patel (New York, USA); Andrew Thomson (Norwich, UK).

The symposium includes five invited Lectures, a number of short oral presentations and a poster sessin. Invited Lectures detail the latest achievements in: i) bioinorganic chemistry including metal clusters (e.g. the Cu₂ cluster) and metal-mediated protein-protein interactions as they occur in metal trafficking processes, ii) pharmacological relevant proteins like G protein coupled receptors and iii) the structural and dynamic bases of functional DNA and RNA interactions.

Q Hot Topics in Nuclear- and Radiochemistry (Jan John)

Invited Lectures by: Heinz H.Coenen (Jülich, D); Heinz W. Gäggeler (Berne, CH); Charles Madic (CEA-Saclay, F), Heino Nitsche (Berkeley, USA), Anthony Ware (Maidstone, UK).

The symposium aims at reviewing the state of the art and outlining the most prospective directions of the field of Nuclear- and Radiochemistry. It will include Lectures on the chemistry of new elements, on radionuclides in the environment, radiopharmaceuticals, the chemistry of the nuclear fuel cycle as well as on teaching of nuclear- and radiochemistry. These Lectures, aimed at the general chemistry community, will be complemented by short oral communications and a poster session on all topics in the field.