

[Martin Albrecht](#), Dublin (IE)

### **Cooperative ligands: an efficient concept for powering catalysis**

This lecture will focus on prospects emerging from ligands that are non-innocent. While not new as a concept, non-innocent ligands have recently received considerable attention in promoting demanding transformations such as oxidation reactions, which often require concomitant transfer of electrons and protons (so-called proton coupled electron transfer, PCET). A number of examples will be discussed to illustrate the role of reactive ligands in assisting metal-mediated C–H, N–H, and O–H bond making and breaking processes.

[Isabel Arends](#), Delft (NL)

### **Nature uses enzymes to catalyze a wealth of biotransformations.**

However in practice these transformations are carried out in-vivo under conditions which are far from suitable for large scale production of chemicals. It is our challenge to engineer or design enzymes in such a way that they can be employed in-vitro as catalysts. Especially for oxidations, the power of enzymes can circumvent the use of halogen-containing and environmentally demanding oxidants, by using oxygen or hydrogen peroxide as clean and selective oxidants. In the lecture it will be discussed how different classes of enzymes can be employed as highly promising catalysts for biocatalytic oxidation of alkenes, alkanes and alcohols and for the reduction of conjugated C=C double bonds.

[Matthias Beller](#), Rostock (D)

### **Catalysis—A Key Technology for a Sustainable Chemistry and Energy Technologies**

More than 80% of all products of the chemical industry are made via catalysis. In this regard catalysis is a key factor for achieving a sustainable production of chemicals today and in the future. In the lecture it will be shown that molecular-defined palladium and iron catalysts enable chemists to perform their organic syntheses more selectively and with improved economics. Examples which demonstrate the superiority of catalytic processes compared to more traditional stoichiometric reactions will include hydrogenations, dehydrogenations, as well as modern CC coupling reactions. In addition, the need of the development of drastically improved catalysts for bulk chemical processes and challenging “dream reactions” will be shown.

[Olga Bortolini](#), Ferrara (I)

### **Transition-metal Ion Chemistry in the Gas Phase: Insight into Catalysis**

Close to half of inorganic chemistry, organic chemistry and bio-chemistry involves ions in solution and, in many cases, these ionic species are active intermediates involved in the crucial steps of the reactions. A precise identification of the intermediates, especially when short-lived, is of enormous importance. Consequently any spectroscopic or spectrometric technique able to shine light on the nature and composition of these short-living species has great meaning. One of these techniques is mass spectrometry in particular when coupled with electrospray ionization (ESI). A number of examples will be discussed to illustrate the potential of ESI-MS in the elucidation of the intrinsic reactivity of the metal-containing active species.

[Stuart Cantrill](#), London (UK)

### **Communicating chemistry**

Go to the library and take a chemistry journal from the 1990s off the shelf — does it look all that different to the journals of today? Now grab one from the 1890s, how does that compare?

The basic unit of scientific publishing (a paper) has not changed for hundreds of years, but with the rise of the internet, how is this changing? And is it changing fast enough? This talk will look at different aspects of communicating chemistry — through traditional methods such as journals (and all that entails), but also via new media including blogs and Twitter.

[Miquel Costas Salgueiro](#), Girona (ES)

### **Bioinspired Oxidations with Non-Porphyrinic Catalysts.**

From Fenton-like Processes to Stereospecific Transformations. Selective oxidation reactions constitute challenging problems in modern synthetic chemistry. The bioinspired approach towards this problem aims at developing oxidation catalysts based on biologically relevant transition metal ions, and that reproduce structural and or functional characteristics of oxidative metalloenzymes. Within this context, non heme iron complexes inspired in iron dependent oxigenasas are emerging as particularly versatile catalysts for challenging C-H and C=C oxidation reactions. Catalyst design has driven evolution of the field from Fenton free-diffusing radical systems, to selective and efficient transformations with synthetic utility.

Mechanistic investigations of these reactions have constituted a matter of continuous scientific controversy, and have put forward a portfolio of rich and subtle, and quite often misleading landscape of reaction mechanisms.

[Livius Cotarca](#), Lonigo (I)

### **Chemical Science Driven Technologies in the APIs Synthesis – A Prosperous Future for the Process Chemistry**

The reproducible manufacture of desired Active Pharmaceutical Ingredients (APIs) following innovative and cost effective routes of synthesis is one of the most difficult tasks for chemical development. The inability to develop a robust process based on successful chemistry often leads to costly project scale-down and delays. There are always “rooms at the top” for developing new synthetic and catalytic methods, replacing, for example, the substitution stages (waste generation) by addition or cycloadditions reactions. Moreover, the scale-up routinely or surprisingly faces the process chemist and chemical engineer with new crystalline forms whether these are thermodynamically stable or less stable crystals. Case studies from ZaCh – Zambon Chemicals development laboratories will show how our group identified and solved some extremely difficult issues for several projects, including recent topics, as new applications of Hydrolytic Kinetic Resolution, “click chemistry”, and relationship between chemical science – and equipment driven – technologies for designing robust and scaleable processes.

[Fahmi Himo](#), Stockholm (SE)

### **Quantum Chemical Modeling of Enzymatic Reactions**

This lecture will discuss methods and models used to study enzyme active sites and reaction mechanisms employing quantum chemical techniques. With density functional theory (DFT) it is today possible to routinely and quite accurately treat systems consisting of more than 150 atoms. This has made it possible to model enzyme active sites in a more realistic way than ever. Indeed, many outstanding mechanistic problems have been addressed and solved for a wide variety of enzymatic systems. Recent advancements of this methodology will be discussed and relevant applications will be given.

[Alceo Macchioni](#), Perugia (I)

### **Investigating the Molecular and Supramolecular Structure of Catalysts by NMR**

#### **Techniques**

Potentialities and limitations of NMR techniques for investigating catalysts and catalytic cycles will be illustrated. Particularly, it will be shown how the evaluation of physical-chemical observables (chemical shift, scalar and dipolar couplings, NOEs, diffusion coefficients, etc ...) by 1D and 2D-NMR experiments leads to precisely disclose the structure and nuclearity of neutral and ionic (pre)catalysts in solution. It will be also shown how informative, but also frustrating, in some cases, can be studying a catalytic cycle by in situ NMR spectroscopy. Examples will mainly concern with the results of the research activity of the speaker, which is focused on organometallic catalysts.

[Per-Ola Norrby](#), Göteborg (SE)

In the last decades, classical methods for the study of reaction mechanisms have been supplemented with theoretical studies. Molecular modeling can now give detailed structures and energies all along the reaction paths. As with experimental studies, computational studies of reaction mechanisms suffer from uncertainties. It is possible to set up experimental and computational studies that complement each other, so that the experiments can select between theoretical models in cases where large uncertainties exist. Good validation methods include competition studies of various kinds, like Hammett correlations and kinetic isotope effect studies.

[Dieter Vogt](#), Eindhoven (NL)

### **Industrial Homogeneous Catalysis**

Selected examples of homogeneous catalytic processes applied on a large scale will be discussed. The lecture spans from the molecular basis of those processes to practical aspects such as reactor technology and catalyst separation and recycling. Economic and ecological aspects will be addressed. Next to well established processes, running since decennia, also very recent developments are presented. Examples include alkene hydroformylation, alkene oligomerization, and telomerization reactions. Important aspects for new processes are feedstock diversification and sustainability. A number of future challenges will be discussed.