# Symposium “Future Directions in Chemistry: From Biology to Advanced Materials”

**Wednesday, September 29, 2021**

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<td><strong>Welcome</strong></td>
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<td>Thomas Henzinger, IST Austria President</td>
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<td>09:15</td>
<td><strong>2D and 3D Halide Perovskites: Remarkable Semiconductors</strong></td>
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<td>Mercouri G. Kanatzidis (Northwestern University)</td>
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<td><strong>Chemistry for Solving the Carbon Problem</strong></td>
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<td>Clare P. Grey (University of Cambridge)</td>
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<td>12:00</td>
<td><strong>Playing with Molecular Rings and Strings: New Directions for Nanoscale Switches, Machines and Motors</strong></td>
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<td><strong>Self-assembly as a Tool to Construct New Materials from Nanoparticles</strong></td>
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Symposium “Future Directions in Chemistry: From Biology to Advanced Materials”

Thursday, September 30, 2021

08:45 Registration

09:00 Dynamic Molecular Systems: From Switches to Motors
Ben Feringa (University of Groningen)

09:45 TBA
Corinna Schindler (University of Michigan)

10:30 Break

11:00 Design of Materials and Solid Catalysts by Bioinspiration
Avelino Corma (Polytechnic University of Valencia)

11:45 NHCs on Surfaces and Imidazolium Salts in Membranes – Reaching the Next Level
Frank Glorius (University of Münster)

12:30 Lunch Break

13:30 Evolving Virus-like Nucleocapsids from a Bacterial Enzyme
Donald Hilvert (ETH Zürich)

14:15 On the Origins of Chemical Evolution
Wilhelm T. S. Huck (Radboud University)

15:00 Coffee Break

Location
Lecture Hall (Central Building, 1st floor)
Two-dimensional (2D) and 3D halide perovskites have emerged as outstanding semiconducting materials thanks to their superior stability and structural diversity as well extraordinary charge transport properties. The latter derive from a peculiar combination of very dynamic Crystal life lattices, unusual chemical bonding which results in defect tolerance and long lifetimes of excited carriers. The ever-growing field of optoelectronic device research using 2D perovskites requires a systematic understanding of the effects of the spacer on the structure, properties, and device performance. So far, many studies are based on trial-and-error tests of random spacers with limited ability to predict the resulting structure of these synthetic experiments, hindering the discovery of novel 2D materials to be incorporated into high-performance devices. In this presentation, we provide guidelines on successfully choosing spacers and incorporating them into crystalline materials and optoelectronic devices. Useful insights are emerging on what kind of spacer cations can stabilize 2D perovskites thanks to an extensive collection of spacer cations, which have been shown to stabilize 2D perovskites. There will be an emphasis on the effects of the spacer on the structure and optical properties.

Reversing the rise of CO\textsubscript{2} in the atmosphere requires a massive transition from fossil to truly sustainable resources. While chemists and engineers have largely mastered high-volume production from crude oil, the ability to utilize CO\textsubscript{2} is in its infancy. This talk will describe our research on simple acid-base reactions to create new processes that turn CO\textsubscript{2} into chemicals and fuels. I will first describe C–H carboxylation chemistry to make carboxylic acids. Conventional carboxylations consume highly resource-intensive reagents. We have developed systems that use alkali carbonate as a regenerable base for C–H carboxylation, resulting in CO\textsubscript{2} insertion into C–H bonds with no reagent consumption or waste production. When applied to inedible biomass feedstocks, this chemistry could enable economical production of high-volume, carbon-negative fuels.
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plastics. Extending this concept to fuel production, we have developed carbonate-based materials that are exceptionally active, selective, and robust CO$_2$ hydrogenation catalysts. I will discuss the combination of carbonate-catalyzed CO$_2$ hydrogenation with available commercial technologies to convert CO$_2$ into liquid fuel with unprecedented efficiency.

PLAYING WITH MOLECULAR RINGS AND STRINGS: NEW DIRECTIONS FOR NANOSCALE SWITCHES, MACHINES AND MOTORS

Alberto Credi

CLAN-Center for Light Activated Nanostructures, Consiglio Nazionale delle Ricerche and Università di Bologna, via Gobetti 101, 40129 Bologna, Italy

Dipartimento di Chimica Industriale “Toso Montanari”, Università di Bologna, viale del Risorgimento 4, 40136 Bologna, Italy

alberto.credi@unibo.it

The construction of molecular scale devices and machines have formidably stimulated the creativity of chemists in the past three decades.$^{1,2}$ The interest on this kind of systems arises from their ability to perform a (useful) function in response to chemical and/or physical signals (e.g., light). Mechanically interlocked molecules exhibit appealing structural and functional properties for the construction of nanoscale devices and machines; molecular shuttles based on rotaxanes constitute common examples.$^2$

We describe investigations undertaken in our laboratories, aimed at exploiting the nanoscale movements in rotaxanes and related species$^3$ to perform functions such as transmitting information and motion between sites$^4$ (see Figure) and activating mechanically chiral structures for enantioselective guest recognition.$^5$ From a fundamental viewpoint these systems behave as molecular switches under thermodynamic control. In appropriately designed architectures, however, kinetics can play a major role in governing intercomponent movements. By exploiting energy and/or information ratcheting effects, directional and autonomous movement of the molecular components can occur.$^{1,2}$ We have combined this strategy with a minimalist chemical design to realize artificial nanoscale pumps powered by light.$^6$ Support from the European Union (H2020 ERC AdG ‘Leaps’ 692981 and FET-OPEN ‘Magnify’ 801378) and the Ministero dell’Università e Ricerca (Grants 20173L7W8K and R16S9XXX3) is gratefully acknowledged.
Self-assembly has emerged as the method of choice for preparing materials made of nanosized particles. Over the past several years, we have been developing new ways to control self-assembly of inorganic nanoparticles into higher-order structures. I will begin this talk by discussing our most recent studies on electrostatic self-assembly of oppositely charged nanoparticles. We have conceived a novel method to induce co-assembly of positively- and negatively-charged nanoparticles, which maintains the high surface charge on these nanoparticles during the self-assembly process, leading to previously unknown assemblies. Next, I will discuss ways to control self-assembly of nanoparticles using external stimuli, such as light, magnetic field, and chemical fuels, as well as emerging applications of the resulting materials. The final part of my talk will focus on post-assembly modifications of nanoparticle aggregates, demonstrating that such aggregates can serve as precursors for further transformations. Specifically, I will discuss selective etching of binary nanoparticle superlattices and its use to prepare a novel family of materials, non–close-packed nanoparticle arrays.
DYNAMIC MOLECULAR SYSTEMS FROM SWITCHES TO MOTORS

Ben L. Feringa
Stratingh Institute for Chemistry, University of Groningen
Nijenborgh 4, 9747 AG Groningen, The Netherlands
b.l.feringa@rug.nl

The fascinating molecular motors and machines that sustain life offer a great source of inspiration to the molecular explorer at the nanoscale. Among the major challenges ahead in the design of complex artificial molecular systems is the control over dynamic functions and responsive far-from-equilibrium behaviour. Chemical systems ultimately require integration of structure, organization and function of multi-component dynamic molecular assemblies at different hierarchical levels. A major goal is to achieve and exploit translational and rotary motion.

In this presentation, the focus is on the dynamics of functional molecular systems as well as triggering and assembly processes. We design motors in which molecular motion is coupled to specific functions. Responsive behavior will be illustrated in self-assembly and responsive materials with a focus on cooperative action, amplification along multiple length scales and 2D and 3D organized systems. The design, synthesis and functioning of rotary molecular motors and machines will also be presented with a prospect toward future dynamic molecular systems and responsive materials.

Information on http://www.benferinga.com

- Molecular Machines: Nature, September 2015
- Molecular Switches: Chemistry World, June 2016

DESIGN OF MATERIALS AND SOLID CATALYSTS BY BIOINSPIRATION

Avelino Corma
Instituto de Tecnología Química, Universitat Politècnica de València-Consejo Superior de Investigaciones Científicas, Avenida de los Naranjos s/n, 46022 Valencia, España
acorma@itq.upv.es

Industrial solid catalysts have been developed, most of the time, on the bases of accumulated knowledge, intuition, trial and error and good chemical sense. Today, the development of advanced material synthesis techniques characterization of solid materials under operando
conditions and molecular modeling, has boosted the molecular design approximation to the synthesis of solid catalysts.

The catalysis model of enzymes with well defined single or multiple sites and their capability to better stabilize one reaction transition state when two or more are competing by a combination of molecular confinement and weak interactions, indicate one potential direction for the synthesis of structured solid catalysts. Certainly, one has to be aware that solid catalysts are much less flexible than enzymes and by requiring higher reaction temperatures, entropic factors may have an important impact on the transition state activation energy. Our aim to synthesize structured solid catalysts will well defined single or multiple active sites located in well defined structures in where short and long range interactions are stablised to stabilize the desired reaction transition state.

I will attempt to show how the introduction of those well defined active sites can be achieved by synthesis, observed by spectroscopic techniques, and modelled by theoretical calculations. We will show that by confining those active sites into crystalline porous materials with cavities prebuild to mimic and stabilize the desired reaction transition state, high catalyst activities and selectivities are achieved, that allow us to go from the molecular design up to the industrial application of our solid catalysts.

Finally, I will try to show how we can synthesize by bioinspiration materials for control release of semiotics, and how we combine enzymes and solid catalyst for multistep chemoenzymatic process.

**NHCs ON SURFACES AND IMIDAZOLIUM SALTS IN MEMBRANES: REACHING THE NEXT LEVEL**

*Frank Glorius*

Organisch-Chemisches Institut, Universität Münster, Germany
glorius@uni-muenster.de

**N-Heterocyclic Carbenes (NHCs)** are powerful ligands in catalysis due to their strong electron-donating properties and their ability to form very stable bonds to transition metals. In addition, they can stabilize and modify nanoparticles or flat metals surfaces, outperforming well established phosphine or thiol ligands regarding structural flexibility, electron-donating properties and stability. Current research is highly interdisciplinary and focusses on the basic understanding of the binding mode, mobility and the elucidation of the impact on the surface properties. Exciting applications in materials science, heterogeneous catalysts and beyond are within reach.

**Biological membranes** and their constituents are some of the most important and fundamental building blocks of life. However, their exact role in many essential cellular processes as well as in
the development of diseases such as cancer or Alzheimer's is still not very well understood. Thus, we design, synthesize and evaluate \textit{imidazolium-based lipid analogs} that can integrate into biological membranes and can be used as probes for \textit{live cell imaging} or to manipulate membranes.

\section*{Evolving Virus-Like Nucleocapsids from a Bacterial Enzyme}

\textbf{Donald Hilvert}  
Laboratory of Organic Chemistry, ETH Zürich, 8093 Zurich, Switzerland  
donald.hilvert@org.chem.ethz.ch

Viruses consist of a protective proteinaceous shell that packages an RNA or DNA genome. The emergence of protein cages that could load, protect, and transfer their own genetic information was therefore likely to be a critical step in the evolution of all primitive viruses. Using a combination of design and directed evolution, this process can now be recapitulated in the laboratory. We have converted a bacterial enzyme called lumazine synthase into an artificial nucleocapsid that efficiently encapsulates its own encoding mRNA, and have elucidated the structural changes in cargo and container that made this transformation possible. In addition to providing insight into the origins of natural viruses, such constructs may serve as non-viral carriers for diverse vaccine and delivery applications.

\section*{On the Origins of Chemical Evolution}

\textbf{Wilhelm T.S. Huck}  
Radboud University Nijmegen, Institute for Molecules and Materials, Nijmegen, the Netherlands  
w.huck@science.ru.nl

The evolution of life from the prebiotic environment required a gradual process of chemical evolution towards greater molecular complexity. Elaborate prebiotically-relevant synthetic routes to the building blocks of life have been established. However, it is still unclear how functional chemical systems evolved with direction using only the interaction between inherent molecular chemical reactivity and the abiotic environment. In this talk, I will discuss how complex systems of chemical reactions exhibit well-defined self-organisation in response to varying environmental conditions. This self-organisation allows the compositional complexity of the reaction products to be controlled as a function of factors such as feedstock and catalyst availability. We observed how Breslow’s cycle contributes to the reaction composition by feeding C$_2$ building blocks into the network, alongside reaction pathways dominated by formaldehyde-driven chain growth. The emergence of organised systems of chemical reactions in response to changes in the environment offers a potential mechanism for a chemical evolution process that bridges the gap between prebiotic chemical building blocks and the origin of life.