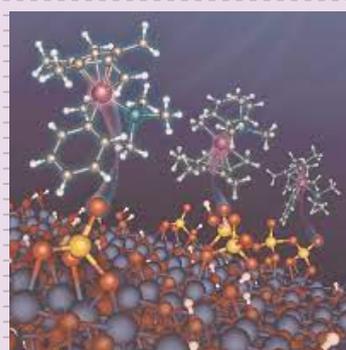
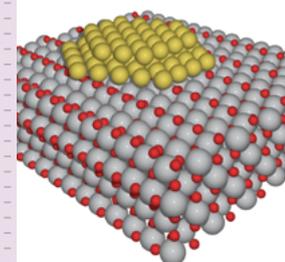
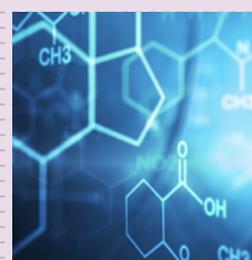
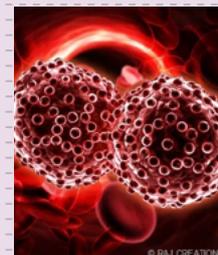


2ND GLOBAL VIRTUAL SUMMIT ON **CATALYSIS &** **CHEMICAL ENGINEERING**

MARCH 14-16, 2022



CHEMICAL CATALYST 2022

Theme:

Contemporary Innovations and
Emerging Novel Research in Catalysis
and Chemical Engineering



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Keynote Forum
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Dong-Pyo Kim

Center for Intelligent Microprocess of Pharmaceutical
Synthesis, Dept. of Chem. Eng., Pohang University of
Science and Technology (POSTECH), Korea

Flow-Assisted Synthesis of Janus and Core-Shell Nanoparticles with Stimuli-Responsive Mobility for Biomedical Applications

Conventional synthetic techniques suffered from complex and time consuming multi-step process in low uniformity, and difficult to endow multi-functions into the produced nanostructures. Continuous-flow technology is emerging for efficient, sustainable and reproducible synthesis of functional nanoparticles (NP). Artificial micro-/nano-motors with asymmetric structures in geometry and chemistry are tiny machines or tools capable of achieving numerous tasks. This work disclosed flow-assisted synthesis of two types of nano-motors with self-propulsion in a process of integrated and scalable manner. Firstly, Janus NPs as triple-responsive nano-motors (m-SiO₂/Fe₃O₄-Pdop/Pt) were manufactured by droplet microfluidic process. Pickering emulsification in flow allowed self-assembly of silica NPs surrounding the spherical interface of resin droplet for anisotropic decoration of polydopamine (Pdop) and Pt

catalyst in a serial process, enabling a scalable manufacturing production of nano-motors with responsive thermophoretic, chemical and magnetic movement. Secondly, enzymatic catalytic core@shell NPs (Pdop@urease@aZIF-8) were prepared by multiple-laminar flow, which allowed to effectively entrapping enzymes into amorphous ZIF-8 shell on Pdop in a serial flow. The novel enzyme-powered nano-motors (A-motor) maintained the activity and photothermal ablation properties with excellent durability upto 5 days due to the protection by shell from external environment. In the biomimic membrane model, the A-motor afforded higher transmigration than bare Pdop NPs, which had a powerful effect on cell uptake and bladder cancer cell ablation via photothermal therapy. This flow approach also facilitates a scalable manufacturing the nano-motors with combinatorial therapeutic functions for nanobiomedicine.

BIOGRAPHY

Prof. Dong-Pyo Kim is a Yonsan chaired professor of POSTECH Chemical Engineering department, and a director of the Center for Intelligent Microprocess of Pharmaceutical Synthesis. He has a Ph.D. in chemistry at Temple University in 1991, post-doctor in MSE at University of Illinois at Urbana-Champaign. He has devoted to a microreaction field, covering from design-fabrication-syntheses of organics/nanomaterials, now forwarding to develop an automated & autonomous synthetic workstation, scale-up production of API and drug delivery systems for biomedical applications. He has published >300 peer-reviewed papers, including Science (2016) on ultrafast organic reaction and several Nature comm. and 43 patents. He received Academic Excellence Award (2017, Korean Chemical Society), POSTECHIAN of the Year (2016, POSTECH), The Scientist of the Month (2016, NRF) and Best 100 Scientific Achievement (2014 & 2007, NRF).



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Michihisa Koyama^{1,2}

¹Shinshu University, Japan

²Kyoto University, Japan

Rapid Screening of Catalytic Reactivity based on Universal Neural Network Potential

The challenges in theoretical catalysis are the prediction of materials with long-term stability and the prediction of activity that arises from the complex and heterogeneous structure of real systems. For this purpose, it is necessary to realize the calculations of large-scale systems incorporating the real-system structure as well as to investigate the catalytic reaction proceeding on it.

When we are to challenge the real system structure of catalyst, typical real-structure models will consist of several hundred atoms or more. To investigate the catalytic reaction based on such a large-scale model is not realistic by the conventional approaches based on density functional theory.

Recent advancement in deep-learning algorithm as well as computer systems, neural network potential (NNP) is attracting much attention. However, applications of traditional NNP is often constrained to a certain material systems due to its limitation in number of elements that can be dealt at the same time. A universal neural network

potential free from such limitation is recently reported [1-2]. It allows the accelerated calculation of chemical reactivity of the catalyst.

In this presentation, the author will introduce applications of universal NNP to the chemical reactivity of catalytic systems.

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BIOGRAPHY

Michihisa Koyama received his Ph.D. from the University of Tokyo in 2002. After serving as Assistant Professor at Tohoku University and Professor at Kyushu University, he is now serving as Professor at Shinshu University, Program-Specific Professor at Kyoto University. Dr. Koyama has authored and co-authored more than 300 review articles, book chapters, and peer reviewed articles. His research activities cover the wide aspects of energy from materials to systems, further to future energy vision. He was awarded The Young Scientists' Prize, The Commendation for Science and Technology by the Minister of Education, Culture, Sports, Science and Technology in 2014, and the Award of the Society of Computer Chemistry, Japan in 2021.



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Richard E. Palmer

Nanomaterials Lab, College of Engineering
Swansea University, UK

Scaling-up Nanoparticle Beam Deposition for Green Synthesis of Advanced Materials: From Atomic Imaging with Aberration- Corrected STEM to Applications in Catalysis

The deposition of size-controlled nanoparticles (atomic clusters) onto supports from the beam is a new, solvent-free, green route to the manufacturing of functional nanomaterials. To translate the beautiful physics and chemistry of clusters into practical applications, e.g., catalysts, coatings, biochips, electrodes, sensors, neuromorphics and photonic materials, significant scale-up of the rate of deposition is needed [1,2]. The deposition rate needed for industrial catalyst R&D is 10mg/hour of clusters, while for bespoke pharmaceutical manufacturing 1-10g/hour is required, a scale-up of 5 to 8 orders of magnitude over traditional mass-selected cluster beam deposition.

In this talk I will discuss both the fundamental aspects of deposited clusters at the atomic-scale – as revealed by aberration-corrected scanning transmission electron microscopy [3,4] – and the status of efforts to meet the scale-up challenge, with emphasis on our “Matrix Assembly Cluster Source” (MACS) [5]. A scale-up by a factor 105 will be shown, and first practical demonstrations [6-12] of deposited clusters in heterogeneous and electrocatalysis will be presented, showing attractive activities and selectivities [1, 6-12].

These also promise exciting advances in a diversity of other application areas.

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BIOGRAPHY

Richard is Head of the Nanomaterials Lab, College of Engineering at Swansea, his hometown; also Professor, School of Physics, Nanjing University, China. His research on atomic clusters includes fundamental studies of atomic structure and dynamics as well as scale-up. Other well-established research topics include atomic manipulation in STM and semiconductor nanofabrication. He was awarded an MA and PhD at Cambridge where he also held 1851, Clare College and Royal Society Fellowships. At Birmingham he founded the UK's first centre for nanoscience. Honours include: IOP Boys Medal, Honorary Doctorate from Hasselt University, British Vacuum Council Yarwood Medal, EPSRC Senior Fellowship and Fellowships of IOP, RSC, Learned Society of Wales. He has published >440 papers, h = 61; also 18 families of patent applications. Spin-out companies: Inanovate, Irresistible, Grove Nanomaterials. He is Editor-in-Chief of the journal Advances in Physics: X (Taylor and Francis) and Editor of the Elsevier Book Series 'Frontiers of Nanoscience'.



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Jean Marie Basset

King Abdullah University of Science and Technology
Kaust Catalysis Center, Jeddah Saudi Arabia

Predictive catalysis by design :

Heterogeneous catalysis, is seeking strategies to render itself more predictable. The main issue is due to the nature of catalytically active sites. One possible solution is to generate single-site catalysts in which most of the sites are structurally identical. Single-site well-defined heterogeneous catalysts can be prepared using concepts of surface organometallic chemistry (SOMC). This strategy has a solid track record to reveal structure–activity relationship to the extent that it is becoming now quite predictable. Almost all elements of the periodical table have been grafted on surfaces of oxides (from simple oxides such as silica or alumina to more sophisticated materials regarding composition or porosity). Considering catalytic hydrocarbon transformations, heterogeneous catalysis outcome may now be predicted based on existing mechanistic proposals and the rules of molecular chemistry (organometallic, organic)

associated with some concepts of surface sciences. A thorough characterization of the grafted metal centers must be carried out using tools spanning from molecular organometallic or surface chemistry. By selection of the metal, its ligand set, and the support taken as a X, L ligands in the Green formalism, the catalyst can be designed and generated by grafting the organometallic precursor containing the functional group(s) suitable to target a given transformation (surface organometallic fragments (SOMF)). The silica-supported catalysts are exhibiting remarkable performances for Ziegler–Natta polymerization and depolymerization, low temperature hydrogenolysis of alkanes and waxes, metathesis of alkanes and cycloalkanes, olefins metathesis, and related reactions, oxidation of olefins into aldehydes by molecular oxygen. Metathesis of Imines.

BIOGRAPHY

Professor Jean Marie Basset was the funding member of the Kaust Catalysis Center (Saudi Arabia). Before he was Director of Research at CNRS (Lyon) at the CPE school of Chemistry Physics and Electronic Jean Marie Basset is member of the French Academy of Science, of the French Academy of Technologies, of the European Academy of Sciences and Arts, and of the Academy of Inventors (US) He is presently Emeritus Research Director (CNRS) at the IRCP - UMR CNRS 8247 Chimie Paris Tech France. He is the author of ca. 700 publications and 50 Patents.



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Roie Yerushalmi



Institute of Chemistry and the Center for Nanoscience and Nanotechnology, The Hebrew University of Jerusalem, Edmond J. Safra Campus, Givat Ram, Jerusalem, 91904, Israel

Customizing Metal Oxide Photocatalysis by Molecular Layer Deposition

Metal Oxides (MOs) are central in a wide range of fields and for numerous applications including catalysis, photocatalysis, sensing, photonics, optoelectronic devices, renewable energy, electrochemistry and more. Atomic and molecular layer deposition utilize surface reactions for layer by layer deposition of thin films. The use of Molecular Layer Deposition (MLD) in the context of photocatalysis and conductive oxides opens new routes towards designing thin films of non-stoichiometric oxides allowing greater tuning and optimizing the reactivity and performances of MOs. Both ALD and MLD are widely used for deposition of thin films with precise control over morphology and composition.

BIOGRAPHY

Prof. Yerushalmi joined the institute of chemistry at the Hebrew University of Jerusalem, Israel in 2008. His research combines molecular level design and surface chemistry in the context of nanoscience and materials science. His main research interests focus on the design and synthesis of hybrid nanostructures for photocatalysis, electrical & optical applications, and energy harvesting. His group study atomic and molecular layer deposition schemes, nanowire synthesis, hybrid nanostructures, ex-situ doping of nanostructures, nanostructure array assembly, and comprehensive application of characterization techniques. Prof. Yerushalmi received a starting grant from the ERC (European Research Council), the Krill Prize from the Wolf foundation, the career development award from the Human Frontier Science Program, and the Kennedy prize.

Our research focus at the interface of material science and surface chemistry by utilizing the precise control offered by vapour phase techniques. An overview of our work demonstrating the versatility of utilizing MLD in materials design, specifically in the context of thin film metal oxide photocatalysis will be presented. MLD is used for depositing organic-inorganic hybrid thin precursor films for enhanced photocatalysis. This approach grants facile route to band gap engineering, defect design and utilizing strain effects as tools for controlling the photo reactivity of metal oxides.



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Irmgard Frank

Leibniz University Hannover,
Theoretical Chemistry, Hannover, Germany

Simulation of chemical reactions and a new view of quantum mechanics

Due to modern high-resolution microscopy methods, we are used to observing atoms and molecules. From Rutherford's experiments with gold foil, we know that what we are seeing is the electronic cloud which surrounds a tiny nucleus. Likewise we are used to classical molecular dynamics simulations which describe molecular systems using empirical force fields. With an appropriate parametrization, condensed phase systems or also bioorganic systems like DNA and proteins can be modelled. These models agree well with the view we obtained from experiment, however, the binding situation must

be defined in the beginning. What happens if we overcome this restriction by introducing quantum chemistry? Indeed, the quantum mechanical description of the electronic structure yields the correct binding situation and hence the structure of matter of any kind. However, from the simulation of chemical reactions, it turns out, that a quantum mechanical description of the nuclear motion is not needed, even more, it is counterproductive. The classical description with Newton dynamics is the better approach. The result is a deterministic version of quantum mechanics, which is free of paradoxa.

BIOGRAPHY

Irmgard Frank studied chemistry at the LMU Munich (1988 – 1993). She went to the University of Bonn where she completed her PhD thesis in 1995. She became a postdoc at the Max-Planck institute for solid state science in Stuttgart where she developed the restricted-open shell Kohn-Sham method (ROKS) for the simulation of photoreactions. She went back to Munich and completed her Habilitation in 2004. Her work focused on the ab-initio simulation of chemical reactions. In 2008 she was appointed associate professor at the University of Hannover. More recently, she develops deterministic quantum mechanics.



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Gianlorenzo Bussetti

Department of Physics, Politecnico di Milano, Italy

Molecules on surfaces: Dodging coupling and ligand effects

One of the most fascinating opportunities offered by organic electronics is the possibility to scale the device architecture down to the molecular level. A prerequisite to this goal is to obtain a scalable arrangement of molecules suitable substrates, which is a major bottleneck in the device development. In fact, substrates act as special ligands, strongly affecting the properties of contact/interfacial molecules. Indeed, the molecule-substrate coupled system often shows specific characteristics that are not suitable for device construction, such as the partial or complete loss of molecules optical or chemical activity. Till now, good couplings have been obtained only following an inefficient trial-and-error approach.

To overcome this crucial problem, different strategies have been considered: e.g., the coupling to low-interacting substrates or the

insertion of spacer layers between the molecules and inorganic surfaces. Either approach however presents some drawbacks, e.g. the magnetic coupling to ferromagnetic substrates (crucial for organic spintronic) is lost if the interposed spacer layer takes the molecule too far from the substrate.

In this talk, a review of different approaches described in the literature is presented. The discussion will be focused on the molecular class of porphyrins that, owing to their extended 2D heteroaromatic macrocycle, usually yield strong electronic interaction with the substrate surfaces. Recent results on the full decoupling of porphyrins from interacting metal substrates will be presented. Dodging the ligand effect opens the route towards fully organic bottom-up constructions, where organic chemistry can be exploited to guide the molecule-molecule directional bonding inside the molecular architecture.

BIOGRAPHY

GB graduated in Physics at the University of Rome with a thesis on the optical properties of semiconducting surfaces. During his PhD, he extended his interests on the optical properties of thin and ultra-thin organic films. His results, applied to organic gas sensors to enhance their sensitivity and selectivity, were honored by the Italian Physical Society Giulotto's prize. He spent many years abroad in France, Austria and Germany to increase his expertise in the growth and characterization of organic films. Currently, GB is professor of Physics at Politecnico di Milano. He is leading a team devoted to the chemical engineering and fine control of the molecule-molecule interaction for the creation of fully organic, bottom-up architectures at the nanoscale.



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Anne M. Gaffney

University of South Carolina,
Columbia, South Carolina, USA

Catalytic Deconstruction of Plasma- treated Single-Use Plastics to Value-added Chemicals and Novel Materials

The rate of plastics production is currently higher than 400 million metric tons per year, with only 10% of global plastic waste is recycled, mostly due to challenges in sorting and depolymerization. Lightweight packaging (LWP) comprises ~50% of total plastics consumption and consists mainly of single and multilayer films and containers. Polyethylene (PE) and polypropylene (PP) makeup more than 65% of the LWP that ends up as reject in a waste materials recovery facility. The North America LWP market is estimated at \$40 billion in 2020 and is expected to grow to \$48 billion by 2026 at a CAGR (Compound Annual Growth Rate) of 3.2%.

To address these challenges, a transformative hybrid approach using low temperature plasma pretreatment to augment conversion of waste polyolefins into monomers, new polymers and value-added chemicals is proposed. The vision is to combine tunable non-equilibrium nonthermal plasma treatment with catalytic depolymerization to offer an improvement in efficiency, cumulative energy demand and selectivity over conventional recycling processes and, in the longer term, a viable environmentally friendly solution to plastic recycling.

BIOGRAPHY

Dr. Anne M. Gaffney is the Chief Science Officer of Idaho National Laboratory and Distinguished National Lab Fellow (2014 – present). She has thirty-four years of experience working in industry inventing and commercializing new technologies for major chemical manufacturing companies including Koch Industries, Lummus Technology, Dow, Dupont and ARCO Chemical Company. She has authored 155 publications and 257 patents. Dr. Gaffney is also a distinguished Joint Appointment Fellow at the University of South Carolina (2018 – present) where she is the Technical Director of the National Science Foundation Center for Rational Catalyst Synthesis. Some of her recent awards include: the 2019 American Chemical Society, Energy & Fuels, Distinguished Researcher Award in Petroleum Chemistry; the 2015 Eugene J. Houdry Award of the North American Catalysis Society; the Chemical Heritage Foundation, Women in Science Inductee, 2014; and the American Chemical Society, Industrial Chemistry Award, 2013. Dr. Gaffney received her BA in chemistry and mathematics from Mount Holyoke College and her Ph.D. in physical organic chemistry from University of Delaware.



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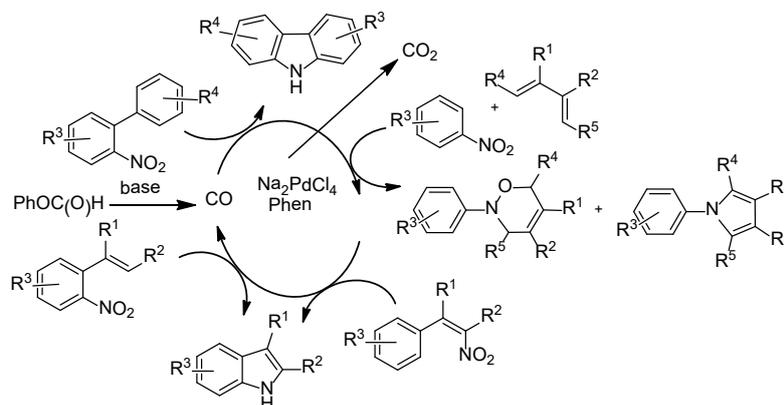
Synthesis of N-Heterocycles by Palladium-catalyzed Reductive Cyclization of Organic Nitro Compounds

Fabio Ragaini¹, Francesco Ferretti¹, Doaa R. Ramadan^{1,2} and Manar A. Fouad^{1,2}

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²Chemistry Department, Faculty of Science, Alexandria University, Alexandria, 21321, Egypt

Indoles and carbazoles can be obtained by reductive cyclization of *o*-nitrostyrenes, β -nitrostyrenes or *o*-nitrobiphenyls, using carbon monoxide as the reductant and a palladium/phenanthroline complex as catalyst. Moreover, the intermolecular reaction between a conjugated diene and a nitrosoarene obtained by reduction of a nitroarene affords oxazines and pyrroles in high yields. However, the use of pressurized CO poses experimental problems to most users. In the last few years, we have developed the use of phenyl formate as a cheap CO surrogate, which liberates carbon monoxide in the presence of a base under the reaction conditions. This allows the reaction to be performed in a cheap glass pressure tube, without the need for any specialized equipment. Excellent results were obtained for the cyclization of *o*-nitrostyrenes to indoles and *o*-nitrobiphenyls to carbazole (almost quantitative yields in several cases, tolerance to sensitive functional groups such as formyl, pyrrolyl, and amino, catalyst loadings as low as 0.1 mol%) and for the synthesis of oxazines, whereas the cyclization of β -nitrostyrenes to indoles proceeded only in fair yields.



Biography

Fabio Ragaini got his PhD at Milan University in 1991 under the supervision of Prof. Cenini. Apart from a visiting scientist period at The Pennsylvania State University with Prof. Geoffroy, he made his entire academic career within Milan University, eventually becoming a Full Professor in 2008. He is the author of around 130 papers and a monograph most of which in the field of the reduction and carbonylation reactions of nitroarenes. h = 42.



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Sulfonic Acid Catalysts for Biomass derived valuated chemicals

Maria Luisa Testa

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Sulfonic acid functionalized silicas have demonstrated excellent catalytic performance in several reactions involved in the biomass conversion for the synthesis of valuated chemicals. In this presentation, the synthesis of several amorphous and mesoporous propyl sulfonic silica were described. The catalytic performance of these sulfonic acid-modified mesostructured silicas were tested in different reactions including the production of biofuel additives as glycerol derivatives. Moreover, the effect of the synthetic procedure, the acidity and textural properties on catalytic activity was considered. The prepared sulfonic acid materials has been benchmarked with other commercial acid catalysts showing higher performance. The surface and structural properties of the catalysts were investigated by several characterization techniques.

Biography

Dr. M.L. Testa, researcher at the CNR-Institute for the Study of Nanostructured Materials, focus her research in heterogeneous catalysis, design and synthesis of hybrid organic-inorganic and metal catalysts. The main applications are -transformation of biomass components in biofuels and added-value products -wastewater purification -gas pollutants abatement. Special attention goes to circular chemistry on use of sustainable and efficient processes and use of waste, both for the synthesis of new materials and added-value products. She is involved in several national and international projects on environmental catalysis and preparation of active materials. She had international research experiences (India-CSIR; Spain-Corboba and Valencia Universities; France-IRCELYON; Ireland-Cork University; Bulgaria-BAS). Part of activity is devoted to Chemistry dissemination, teaching, tutoring and thesis supervision.



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Metal Nanoparticles as Catalyst in Ionic Liquids

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The use of metal nanoparticles still represents a good compromise on the fringes of a heterogeneous and homogeneous chemistry. Combined with alternative solvents such as ionic liquids, metal nanoparticles can perform very unusual reactions. Furthermore, the nature of the ionic liquids can also influence the reaction path and, at times, a small change in the composition of the ionic liquid can greatly vary the result of the reaction. In this presentation some examples of the use of ligand-free metallic nanoparticles in ionic liquids will be shown with some mechanistic implications.

Biography

The research carried out by Dr. Monopoli can be traced back to four main themes: a) use of ionic liquids as alternative solvents in organic synthesis and study of their effect on the catalytic activity of metal nanoparticles (palladium, copper, gold, etc ...); b) applications of ionic liquids as solvents for non-catalytic reactions; c) use of catalysts in organic synthesis and green chemistry d) new synthetic approaches for the valorisation of CO₂ and biodiesel production; d) development of innovative analytical protocols (including synthesis of new matrices) for applications in MALDI mass spectrometry.



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The thiamine diphosphate-dependent lyase acetoin:dichlorophenolindophenol oxidoreductase as a versatile tool for the implementation of biocatalytic synthetic pathways

Pier Paolo Giovannini, Francesco Presini and Valentina Venturi

Department of Chemical Pharmaceutical and Agricultural Sciences, University of Ferrara, Italy

The acetoin: dichlorophenolindophenol oxidoreductase (Ao:DCPIP OR) is an enzyme making a part of the acetoin dehydrogenase multi-enzyme system, where it catalyzes the acetoin cleavage assisted by the thiamine diphosphate (ThDP) cofactor. We exploited for the first time the catalytic promiscuity of the Ao:DCPIP OR which allow it to catalyze the reverse reaction with respect the physiological one, namely the formation of a C-C bond formation in place of the C-C bond cleavage. This promiscuous activity, together with the broad substrate specificity of the Ao:DCPIP OR, allowed us to employ this enzyme as a catalyst for a number of asymmetric benzoin-type condensation between different carbonyl compounds. Two different donors, namely the 3-hydroxy-3-methylbutane-2-one and the 4-hydroxy-4-methylhexane-3-one have been coupled with various aromatic and aliphatic aldehydes or with activated ketones as well. Through this approach, a wide set of enantioenriched α -hydroxy ketones, even with tertiary alcoholic groups has been produced which, thanks to their multi-functionality, represents valuable chiral synthons. In this perspective, several studies on the combined use of the Ao:DCPIP OR with other enzymes such as NAD-dependent dehydrogenases, and lipases, either in multi-step or one-pot processes devoted to the preparation of bioactive natural compounds or parts of them. These studies contributed to highlight the synthetic potential of the of ThDP-dependent enzymes in the implementation of sustainable asymmetric synthetic pathways.

Biography

Pier Paolo Giovannini PhD., is an associated professor of Industrial chemistry at the University of Ferrara (Italy), where he teaches Industrial chemistry and Sustainable chemical processes. He is author of more than sixty papers published on peer reviewed international journals, most of which are focused on the development of biocatalyzed synthetic strategies.



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From Naphthalene to Polycyclic Molecular Architectures

Damien Prim

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Naphthalene is a central building block for the construction of elaborated polycyclic architectures with applications in broad domains such as life and material sciences. As a result, C-H functionalisation strategies specially designed for naphthalene substrates have become essential to install valuable substituents at one or both rings of the naphthalene unit. Our approach towards extended fluorenones and benzo-fused phenanthridinones is based on dual role of N-tosyl carboxamides acting jointly as a directing group in a first C-H arylation step and as a “CO” or “CO-NH” fragment precursor. In this context, the C-H arylation and cyclisation sequence represents a useful way to the preparation of novel tetra- and pentacyclic molecular architectures in various substitution patterns. Additionally, both the regioselectivity and the reaction paths of the cyclization was studied by DFT calculations which fully complement experimental observations.

Biography

Damien Prim studied chemistry at the Paul Verlaine University of Metz, where he received his PhD in organic chemistry in 1994 under the guidance of Prof. Gilbert Kirsch. After a postdoctoral period with Prof. Léon Ghosez at UC Louvain-la-Neuve, Belgium, he was appointed Professor assistant at Paul Verlaine University of Metz. He then successively moved to Pierre et Marie Curie University in Paris as CNRS research associate from 1999 to 2001 and to the University of Versailles St Quentin as Professor assistant in 2001. In 2005, he was appointed Full Professor of Chemistry at the University of Versailles St Quentin. His research focuses on homogeneous and heterogenous catalysis and the syntheses of polycyclic molecular architectures.



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Noncovalent Interactions, a New Perspective for a Rational Engineering in Homogenous Catalysis ?

Jean-Pierre Djukic, Yann Cornaton, Christophe Deraedt and Fule Wu

Laboratoire de Chimie et Systématique organométalliques, UMR 7177 Université de Strasbourg, Strasbourg, France

The recent outburst of interest for C-H bond functionalization led us to address the broader question of reaction and catalyst engineering. Although one can now satisfactorily analyze bonding and molecular cohesion in transition metal-based organometallic systems, can modern theoretical methods guide reactivity exploration and the engineering of novel catalytic systems ? We addressed this question by investigating the Ambiphilic Metal–Ligand Activation/Concerted Metalation Deprotonation (AMLA/CMD) mechanism involved in the transition metal-catalysed directed C-H bond functionalization. This endeavor was initiated having in scope the construction of a rationale for the transposition of 4-5d metal chemistry to earth-abundant 3d metals. In this base-assisted mechanism of C-H bond metalation, agostic interactions are necessary but not sufficient, for C-H bond breaking actually relies on the attractive NCI-coding of a proton-transfer step and the minimization of metal-H repulsion. We will introduce the recent shift of our research towards the construction of a noncovalent -inclusive paradigm of chemical reactivity engineering based on experimental efforts propped up by state-of-the-art theoretical tools.

Biography

Jean-Pierre Djukic, obtained a PhD in chemistry from the University Pierre and Marie Curie in Paris in 1992. He was post-doctoral research fellow at the Iowa State University in 1993-94 in the group of L. Keith Woo. He was hired as researcher at the CNRS in Strasbourg in the group of Michel Pfeffer in 1994. In 1996-97 he was a A. von Humboldt foundation fellow in the group of Karl-Heinz Dötz at the University of Bonn. Since 2014 he heads as Director of Research the Laboratory of Organometallic Chemistry and Systemics of the Institute of Chemistry of Strasbourg. His research interests focus on theoretical studies of noncovalent interactions in organometallic chemistry.



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Solar Energy for the Sustainable Synthesis of Pharmaceuticals and Fuels

Shoubhik Das

Department of Chemistry, University of Antwerp, Belgium

Currently, human beings are completely dependent on the extended use of fossil fuels as primary energy resource. In contrary, solar energy, contains huge amount of energy. The average intensity of the total solar irradiance is about 1366.1 Wm^{-2} which provides roughly $4.3 \times 10^{20} \text{ J}$ energy only in 1 h. Therefore, if it is harvested properly and is utilized in organic synthesis or in fuel generation, can provide sustainable solutions in the society. In fact, a very small fraction of solar energy, about 0.1%, is converted by natural photosynthesis into biomass. Chemists are learning to exploit the huge amount of solar energy by artificial photochemical reactions for two important applications: (i) to convert sunlight into chemical or electrical energy, and (ii) to perform organic synthesis that cannot be obtained by conventional chemistry. Light excitation of a molecule or a semiconductor leads to an electronically excited state capable of performing as a stronger one-electron oxidant/reductant compared to the ground state. This means that light excitation promotes a primary electron-transfer reaction. The primary photoinduced electron-transfer reactions can later be converted into desired products via radical formations during photocatalysis. Based on this consideration, we are working on the synthesis of pharmaceuticals, fine chemicals and fuel molecule generation.

Biography

Shoubhik Das completed his PhD in 2012 under the supervision of Prof. Matthias Beller in Rostock, Germany. After a postdoctoral stay with Prof. Matthew J. Gaunt at the University of Cambridge, he worked at the École Polytechnique Fédérale de Lausanne (EPFL), Switzerland until 2015. Then, he started as an independent research group leader at the Georg-August-Universität Göttingen, Germany after which he moved to the University of Antwerp in 2019. Very recently, he has won Francqui lecturer award and Odysseus award.



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Predicting Catalytic Activity with Electric Fields

Valerie Vaissier Welborn

Theoretical and computational chemistry, Virginia Tech December 30, 2021

In condensed phase, the function of macromolecules is determined by the motion of charged particles, from electrons for chemical reactivity and catalysis to ions or ionic complexes for signal transduction, transport and chelation. Therefore, macromolecular function can be predicted from electric fields, the driving force behind the motion of charged particles. In complex systems, each molecule or molecular fragment will produce an electric field that contributes, constructively or destructively, to these electric fields (superposition principle). Further, since electric fields are relevant across length scales, they are a great metric to quantify the role environmental factors play in regulating macromolecular function. In this talk, I will present electric field calculations estimating the catalytic power of synthetic enzyme KE15 in presence of a nearby DNA fragment. More specifically, I will show how the catalytic activity of the enzyme can be regulated by DNA, whose structure and sequence can be easily controlled outside of the protein. This thought experiment combines potential functional application of DNA origamis and synthetic enzyme tuning, illustrating the predictive power of electric field calculations.



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Thermal-tuning of one-pot multienzymatic cascades by nanoactuation (HOTZYMES PROJECT)

Valeria Grazú^{1,2}

¹BioNanoSurf Group, Instituto de Ciencia de Materiales de Aragón (ICMA), CSIC/Universidad de Zaragoza, c/ Edificio I+D, Mariano Esquillor Gómez, 50018, Zaragoza, Spain.

²Centro de Investigación Biomédica en Red de Bioingeniería, Biomateriales y Nanomedicina (CIBER-BBN), Av. Monforte de Lemos, 3-5, 28029 Madrid, Spain

Enzymatic cascades open a path to the efficient implementation of complex biotransformations for producing from high-cost pharmaceuticals to low-cost biocommodities. However, for multi-step synthetic schemes catalyzed by incompatible or unpaired enzymatic cascades, efficient cell-free one-pot systems, where enzymes are perfectly orchestrated and regulated, have yet to be developed. The FET-OPEN project HOTZYMES (<https://www.hotzymes.eu>), we propose to develop a new ground-breaking concept to exert functional control over different enzymes using magnetic heating. We expect to control enzyme activity by conjugating enzymes and magnetic nanoparticles and tuning temperature gradients at the nanoscale to precisely and locally reach the optimal temperature of each immobilized enzyme. This will allow an unprecedented spatio-temporal control over the kinetics of multi-enzymatic cascades by remotely applying alternating magnetic fields.

In this sense we were able to demonstrate the feasibility of HOTZYMES's main hypothesis of triggering simultaneous or sequential multiple hotspots within the same vessel without raising the global temperature of the media by using magnetic particles with different magnetic heating properties under the application of Alternating Magnetic Fields (AMFs). This concept is being currently used by consortium members to gain simultaneous or sequential control over model multienzymatic cascades of industrial interest. To meet this technological break-through, a new generation of magnetic bio-reactors specific to the field of biocatalysis is also being designed and tested.

Acknowledgements : The research for this work has received funding from the European Union (EU) project HOTZYMES (grant agreement n° 829162) under EU's Horizon 2020 Programme Research and Innovation actions H2020-FETOPEN-2018-2019-2020-01.

Biography

Dr. V. Grazú has more than 20 years of experience in biofunctionalization of micro/nanostructured materials for their use in biotechnological and biomedical applications. Her current line of research is focused on the development of pioneering non-traditional uses of magnetic heating to trigger remote activation of therapeutic enzymes for biomedical applications or multienzyme cascades for efficient production of pharmaceutical and biocommodities. She is a member of BioNanoSurf Group and scientific researcher at "Instituto de Nanociencia y Materiales de Aragón" (INMA, CSIC-UNIZAR). She has also large experience on the successful transfer of technology having 7 licensed patents and having been Chief Technology Innovation Officer of Nanoimmunotech, a company that she has also co-founded. She is the coordinator of the FET-OPEN project HOTZYMES.



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Manipulating Surface Acidity and Basicity for Heterogeneous CO₂ Photoreduction

Kulbir Kaur Ghuman

Institut national de la recherche (INRS), Centre Énergie Matériaux Télécommunications, Quebec, Canada

The significant challenge faced by our global society, from issues of climate change to questions of energy security could be solved if we can find a champion catalyst that can convert atmospheric CO₂ to carbon-based fuels. However, designing catalytic nanostructures that can thermochemically or photochemically convert gaseous CO₂ into fuels is a significant challenge that requires a keen understanding of the physical and chemical properties of complex materials and the processes happening on them at the atomic and electronic level. In this presentation, I will talk about one such active catalyst, In₂O₃-x(OH)_y, capable of reducing CO₂ in the presence of light and temperature. I will specifically highlight the electronic- and atomic-level insights provided by the advanced modeling techniques (such as density functional theory (DFT), time-dependent DFT, and metadynamics) into the surface chemistry of CO₂ reduction reaction on In₂O₃-x(OH)_y nanoparticles. Finally, a new class of frustrated Lewis pair (FLP) heterogeneous catalysts discovered through this work will be discussed, which among many reaction possibilities can enable efficient gas-phase hydrogenation chemistry of CO₂ to fuels and chemicals.

Biography

Kulbir Kaur Ghuman is an early-career researcher, recently appointed as Assistant Professor at Institut national de la recherche scientifique, Centre Énergie Matériaux Télécommunications (INRS-EMT) and a Tier-2 Canada Research Chair in 'Computational Materials Design for Energy and Environmental Applications'. She is also the head of a well-established lab equipped with advanced software and computational infrastructure, dedicated to understanding the theoretical underpinnings of the behavior of complex materials and chemical reactions. She has established several novel structure-property relationships and mechanisms for optimizing fuel cell materials and designing efficient catalysts. Her influence in the field of computational materials science is demonstrated through her publications (h-index: 16) in top-ranked journals such as Chem. Rev. Soc., Energy Environ. Sci., Adv. Energy Mater., Nat. Comm., etc.



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Cheng Tang

The University of Adelaide, Adelaide, Australia

Electrocatalysis for Renewable Chemicals and Fuels

Access to green, flexible and reliable energy and chemicals is the key to global sustainable development and increasing prosperity, especially in the post-COVID-19 and carbon-neutral economy. Aiming at creating changes in energy technologies and chemicals manufacturing, we proposed the electrocatalytic refinery (e-refinery) to defossilize, decarbonize and decentralize present chemical industry. We for the first time established the concept, principles, and methodologies of e-refinery. Based on it, we aim to develop new technologies that can creatively produce some key chemicals (e.g., H₂, hydrogen peroxide, ammonia, formate, urea) directly from abundant sources (e.g., water, air, CO₂) and powered by renewable electricity.

Specifically, we developed an efficient e-refinery strategy for producing H₂O₂ directly from water and oxygen via two-electron oxygen reduction, which is of high flexibility to be operated in small scales and on demand. Our work innovatively

engineers the structure of electrocatalysts at the molecular level, and has achieved present best activity and selectivity (> 95%) for H₂O₂ production in both alkaline and acidic conditions. The obtained concentration of H₂O₂ (> 1%) is high enough for practical applications such as disinfection and electro-Fenton water treatment. Besides, we also innovated the ammonia production technologies by electrocatalysis directly from air (N₂ and O₂) and water. We proposed for the first time bismuth catalysts for direct electrocatalytic nitrogen fixation into ammonia at ambient conditions. To address the significant drawbacks of tough N₂ activation and poor NH₃ selectivity, we developed a new two-step process through integration of plasma oxidation with electrocatalytic reduction, leading to ~2500 times higher yield and ~100% Faradaic efficiency. All the research in materials design and mechanism elucidation are achieved by combining atomic-level material engineering, electrochemical evaluation, theoretical computations, and advanced in situ characterizations.

BIOGRAPHY

Cheng Tang received his B.Eng. and Ph.D. from the Department of Chemical Engineering, Tsinghua University in 2013 and 2018, respectively. Currently, he is a Lecturer at The University of Adelaide. His research focuses on functional nanomaterials and carbon-neutral energy and chemistry, including 3D graphene, single-atom materials, next-generation batteries, electrocatalytic refinery for renewable fuels and chemicals, etc. He has published 1 authored book, 1 book chapter and > 80 research papers in refereed journals (over 9000 citations, h-index: 48, Google Scholar). He was recently honored with the ARC Discovery Early Career Researcher Award (2022), the MIT TR35 Asia Pacific (2021), the Thomson Reuters/Clarivate Analytics Highly Cited Researcher (2020, 2021), and The Chorafas Foundation Award in Chemistry (2019).



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Giovanni Barcaro

Institute for Physical and Chemical Processes (IPCF)

Multi-scale modeling as a powerful tool in catalysis

As attested in the pillars of the main funding schemes worldwide, developing and optimizing the performances of new catalysts for sustainable processes is a scientific challenge with remarkable economic and societal repercussions. In this presentation, it will be shown how hierarchical multi-scale computational modeling offers a powerful tool aimed at elucidating, but especially predicting and optimizing, the structure and the structure/properties relationships in realistic working conditions of catalytic systems with a diffuse interest in both fundamental science and technological applications. More specifically, the discussion will focus on some selected case studies providing mechanistic insights into (as

an example) (i) the lignin β -O-4 linkage acidolysis catalyzed by mineral acids as a key resource for the production of important aromatic chemicals and (ii) TiO₂-catalyzed glycine polymerization and its conjunction to prebiotic chemical reactions on the primitive Earth. The discussion will also focus on the development of a novel computational protocol based on the use of Reactive Force Field (ReaxFF) massaging (DynReaxMas) applied to the study of amorphous-carbon systems (of large interest as a promising catalytic material) able to simulate the synthesis at temperatures close to the experiment, correctly capturing the interplay of activated vs entropic processes and the resulting phase morphology.

BIOGRAPHY

Dr. Giovanni Barcaro got his Master in Materials Science in 2003 and his PhD in Chemistry in 2007 at Pisa University. Since 2021 he is a senior researcher at CNR-IPCF. He is author of about 130 publications on peer-review International Journals and as book chapters in the period from 2005 to 2020 with about 3500 citations and an h-index of 35 (source: WOS, September 2021). Dr Barcaro is a leading expert the computational modeling of systems at the nanoscale, having played a pivotal role in developing advanced computational tools for structural search and structure/properties relationships assessment via the hierarchical application of multi-scale methods, ranging from accurate electronic (mainly DFT) to Reactive Force Fields (ReaxFF) simulations.



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Salvador Eslava

Dept. of Chemical Engineering, Imperial College
London, SW7 2AZ, United Kingdom

Engineering photoelectrochemical and photocatalytic materials for solar fuels

Photoelectrochemical and photocatalytic conversion of water and carbon dioxide using solar energy offers a clean solution to the world energy requirements of a sustainable future. Achieving its full potential depends on developing inexpensive photoelectrodes and photocatalysts that can efficiently absorb solar light and drive the photoinduced charges to react with water and carbon dioxide. In this talk, I will present recent developments we have achieved in the preparation of inexpensive photoanodes, photocathodes and photocatalyst composites. For example, we have achieved nanostructured TiO₂ with exposed {0 1 0} facets for photoanodes, ferrite perovskites for photocathodes or halide perovskite composites with graphene or graphite for photoanodes and CO₂ photocatalysts, following vapor deposition techniques, solution processing or mechanochemical syntheses. 1-6 An extended characterisation help us relate their physical and charge-transfer properties to their performance, guiding us in their rational design for their optimization and future application.

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BIOGRAPHY

Dr Salvador Eslava is a Senior Lecturer (Assoc. Prof.) and EPSRC Early Career Fellow in the Department of Chemical Engineering at Imperial College London. He was recently awarded the Warner prize from the Institution of Chemical Engineers (IChemE). Before Imperial, he was a Lecturer at University of Bath (2014-2019), research associate in the Materials Department at Imperial College London (2011-2014) and in the Chemistry Department at The University of Cambridge (2009-2011). He defended his PhD degree in 2009 conducted in the Centre for Surface Chemistry and Catalysis (COK) at Katholieke Universiteit Leuven and IMEC, Belgium. He holds a Taught Master in Materials Science from Università degli Studi di Pavia, Italy, and an MEng in Chemical Engineering from Autonomous University of Barcelona, Spain. He has published more than 60 articles and received funding from different sources such as EPSRC and The Royal Society.



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Martin Schmal

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University of São Paulo, Av. Prof. Luciano Gualberto, Tv. 3, nº.
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Graphene-Supported Metal Oxide Nanoparticles for Catalysis Applications

This project proposes the use of environmentally friendly, simple and versatile methodologies for the synthesis of controlled metal oxides nanoparticles supported on graphene with a high level of distribution, morphology, size and defined composition for applications in catalysis. The different synthesis routes will be tested in order to systematically correlate the effect of nanoparticles on dispersion and uniformity on the surface of graphene sheets. The control over the structure and composition of the nanoparticles will serve to generate higher performance.

The catalyst was characterized before and after

reaction by several techniques. XPS results revealed a higher concentration of ion species at the surface and electrostatic interaction with the support. Diffuse Reflectance Infrared Fourier Transform Spectroscopy analysis (DRIFTS) suggested formate species formation on the catalyst surface and the absence of bridge-bonded adsorbed CO. The electronic interaction between cobalt nanoparticles and graphene affected carbon monoxide dissociation. Tests to generate photocatalysts with greater photocatalytic performance will also be shown. The photocatalytic activity of the produced nanostructures will be tested using catalysts for the photodegradation.

BIOGRAPHY

MARTIN SCHMAL is professor since 1970, became Full Professor in 1985 and Emeritus since 2008 at the Chemical Engineering Department of the Federal University of Rio de Janeiro and actually visiting professor at the University of São Paulo since 2014 – He graduated Chemical Engineering at the Engineering Faculty of the Catholic University of S. Paulo (1964), Master Science degree - 1966 at the Federal University of Rio de Janeiro/COPPE, Brazil, Doktor Ingenieur degree (Dr. Ing.) at the Technische Universität Berlin, Germany. He specialized at the Institut du Recherche sur la Catalyse, Lyon, France and University of Karlsruhe, Germany. He has more than 320 publications in international journals; 250 papers H=51.

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B. Frank Gupton

Virginia Commonwealth University,
Richmond, VA (USA)

Novel Carbon Support Systems for Transition Metal-Catalyzed Chemical Reactions

Recent work has demonstrated that novel carbon support systems such as graphene and multi-wall carbon nanotubes impart unusual and advantageous catalytic properties to metal nanoparticles that have been deposited onto the surface of these substrates. By treating these materials with microwave radiation, we have been able to create essentially a solid-state ligand system that can be applied in specific organic transformations. The conductive properties of

these substrates provide a platform for accelerating reaction rates by promoting both oxidation and reduction components of catalytic cycles. Furthermore, the enhanced binding energies imparted by the interaction between the substrate and the metal nanoparticles provides remarkable stability. Computational and experimental results have provided insights into the nature of these catalytic systems and will be provided in the presentation

BIOGRAPHY

Dr. Frank Gupton is a professor at Virginia Commonwealth University and holds joint appointments in the Departments of Chemistry and the Department of Chemical and Life Science Engineering. He is the Floyd D. Gottwald Chair of Pharmaceutical Engineering and also serves as Department Chair of the Chemical and Life Science Engineering Department. His thirty-year industrial career centered on the development and commercialization of chemical processes for pharmaceutical applications. Dr. Gupton's research group is currently focused on the development of continuous processing technology to facilitate the discovery, development and commercialization of drug products. Dr. Gupton's research efforts have focused on streamlining pharmaceutical processes, particularly in the area of active ingredients, by employing the principles of process intensification which include the use of innovative chemistry, novel continuous manufacturing platforms, and new and more efficient catalysts for pharmaceutical applications. The research group's efforts are guided and driven based on both financial and economic impact that can be derived from this effort. Dr. Gupton is the recipient of the 2018 American Chemical Society Award for Affordable Green Chemistry, and in the same year, he received the Presidential Award for Green Chemistry. In 2019 he received the Peter J. Dunn Award for Green Chemistry and Engineering Impact in the Pharmaceutical Industry from the ACS Green Chemistry Institute Pharmaceutical Round Table. These awards were associated with Professor Gupton's work on the development of a highly efficient process to produce nevirapine, a first-line treatment in HIV therapy.



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Horia Metiu

Department of Chemistry & Biochemistry, University of
California, Santa Barbara California 93106-9510, USA

Hydrogen Manufacture Without Carbon Dioxide

One of the most conspicuous problems in heterogeneous catalysis of carbon-containing reactants is the deactivation of the catalyst by coke formation. The problem is particularly common for reactions taking place at high temperature. In the last few years we have investigated the possibility of performing such reactions with the aid of molten metal alloys or molten salts, in which the melt is the catalyst. This has two important advantages. (1) The reaction is performed in a bubble reactor, and the carbon produced is lifted with the bubbles and is deposited on the surface of the melt. Use of the bubble reactor avoids coking because each bubble is in contact with fresh liquid catalyst. (2) In this system there is no coarsening. Based on this

idea we have searched for active, molten catalysts for two reactions: methane pyrolysis to hydrogen and carbon, and a combination of pyrolysis and dry reforming. The advantage of performing pyrolysis in such a system is that the process produces no CO₂, unlike steam reforming, which is the current industrial process for hydrogen production. The advantages of pyrolysis combined with dry reforming is that one can prepare syngas having any desired H₂-to-CO ratio, the reaction does not produce water, and coking problems are avoided. Potentially this opens the way for a new method of syngas fabrication. In the talk I will present the catalysts discovered so far and discuss various methods for theoretical and experimental analysis.

BIOGRAPHY

Horia Metiu, Professor of Chemistry.

Horia Metiu obtained his Ph.D. at MIT in 1974. After postdoctoral research at MIT and the University of Chicago, he joined the UCSB faculty in 1976. His awards include the Exxon Solid State Chemistry ACS award (1979), the UCSB Faculty Research Lectureship (1987), a Humboldt Senior Scientist Award (2003), and the American Chemical Society Division of Physical Chemistry Award in Theoretical Chemistry (2015). He was an Associate Editor of the Journal of Chemical Physics from 1999 through 2012. His current research, in collaboration with experimentalist colleagues, focuses on the search for new catalysts for converting natural gas or CO₂ into useful chemicals.



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Theoretical Design of CO-tolerant Catalysts for Fuel Cells

Elisa Jimenez-Izal^{1,2}, Andoni Ugartemendia¹, Abel de Cózar^{1,2} and Jose M. Mercero¹

¹Polimero eta Material Aurreratuak: Fisika, Kimika eta Teknologia, Kimika Fakultatea, Euskal Herriko Unibertsitatea UPV/EHU & Donostia International Physics Center (DIPC) PK 1072, 20080 Donostia, Euskadi, Spain.

²IKERBASQUE, Basque Foundation for Science, Bilbao, Euskadi, Spain

A major drawback affecting the efficiency and the long-term performance of platinum catalysts in fuel cells is the vulnerability towards CO poisoning. Moreover, with increasing environmental concerns worldwide as well as the scarcity and cost of noble metals, the use of nanocatalysts is a novel way to exploit resources more efficiently and minimize waste. They are also good models to look for catalysts with optimized properties.[1] In this talk we will show that doping Pt nanoclusters with Ge can be an efficient alternative to mitigate the CO poisoning on Pt-based catalysts. The ability of Ge to weaken the Pt-CO interaction was predicted and rationalized theoretically, as well as confirmed by mass spectrometry experiments.[2] In addition, the dopant concentration is pinpointed as a crucial factor to tailor the catalytic properties of Pt. Importantly, the newly designed PtGe clusters remain catalytically active towards H₂ dissociation. Ge can be a promising alloying agent to tune the selectivity and improve the durability of Pt particles, and could open the way to novel catalytic alternatives for fuel cells.

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Biography

Dr. Elisa Jimenez-Izal received her PhD degree in 2014, under the supervision of Prof. Ugalde at the University of the Basque Country, Spain. She then moved to the University of California, Los Angeles (UCLA) to continue with her postdoctoral studies under the supervision of Prof. Alexandrova. After four years she obtained an Ikerbasque research fellowship at the University of the Basque Country and the Donostia International Physics Center, both in Donostia, Spain. She has experience working in Theoretical Chemistry groups in Mexico, Italy and France, and she has published more than 25 research papers during her short career.



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CORRELATING STRUCTURE AND REACTIVITY ON ENERGY MATERIALS BY IN SITU SPECTROSCOPY

Christoph Rameshan

Institute of Materials Chemistry, TU Wien, Getreidemarkt 9, 1060 Vienna, Austria

In heterogeneous catalysis surfaces decorated with uniformly dispersed, catalytically highly active particles are a key requirement for excellent performance. One of the main tasks in catalysis research is the continuous improvement or development of new catalytically active materials and the search for efficient catalyst synthesis routes.

Based on model catalysts we present different innovative approaches in catalyst design that allow precisely tuning the complexity of the surface structure. Furthermore, characterization under catalytically relevant reaction conditions (operando studies) with simultaneous gas analysis allows obtaining correlations between structure and reactivity.

Atomic layer deposition (ALD) can be utilized for controlled synthesis of catalysts with various surface structures (e.g. from small particles up to closed coatings) and the process can be easily scaled. We present results on supported Pt model catalysts with different surface morphology and the resulting impact to catalytic reactivity.

Alternatively, an emerging concept in catalyst design is to selectively and reversibly tune and modify the surface chemistry by either electrochemical polarization or reductive treatment. Perovskite-type catalysts raise the opportunity to incorporate guest elements as dopants. Upon reduction (or in reducing reaction environment) these dopants emerge from the oxide lattice to form catalytically active clusters or nanoparticles on the surface (by exsolution). In consequence, this leads to a strong modification or enhancement of catalytic selectivity and activity.

Highlighted are studies for Pt/ZrO₂ model systems and different acceptor doped perovskite-type catalysts, which can be applied for CO₂ utilization via rWGS. We show a direct correlation of surface chemistry with catalytic activity, selectivity.



Selective Alkyne Hydrogenation by Poly(lactic acid) Supported Pd-Cu Alloy Nanoparticles

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Claudio Evangelisti³ and Peyman N. Moghadam⁴

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Functional polymers are highly suitable support materials, because they favor the NPs' dispersion on the support surface and thus stabilize them under real catalytic reaction conditions, avoiding aggregation, which is the most frequently encountered catalyst deactivation process. In addition, functional groups present on the polymer support tailor the chemical environment of the supported NPs, contributing to chemical selectivity achieved in catalytic substrate conversions. In this context, enantiomerically pure 2,2'-bipyridine end-functionalized poly(lactic acid) (PLA) of opposite stereochemistry has been used to anchor separately palladium- and copper acetate. A simple mixing of both macrocomplexes in dichloromethane and successive drying, gave anchored palladium- and copper acetate onto stereocomplexed poly(lactic acid) (sc-PLA). By treating the obtained polymer material with hydrogen gas in an autoclave well-defined Pd-Cu (1:1) NPs have been obtained, which have been successfully applied in the selective hydrogenation of industrially important alkynols. A clear alloy effect emerged from the catalytic screening and comparison of the catalytic performance with that of a related Pd-based catalyst. The sc-PLA-supported Pd-Cu catalyst showed high selectivity for cis-olefins in different reaction media and under different hydrogen pressure. Isomerization and over-hydrogenation reactions, which are known to occur with Pd-based catalysts, have been almost completely suppressed. Several physical measurements, such as HRTEM, XRD and XPS, carried out on the recovered Pd-Cu catalyst along with successive recycling experiments confirmed the stability of the catalyst even when recovered in air atmosphere.

Biography

Werner Oberhauser studied chemistry at the University of Innsbruck and received his Dr. rer. nat. at the same University in 1997 under the supervision of Prof. Peter Brügge. Afterwards he spent three years of Post-doc in Claudio Bianchini's laboratory in Florence, before becoming a permanent researcher at the institute of Chemistry of Organometallic Compounds (ICCOM) of the Italian National Research Council in 2001 and a senior researcher in 2010. His recent research interests are: (i) the study of nanostructured materials by means of X-ray diffraction; (ii) the synthesis and application of nanoparticle-based catalysts for aerobic polyol oxidation reactions. He has authored or is coauthor of 142 papers. H-index = 36 (www.scopus.com).



Zinc and magnesium catalysts for the synthesis and chemical depolymerization of polyesters

Mina Mazzeo, Federica Santulli and Marina Lamberti

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The oil derived plastics offer the advantages of high durability and low costs. Nevertheless, these properties represent a grave drawback for their end-of-life management. Every year more than 50 million tons of plastic waste are retained into landfills or spread into the environment. The severe consequences of plastic pollution require the introduction of new strategies and materials to convert the current linear economy of plastics to a circular model. In this context, biodegradable polymers such as aliphatic polyesters offer great opportunities because they combine good mechanical properties with biodegradability.

The chemical recycling of polymers to their starting monomers or small molecules as chemical platforms may represent a strategic approach to design virtuous productive model for plastics, in which a material can be recycled virtually ad infinitum.

Herein we report the synthesis of new and easy-to-obtain pyridyl imino-phenolate zinc complexes and magnesium catalysts which revealed to be exceptionally efficient to promote both the synthesis and the chemical degradation of polyesters.

Biography

Mina Mazzeo received her Ph.D. in Chemistry in 2001. From 2002 to 2016, she was Assistant Professor at Chemistry Department of the University of Salerno. In 2006 she was visiting professor in the Prof. Jonas Peters's group at California Institute of Technology. From 2016 she is Associate Professor at Chemistry and Biology "Adolfo Zambelli" Department of the University of Salerno. Her research interests include the synthesis of biodegradable polymers by ring opening polymerization of cyclic esters and ring opening co-polymerization of epoxides with cyclic anhydrides or CO₂ and depolymerization catalysis.



Nanoporous Gold: a tunable material for electrochemical applications

Federico Scaglione, Eirini Maria Paschalidou, Yanpeng Xue and Paola Rizzi

Department of Chemistry and Interdepartmental Center NIS (Nanostructured Surfaces and Interfaces), University of Turin, Turin, Italy

Nanoporous gold (NPG) is constituted by metallic ligaments and porosities and is obtained by de-alloying less noble elements while the more noble one forms ligaments by surface diffusion. NPG has sparked interest because of the versatile size of morphology and the intriguing properties in the field of electro-catalysis. We report studies of de-alloyed Au-based amorphous precursors then successfully used as electro-catalysts for methanol oxidation and hydrogen evolution reaction (HER). Arc melted $\text{Au}_{40-x}\text{Si}_{20}\text{Cu}_{28+x}\text{Ag}_7\text{Pd}_5$ (at.%) ($x = 0, 10, 20$) alloys were melt spun into amorphous ribbons, 20 μm thick and 2mm wide. NPG was prepared by chemical or electrochemical de-alloying, setting properly the etching conditions. HER and methanol oxidation reaction were studied in 0.5M H_2SO_4 aqueous solution and 0.5 M KOH and 5 M CH_3OH respectively. When applied as electrodes for methanol electro-oxidation, NPG remained active to more than 60% of the initial current density after five hundred cycles, without further apparent decay. For HER, NPG exhibited a Tafel slope of 160 mV/dec decreased at 90 mV/dec after 1000 cycles and could support MoS₂ nanoparticles. It was shown that NPGs can be synthesized by chemical and electrochemical means with size between 40 to 200 nm and applied as electrodes for electrocatalysis. In electrochemical applications NPG can be envisaged as an electrode in methanol fuel cells not being subject to CO poisoning. A synergic effect was found between NPG and MoS₂ for hydrogen evolution reaction.

Biography

Federico Scaglione graduated in Material Science at the University of Torino in 2008, where he obtained in 2012 his Ph.D. degree in Science and Technology of Materials and Nanosystems. From 2012 to 2018 he worked as Postdoc, and in this period his scientific work was committed to the synthesis of nanoporous and nanostructured metals and alloy by chemical or electrochemical de-alloying of crystalline and amorphous precursors. Since 2018 he works as Researcher in the same group of the same University. Currently, his scientific interest is not only focused on the production and characterization of nanostructured metallic materials but also devoted to applications of these promising materials as electrodes for electrocatalysis in general and water splitting in particular, and as active substrates for surface enhanced Raman scattering.



Solar activated-TiO₂ nano-photocatalysis grown on different substrates

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CENIMAT/i3N, Department of Materials Science, School of Science and Technology, NOVA University Lisbon and CEMOP/UNINOVA, Caparica, Portugal

The interest in advanced photocatalytic technologies with metal oxide-based nanomaterials has been growing exponentially over the years due to their green and sustainable characteristics. The use of metal oxides is widely spread in photocatalysis, mostly since these materials display enhanced photocatalytic activities, allied to their chemical stability, non-toxicity, and earth abundance, despite being inexpensive and compatible with low-cost wet-chemical synthesis routes. Photocatalysis has been employed in several applications ranging from the degradation of pollutants to water splitting, CO₂ and N₂ reductions, and microorganism inactivation. However, to maintain its sustainable aspect, new solutions must be identified, including the use of eco-friendly and flexible substrates adaptable to unlike surfaces. Moreover, it is imperative to use substrates that are inexpensive, recyclable, earth abundant and lightweight. Such as plastic, cellulose- and cork-based substrates are flexible materials that start to appear as options in photocatalysis. This talk will focus on titanium dioxide (TiO₂) nano- photocatalysts grown on different substrates for water purification under solar radiation. Cork, paper, plastic, 3D printing resin, and water filters were tested as substrates where the photoactive TiO₂ layers were deposited using microwave synthesis. The main characteristics of the TiO₂ nanostructured films produced will be correlated to their photocatalytic activity.

Keywords: TiO₂; photocatalysis; water purification; microwave synthesis; different substrates.

Biography

Daniela Gomes (born 1983) received the Ph.D. degree from Instituto Superior Técnico in 2012, in Materials Engineering, with the dissertation "Carbon dispersions in nanostructured metals". The degree was obtained with merit. She became a Post- doctoral researcher at the CENIMAT/i3N of NOVA School of Science and Technology in 2013. The post-doctoral work is entitled "Design of new functional materials for electronics applications", which is financed by Fundação para a Ciência e Tecnologia through the scholarship 84215/2012. She is also working at the Nanofabrication lab at CENIMAT, which she is the main operator of the dual-beam SEM-FIB microscope. Since October of 2015, she became Assistant Professor at the Materials Science Department of NOVA School of Science and Technology. She is co- author over 70 peer-reviewed papers (h-index=26, as February 2022). She co-authored 1 book and 2 book chapter. She participated on the EU project, CEOPS project with the grant agreement no: 309984.



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March 14-16, 2022

Theme: Contemporary Innovations and Emerging Novel
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Fluorinated alkenes: synthesis and applications

Samuel Couve-Bonnaire

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Fluorinated alkenes are relevant molecules that have found many applications such as peptidomimetics, bioactive compounds and materials. The fluoroalkene moiety is also recognized as a stable isosteric and isoelectronic mimic of the amide bond. So, it can therefore be used as a bioisostere in structure- activity relationship studies in pharmaceutical or agrochemical domains or to overcome problems associated with the instability of peptides. Some fluorinated alkenes building blocks can also serve as platform for further transformation by radical chemistry or conjugated addition. Among the various methods reported to synthesize fluoroalkenes, we have developed several catalyzed-access to these molecules including CH-functionalization, cross-coupling reaction or metathesis. In this presentation I will focus on our recent developments (Mizoroki-Heck reaction, metathesis...) regarding the synthesis and the application of fluorinated alkenes.

Biography

Samuel Couve-Bonnaire received his Ph.D. in 2001 under the supervision of Pr. J.-F. Carpentier and Y. Castanet at the Laboratory of homogeneous catalysis of Lille directed by the Pr. A. Mortreux. Then he carried out his postdoctoral studies in Canada at the Steacie Institute for Molecular Sciences in Ottawa with Pr. Prabhat Arya. Back to France, he was post-doctoral researcher with Sanofi-Aventis as industrial partner. Since February 2005, he is working in the group of "fluorinated biomolecules synthesis" as an associate professor, in COBRA laboratory. His main thematic research deals with fluorinated alkenes, from their synthesis (by radical chemistry, C-H bond functionalization, metathesis...) to their application as biorelevant fluorinated molecules and fluoro-peptidomimetics.



The bio-catalysis of the vitamin B12 active forms in human body. The preliminary step

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The cofactor methylcobalamin catalyzes the transfer of the methyl group from 5-methyltetrahydrofolate systems to ion homocysteine negative ion synthesizing the methionine. Adenosylcobalamin cofactor in turn catalyzes a number of transformations and rearrangements of biochemical substrates. The B12 cofactors structure is well known. The -CH₃ or -5'- deoxy-5'-adenosyl radical groups are bonded to the central cobalt atom above the plane of the corrin ring position and the 5,6-dimethylbenzimidazole base is bonded to the central cobalt atom below the corrin ring plane. The dimethylbenzimidazole ligand in both vitamin B12 cofactor-dependent processes is replaced by the histidine ligand, as confirmed by kinetic and X-ray studies.

We have built models in which in addition to the molecules of each methylcobalamin or adenosylcobalamin cofactors we added one, two, three, or four molecules or models of the substrates, present in the cavity of the vitamin B12 cofactors. The geometry optimization of these models by using the CASSCF method described above showed that, the breaking of the Co-N bond, i.e. the removal of the dimethylbenzimidazole ligand from the central atom occurs in most cases with energy barriers except for three models, in which the breaking of the Co-N bond, that is, the removal of the dimethylbenzimidazole ligand from the central atom occurs in the absence of a total energy barrier. The Pseudo-Jahn-Teller-Effect e.g. the mixing of the occupied and unoccupied molecular orbitals plays a determinant role in the removal of the dimethylbenzimidazole ligand from the central Co ion.

Biography

Tudor Spataru earned in the year 1983 his Ph.D. in the Inorganic Chemistry field with the topic "Electronic Structure and Properties of the Dioximates" under direction of Isaac Bersuker. From 1999 until 2004 he was a fellow associate researcher in the Mechanical Engineering Department at Padua University, Italy, where he studied with Prof. Giovanni Principi the intermetallic and hydrogen storage materials. From 2004 until 2007 he was a fellow associate researcher at City College, CUNY, US, where he studied with Prof. Ronald Birke the electronic structure and properties of forms of Vitamin B12. In 2007 he joined the Chemistry Department of Columbia University.



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Electrochemical Impedance of a Single Electrocatalyst

Lior Sepunaru and Brian Roherich

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Heterogeneous electrocatalysis is a chemical process driven by electricity. A better understanding of the function and mechanism of an electrocatalyst is essential for process optimization but is often masked by concurrent Faradaic and non-Faradaic (capacitive) routes. Electrochemical impedance is often used for studying these materials because of the method's inherent ability to separate events by their characteristic time scales. However, impedance is a quantity measured at the "bulk" level and cannot differentiate the contribution of each individual catalyst to the total electrocatalytic process. We present a new electrochemical methodology for studying catalysis at the single-particle level. This framework demonstrates the ability to simultaneously investigate charge transfer, capacitive and diffusional events of a single freely diffusing electrocatalyst interacting with a conductive solid interface. The proposed single entity electrochemical impedance can be applied to study energy storage and power devices at the molecular scale.

Biography

Lior completed his post-doctoral studies as a Marie Curie research fellow at the University of Oxford, working on bio-nanoelectrochemistry under the tutelage of Prof. Richard G. Compton. Before this, he completed his Ph.D. at the Weizmann Institute of Science in 2014, working on solid-state bioelectronics under the supervision of Prof. David Cahen and Prof. Mordechai Sheves. Lior's research is focused on electrocatalysis at the nanoscale, including the study of enzyme catalysis and development of a new generation of biosensors.



Dual Function Materials, comprised of supported mixtures of catalyst and sorbent, for direct air capture of 400 ppm CO₂ in ambient air followed by catalytic methanation

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A dual function material (DFM), comprised of Ru in intimate combination with a NaO supported on high surface area γ -Al₂O₃ is being investigated for direct air capture (DAC) of 400 ppm CO₂ followed methanation for production of renewable natural gas (CH₄). The process will be operated at ambient air conditions with waste or preferably green H₂ in a temperature swing mode. The data to be presented was generated using in simulated CO₂/air at ambient temperature and high humidity

Experiments were conducted with DFM/Al₂O₃ granules with demonstrated stability in cyclic operation of CO₂ capture and conversion to RNG. Preliminary stability data on DFM washcoated ceramic monoliths will also be shown.

Our future reactor design will include deposition of the DFM on high cell density thin wall ceramic monoliths, typical of those used in the automotive catalytic converter. This design provides low pressure drop with suitable thin DFM/washcoat layers for high CO₂ capture allowing for rapid surface heating during temperature swing methanation.

The impact of humidity on different sorbents demonstrates the importance of laboratory evaluations under expected realistic DAC conditions.

Biography

Bob retired from BASF (formerly Engelhard), Iselin, NJ as a Vice President of Research in 2012. He immediately joined Columbia University, as a Professor of Professional Practice in the Earth and Environmental Engineering (EEE) Department. He is the author (co-author) of 138 journal publications and 56 US patents. He is co-author of three catalyst textbooks, published by Wiley and Sons. He is the recipient of a number of research awards. He has a Google scholar rating of 54. He received a BS from Manhattan College, Bronx, New York and PhD from Rensselaer Polytechnic Institute, Troy, New York.



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Understanding the Mechanism of Solar Water Oxidation in Natural and Artificial Water Oxidation Catalysts

K. V. Lakshmi

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The solar water-splitting protein complex, photosystem II (PSII), catalyzes one of the most energetically demanding reactions in Nature by using light energy to drive water oxidation. The four-electron water oxidation reaction occurs at the tetra-nuclear manganese-calcium-oxo (Mn₄Ca-oxo) cluster that is present in the oxygen-evolving complex of PSII. The electronic and geometric structure of the Mn₄Ca-oxo cluster, which is exquisitely tuned by smart protein matrix effects, is central to the water-oxidation chemistry of PSII. However, the mechanism of water oxidation at the Mn₄Ca-oxo cluster is not well understood because of the inability of conventional methods to directly probe the reaction intermediates. We are developing high-resolution two-dimensional (2D) hyperfine sublevel correlation spectroscopy methods that provide direct 'snapshots' of the photochemical water oxidation intermediates of the Mn₄Ca-oxo cluster of PSII. Moreover, we are using the design principles of the oxygen-evolving complex of PSII to synthesize bio-inspired catalysts that mimic the electronic and geometric structure of the Mn₄Ca-oxo cluster. I will describe ongoing efforts in our laboratory to understand the mechanism of water oxidation in both natural and bio-inspired artificial systems.

Biography

K. V. Lakshmi is a Professor in the Department of Chemistry and Chemical Biology and Director of the Baruch '60 Center for Biochemical Solar Energy Research at Rensselaer. She is trained in the development and application of advanced biophysical spectroscopy at Brandeis University, the Francis Bitter Magnet Laboratory at MIT, and Yale University. She is recognized worldwide as a leader in the current generation of physical chemists and biophysicists for her research on the development of state-of-the-art multi-frequency multi-dimensional pulsed EPR spectroscopy, solids NMR spectroscopy and electron-nuclear spectroscopy methods. She applies her advanced training in magnetic resonance spectroscopy, molecular genetics, biochemistry, inorganic chemistry, computational chemistry and in situ observation of light-driven intermediates to address the molecular mechanisms of solar energy conversion in natural and artificial systems.



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Keynote Forum
Day 3

CHEMICAL CATALYST 2022



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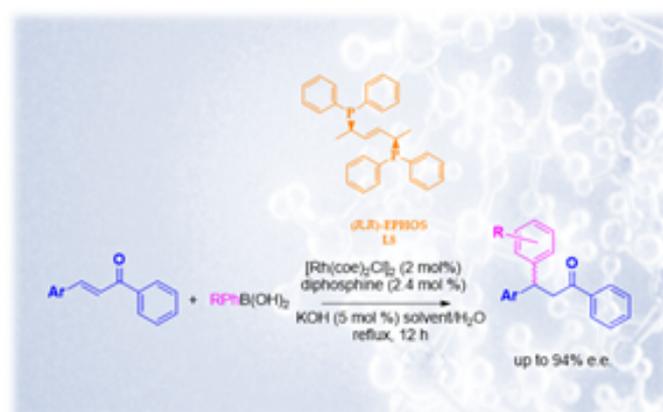
Giorgio Facchetti

Department of Pharmaceutical Sciences, Via Venezian 21,
20133 Milano, Italy, University of Milan

New rhodium-sp³ diphosphine catalytic systems for the asymmetric addition of aryl boronic acids to azaarenes

Catalytic asymmetric conjugate reaction stands out as one of the most useful synthetic tools for the preparation of chiral compounds although its application to the synthesis of chiral azaarenes has been scarcely investigated till now (*Ad. Synth. Catal.* 2020, 362, 3142). Starting from the established expertise gained in my research group in the synthesis of chiral phosphine ligands and their application in homogeneous catalysis (*Inorg. Chem.* 2021, 60(5), 976; *Catalysts* 2020, 10(8), 914) we prepared a novel chiral phosphorus ligand, called (*R,R*)-EPHOS, designed and synthesized starting from the optically active 1,4-(*E*)-2-butene. Its *cis* analogue, called (*R,R*)-ZEDPHOS had been already successfully employed in the enantioselective reduction of carbonyl groups affording satisfactory enantioselectivity. This new diphosphine features a stereogenic sp³ carbon atom combined to the presence of a C₂ axial chirality, the one featuring the atropisomeric diphosphines. A combined 31P-NMR and computational approach shed light on the different coordination mode to the rhodium

centre respect to (*R,R*)-ZEDPHOS, suggesting the ability of (*R,R*)-EPHOS to form complexes with phosphorus atoms in *cis* configuration and revealing the asymmetric disposition of the aryl groups responsible for the chiral recognition of the substrate enantiofaces. Thus, (*R,R*)-EPHOS was applied to the asymmetric rhodium catalyzed 1,4-addition of different substituted arylboronic acids to azaarenes in comparison with other. When applied to (*E*)-1-phenyl-3-(pyridin-2-yl)prop-2-en-1-one (1), (*R,R*)-EPHOS-Rh(catalytic system afforded the product 1a in a remarkable 94% e.e.



BIOGRAPHY

Dr. Giorgio Facchetti is actually a researcher fellow and Adjunct Professor of Organometallic Chemistry at the Department of Pharmaceutical Sciences, University of Milan. In 2015 he was awarded of the prestigious fellowship "Fondazione Confalonieri" soon after receiving his PhD in Chemical Sciences in 2014 at the University of Milan with a thesis entitled "New antiproliferative transition metal complexes: development and synthesis". His research interests deal with the synthesis of hybrid catalysts ("artificial metallo-enzymes"), the design and synthesis of new chiral ligands for homogeneous catalysis and with theranostic metal-based complexes.



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Advanced materials for wastewater remediation by solar light irradiation

In the last decades, freshwater scarcity has become a global issue mainly caused by overwhelming industrialization and the expansion of agriculture. In this regard, heterogeneous photocatalysis could offer a feasible solution to this problem aiming at the development of photoactive devices suitable for water remediation. Although TiO₂ is still the most used semiconductor due to its chemical and physical stability, good photoactivity and low cost, researchers are willing to replace it with new smart materials because of its suspected carcinogenic nature and limited activity under solar light. Among them, g-C₃N₄ has promising features as metal-free photocatalyst for water-remediation considering its visible-light response, simple synthetic pathway, and peculiar layered structure and cheap

production cost. Moreover, the use of floating materials can overcome problems related to the use of slurry systems. Recently, buoyant materials are emerging as promising alternative to traditional photocatalysts for water decontamination, thanks to their characteristics in terms of efficiency due to the high oxygenation of the photocatalyst surface, full sunlight irradiation, easy recovery and reuse. In the present study, g-C₃N₄ photocatalysts immobilized in floating alginates were properly developed and studied for photodegradation of rhodamine B, sodium diclofenac and isoproturon in water under solar light irradiation. These materials, subjected to recycle tests, exhibited high activity and stability.

BIOGRAPHY

Ermelinda Falletta is a researcher at the Department of Chemistry of the University of Milan. Her research activity deals with: i) development of innovative environmentally friendly approaches for the preparation of intrinsically conducting polymers and their composites and their application in the field of environmental remediation and piezoresistors, ii) development of heterogeneous catalysts for the selective oxidation of organic compounds and photodegradation of emerging pollutants, iii) development and optimization of new analytical methods (in particular UHPLC-MS/MS, GC/MS and SPME/GC/MS) for the identification and determination of target and non-target species in the environment and biological sectors. She is author and co-authors of about 75 ISI papers, 3 books, 8 book chapters and 2 patents. H-index: 23 (Scopus); 24 (Google Scholar).



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Luca Vattuone^{1,2}

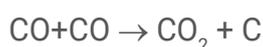
¹Università degli Studi di Genova, DIFI, Italy

²IMEM-CNR, Italy

Boudouard reaction under graphene cover

It has been shown recently that the space between graphene and the substrate can act as a nano-reactor where the activation barrier for catalytically relevant reactions such as CO oxidation is effectively reduced [1].

Ni is known to be a catalyst for the Boudouard reaction



Such a reaction is favoured by high pressure and for this reason it escaped until now direct investigation under operando conditions. We report here about a Near Ambient Pressure XPS study performed at Soleil (Tempo Beamline).

Exposing bare Ni(111) to CO at a pressure $P_{\text{CO}} \sim 2$ mbar we observed graphene growth already at 550 K [2], a temperature significantly lower than

the one (670 K) at which growth of graphene by segregation of dissolved carbon has been reported. The formation of CO₂ is proved by the presence of a C1s line at 291.3 eV and an O1s line at 533.4 eV.

Indeed, exposing single layer Graphene on Ni(111) to CO at 3.7 mbar, i.e. at a pressure more than one order of magnitude higher than previously explored, CO intercalates under the graphene layer causing its detachment from the substrate. The so obtained high local CO coverage under graphene cover enables the formation of CO₂ via the Boudouard reaction catalysed by the Ni(111) surface. The carbon produced by the reaction is used to transform carbide into graphene.

[1] Q. Fu and X. Bao, Chem. Soc. Rev. 46, 1847 (2017)

[2] R. Davì et al. Chem. Phys. Lett. 774, 138596 (2021).

BIOGRAPHY

L. Vattuone obtained his Ph.D. in Physics at the University of Genova in 1994 under the supervision of Prof. M. Rocca. After a postdoctoral stay in the University of Cambridge under the supervision of Prof. Sir. David King, he returned to Genoa where he is now associated professor of Condensed Matter Physics and serves as Coordinator of the Material Science Programme. L.V research focused on the experimental investigation of gas surface interaction by High Resolution Electron Energy Loss Spectroscopy, Supersonic Molecular beams and Single Crystal Calorimetry, on the stereodynamics of adsorption, on the growth and chemical properties of ultrathin oxide films and graphene and on surface plasmons.



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Michael J. Heller

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Department of Nanoengineering, La Jolla, CA, 92093 USA

The Histidine Imidazole Group and Enabling Enzyme-Like Catalysis in Synthetic Nanostructures

Our research work on incorporating bio-catalytic mechanistic properties into synthetic peptide nanostructures has given us new insight into the unique properties of the histidine imidazole group. Numerous “synzymes” for ester/amide bond hydrolysis based on peptides, macromolecules and nanostructures have been designed to closely resemble the active site of serine and cysteine proteases. Such proteases (Trypsin, Chymotrypsin, and Papain) contain the catalytic triad amino acids (serine hydroxyl or cysteine thiol, histidine imidazole, and aspartate carboxyl) which are in close proximity in the enzyme active site. Nevertheless, while the synthetic structures look similar to the enzyme active site they do not have the unique dynamic mechanical catalytic properties to transform substrate molecules into product molecules i.e., turnover. Our work has centered on designing and synthesizing peptide structures where a

cysteine sulfhydryl group (nucleophile) and histidine imidazole group (nucleophile & general base) are in extremely close proximity. Ellman’s reagent trapping experiments showed that rapid acetyl group exchange exists between the thiol and imidazole groups. This exchange rate increased significantly in peptides with bulky R-groups (phenylalanine) between the cysteine and histidine amino acids. A reduction of the cysteine thiol pKa and NMR results supports that closer proximity of the thiol and imidazole groups in these peptides produces faster acetyl group exchange. While the synthetic peptide structures demonstrated only slight improvement in turnover, due the slow acylation step, the de-acylation step was significantly accelerated. Our better understanding of the uniqueness of the histidine imidazole group will be important in designing novel synzymes with improved turnover.

BIOGRAPHY

Michael J. Heller, PhD – Professor, University California San Diego, Departments of Nanoengineering and Bioengineering (2001–Present). PhD Biochemistry, Colorado State University 1973; NIH Postdoctoral Fellow, Northwestern University; Supervisor DNA Technology Amoco, 1976-1984; Director Molecular Biology, Molecular Biosystems, 1984-1987; Co-founder/President, Integrated DNA Technologies (IDT), 1987-1989; Co-founder/CTO, Nanogen, 1993-2001; Co-Founder and Scientific Advisory Board, Biological Dynamics (2012-present). In addition to work on synthetic enzymes and bio-catalytic mechanisms, other research work includes development of sample to answer systems for cf-DNA, RNA and exosomes biomarkers, protease biomarkers, liquid biopsy diagnostics for cancer and other diseases. Dr. Heller has over 100 publications and 60 issued US patents on new molecular diagnostic devices, genotyping electronic microarray technologies, FRET DNA detection and in nanofabrication and bionanotechnology areas.



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Richmond, VA, 23284-2006, USA

Heterogeneous Catalysis on Oxide and Carbon-based Supports Surpassing Homogeneous Catalysis for Carbon-Carbon Bond Forming Reactions

Palladium catalyzed cross-coupling reactions represent a significant advancement in contemporary organic synthesis as these reactions are of strategic importance in the area of pharmaceutical drug discovery and development. This talk will address the development of heterogeneous Pd catalysts anchored on oxide and carbon-based supports that match the high activity and selectivity of homogeneous catalysts and also eliminate catalyst's leaching and sintering and allow efficient recycling of the catalysts. In the first approach, strong electrostatic adsorption is used to synthesize ultrasmall (1-2 nm) Pd and the bimetallic Pd-Cu, Pd-Ni and Pd-Co catalysts on silica supports. These catalysts demonstrate very high turnover frequencies (TOF = 100,000 h⁻¹ at 60 °C) for Suzuki coupling reactions and are easily recovered and recycled under batch reaction conditions. In the second approach, highly active larger Pd nanoparticle catalysts (3-4 nm) encapsulated within novel carbonaceous and N-doped carbonaceous TiO₂ or ZrO₂ support nanomaterials are developed via the laser

vaporization of Ti or Zr metal organic frameworks (MOFs), respectively. The resulting hollow carbon spheres decorated with TiO₂ or ZrO₂ nanoparticles provide highly improved support for the Pd nanoparticles for high activity and no significant Pd leaching in the Suzuki coupling reactions. Finally, in the third approach, functionalization of the reduced graphene oxide (RGO) support by the covalent attachment of aromatic amines such as p-phenylenediamine (PPD) or benzidine (BZD) results in further enhancement of the activity of the Pd nanoparticles in the solid Pd/(RGO-PPD) or Pd/(RGO-BZD) catalysts for the Suzuki coupling reactions with unprecedented catalytic activity showing TOF values of 408,000 h⁻¹ and 378,000 h⁻¹, respectively at 80 °C. The three approaches presented for the supported Pd catalysts attest to function via a heterogeneous pathway where the dispersity of Pd nanoparticles and the influence of the carbon support appear to play major roles in achieving catalytic activity that matches or exceeds that of the best homogeneous Pd catalysts.



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BIOGRAPHY

Mary Eugenia Kapp Endowed Chair in Chemistry and Commonwealth Professor, Department of Chemistry at Virginia Commonwealth University, USA. El-Shall received his B.S. and M.S. degrees from Cairo University, and a Ph.D. from Georgetown University. He did postdoctoral research in nucleation and clusters at UCLA. His research interests include nanostructured materials, graphene and nanocatalysis for energy and environmental applications, gas phase clusters and nucleation. He has published over 285 refereed papers and review chapters (Google Scholar h-index = 57, citations > 12,800), and he holds ten US patents on the synthesis of nanomaterials, nanoparticle catalysts, graphene, and graphene-supported catalysts. Dr. El-Shall received the *Outstanding Faculty Award* of the State Council of Higher Education of Virginia (SCHEV), Virginia's highest faculty honor in 1999; the *Distinguished Research Award* from the Virginia Section of the American Chemical Society in 2009; the *VCU Distinguished Scholarship Award* in 2011, and the *VCU Award of Excellence* in 2016. He was selected as a Jefferson Science Fellow and worked as a Senior Science Advisor at the U.S. Department of State in 2012-2013. Dr. El-Shall received the Virginia Outstanding Scientist in 2018 awarded by the Governor of Virginia. He is an elected Fellow of both the American Physical Society (APS) and the American Association for the Advancement of Science (AAAS).



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William A. Goddard III

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Mechanisms, design, and characterization of electrocatalysts for water splitting, CO₂ reduction, and N₂ reduction using Grand Canonical Quantum Mechanics

Recently, we modified the traditional QM methods (that use fixed numbers of electrons) to enable the prediction of the current density and turn-over-frequencies (TOFs) as a function of applied potential. In grand canonical QM, the net charges at the electrode surface changes continuously as each reaction step goes from the initial state through the transition state to the product, keeping the applied potential constant. This has been formulated into the grand canonical potential kinetics (GCP-K) formulation for practical predictions on complex systems. The accuracy of

GCPK was validated recently for single-crystal Co/TiO₂ nanoparticles, for which the predicted TOF versus applied potential and Tafel slope are in a nearly exact agreement with the experiment.

We will illustrate here recent applications to electrocatalysts important to energy and environment such as CO₂ reduction to C₂ products, hydrogen reduction reaction, oxygen evolution reaction, or N₂ reduction reaction, or oxygen reduction reaction.

In each case we will use the new reaction mechanism to suggest improved electrocatalysts.

BIOGRAPHY

Goddard obtained his PhD from Caltech and has been on the Caltech faculty since November 1964. He has been a member of the National Academy of Science since 1984, and has published over 1496 papers (H index = 173, I10 index = 1293). Goddard continues to be a pioneer in developing methods for quantum mechanics (QM) and reactive force fields (ReaxFF, RexPoN), with the goal of making the methods sufficiently accurate that experimental validation can be restricted to the predicted best systems. He applies these methods to a variety of materials related problems [catalysis (heterogeneous, organometallic, electrochemical), batteries (new electrolytes, cathodes, and anodes), nanotechnology, energetic materials] and bio related problems (predicted structures and activation of GPCR-G-Protein by agonists).



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Huiyao Wang

Department of Civil Engineering,
New Mexico State University, USA

Photo-reforming and degradation of microplastics in aqueous solution for H₂ production using nanocomposite photocatalysts

Plastics are recalcitrant and difficult to remove from wastewater and the natural environment. As a result, many plastics accumulate in the environment and food chain, causing adverse effects on living organisms. Photo-reforming, a process of generating H₂ from an organic substrate in aqueous solutions using catalysts, is found promising to address the challenge of treating plastics. TiO₂ nanoparticles were doped with Au and Pt in this study to enhance the light utilization efficiency and catalytic activity. The preliminary photodegradation experiments using Rhodamine B as an organic indicator revealed that 5% Au doped TiO₂ (Au/TiO₂) was the most photo-active catalyst among the developed samples. The change of the Au/TiO₂ properties was characterized using a transmission electron microscope (TEM), powder X-ray diffraction (XRD), UV-Vis spectrophotometer, X-ray photoelectron spectroscopies (XPS), and Fourier transform

infrared (FTIR). Computational simulation using Quantum EXPRESSO was performed to predict the narrowed bandgap of TiO₂ when the surface of nano-TiO₂ particles was modified with nano-Au particles.

Polyethylene terephthalate (PET) was selected as a representative plastic for photo-reforming experiments. Microscopic examination and FTIR analysis were conducted to identify the morphology and functionality change during photo-reforming of PET after UV irradiation at different time. The gaseous phase of a closed photoreactor with plastics and catalysts (Au/TiO₂ and pure TiO₂) was analyzed using gas chromatography equipped with a thermal conductivity detector. H₂ was observed under both UV and visible light conditions. It can be concluded that the developed catalyst can produce H₂ using solar energy and production increased with exposure time.

BIOGRAPHY

Dr. Huiyao Wang studied Physics at the Lanzhou University, Lanzhou, China and graduated as MS in 1993. He then joined the research group of Prof. Tianmin Wang in the Department of Material Science at the Lanzhou University. He received his PhD degree in 1998 at the same University. After two years postdoctoral fellowship and several research associate works, he obtained the position of an Associate Professor at the New Mexico State University. He has published more than 50 research articles in SCI journals.



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CHEMICAL CATALYST 2022



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Synthesis, characterization, photo-and-electrochemical properties of cationic iridium(III) complexes by using 1,3,4-oxadiazole cyclometallating ligand

Mansoor Akhtar, Shifa Ullah Khan, Dong-Xia Zhu, Guo-Gang Shan and Zhong-Min Su

Institute of Functional Material Chemistry, Faculty of Chemistry, Northeast Normal University, Changchun 130024, Jilin, People's Republic of China

Three new cationic iridium(III) complexes, namely $[\text{Ir}(\text{OXD})_2(\text{bpy})]^+(\text{PF}_6^-)$, $[\text{Ir}(\text{OXD})_2(\text{phen})]^+(\text{PF}_6^-)$, $[\text{Ir}(\text{OXD})_2(\text{dpq})]^+(\text{PF}_6^-)$ by utilizing the electron deficient 2,5-diphenyl-1,3,4-oxadiazole ligand with variety of electron rich ancillary ligands. Their photophysical, electrochemical and density functional theory (DFT) has been investigated. In addition, complex 2 was characterized by single X-ray diffraction while complex 1 and 3 was unsuccessful to crystalize. DFT shows that the electronic state for the complex 2 has the characteristic mixed 3MLCT (Ir \rightarrow the ancillary ligand) and 3LLCT (the cyclometallated ligands \rightarrow the ancillary ligand) structure.

Biography

Dr. Mansoor Akhtar received his bachelor degree in Bachelor of Science Education from University of Sindh in 2011 and his Master in Chemistry from Institute of functional material chemistry, Northeast Normal University, China in 2015. He served Institute of functional material chemistry as student demonstrator in Supramolecular Lab for one year (2014-2015). In 2013, he won Cultural Scholarship announced by Ministry of Education for Masters and joined Institute of functional material chemistry, Northeast Normal University in September 2013 as Masters Scholar and he completed Masters degree in 2015 under the supervision of great scientist Prof Zhu Dongxia. In continual same year, he earned Chinese Government Scholarship for PhD degree under supervision of Prof Su Zhongmin. During his PhD, he did research work on Luminescent material by synthesizing oxadiazole derivatives and published five research articles in international journals.



Increase of form-stability by using modified graphene aerogel supported phase change materials (PCMs)

Chengbin Yu¹ and Young Seok Song²

¹Researcher, Seoul National University, Korea

²Professor, Dankook University, Korea

The phase change material (PCM) can absorb or release a large amount of heat during the phase transition process. However, the leakage problem is occurred among the PCMs and restricts the applications. The graphene aerogels are widely utilized as supporting materials due to their lightweight and high porosities. Though the graphene aerogel-supported PCM composites can forbid the leakage problem, the volume shrinkage of graphene aerogels under the infiltration process becomes a new problem and which makes a mass loss of the PCM matrix. Therefore, polydimethylsiloxane (PDMS) embedded and cysteamine cross-linked graphene aerogels are mentioned to reduce the volume shrinkage effectively. These modified graphene aerogels supported PCM composites contain more PCM than that of originals and increase the thermal energy storage abilities. In addition, the form stability of PCM composites is measured under high temperatures with external force. Though both original and PDMS-embedded graphene aerogel-supported PCM composites occur volume damage, the cross-linked graphene aerogel-supported PCM composite shows an excellent mechanical property without any leakage. It is clear that the cysteamine cross-linked graphene aerogel can sustain the initial state of PCM composite even over the melting point.

Biography

Chengbin Yu, Researcher.

Degree of Bachelor: 2009.09 ~ 2013.06 Beijing University of Chemical Technology (BUCT). Polymer Science and Engineering.

Degree of PhD: 2013.09 ~ 2019.02 Seoul National University (SNU). Material Science and Engineering.

Have published 18 papers (13 first author, 5 co-authors), and 4 papers (2 first author, 2 co-authors) are under revision process. The published journals are Energy Conversion and Management, Macromolecular Research, Fibers and Polymers, Polymers for advanced technologies, Journal of Sound and Vibration, Materials & Design, Journal of Polymer Research, ACS Applied Energy Materials, Applied Energy, and Chemical Engineering Journals. The research area contains nanocomposite, polymer processing, energy storage and harvesting.



Effective Utilization of Wide Range Wavelength of Light Composing Sunlight to Promote CO₂ Photocatalytic Reduction Performance

Akira Nishimura

Mie University, Japan

One of promising CO₂ utilization technologies is CO₂ photocatalytic reduction. TiO₂ is the most popular photocatalyst used for CO₂ reduction. Though there are some reports investigating the CO₂ reduction performance of TiO₂, it is still low. The author sets the strategies to promote the CO₂ reduction performance of TiO₂ as follows: (i) to extend the wave length absorbed from ultraviolet light to infrared lay including visible light, (ii) to utilize the infrared ray for the mass transfer around the photocatalyst via the radiation. The strategy (i) is carried out by doping phosphorus on TiO₂. Though some papers reported the effect of metal doping aimed for the visible light absorption on the CO₂ reduction performance, there is no report to investigate the effect of doping for absorption of infrared ray as well as visible light on the CO₂ reduction performance of TiO₂. The strategy (ii) is based on the previous study by the author which reported the products above the photocatalyst disrupts to contact the reductants with photocatalyst and attract the reverse reaction from products to reductants, resulting in small amount of product. Therefore, the author suggests to promote the mass transfer by the black body material located under the photocatalyst with porous structure which can penetrate the light. Due to radiation from the black body, the gas temperature around the photocatalyst rises, which expects the promotion of mass transfer by natural convection heat transfer. This study reports the effect of these strategies on the CO₂ photocatalytic reduction performance of TiO₂.

Biography

Dr. Akira Nishimura is an associate professor in Division of Mechanical Engineering at Mie University, Japan. He received the B.S. Eng., the M.S. Eng. and Dr. Eng. degrees in Chemical Engineering from Nagoya University, Japan in 1995, 1997 and 2000, respectively. He worked at Center for Integrated Research in Science and Engineering, Nagoya University as research associate from 2000 to 2002. He moved to Mie University in 2002 as an assistant professor and promoted to associate professor from 2014. He has published 80 journal papers which are reviewed. His current researches are CO₂ reduction by photocatalyst, H₂ production from biogas, smart city utilizing renewable energy actively, clarification on heat and mass transfer mechanism of polymer electrolyte fuel cell.



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Biocatalytic membrane reactors for simultaneous production and separation of bioactive molecules

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Catalysts of biological origin such as enzymes have unpaired selectivity and catalytic performance. Their use in industrial production is hindered by their macromolecule instability. Heterogeneization of enzymes to solid supports is a strategy to stabilize them. Membranes are among the supports that best suit for enzyme immobilization, probably because they mimic the compartmentalization of biological systems. In addition to host the enzyme, membranes can promote mass transfer under different driving forces as well as can restrict the passage of some components compared to others in a selective way. This means that enzyme-loaded membranes can combine the selective catalytic ability of the enzyme with the selective transport properties of the membrane leading to potentially outperforming biocatalytic membrane reactors (BMR) for continuous bioconversion and separation in a single step. They are intensified and clean processes, can work in mild conditions of temperature, pH and pressure. They do not produce by-products thanks to their high selectivity. Therefore, BMR can be considered an ecofriendly technology with great potential. Traditionally, BMR have been used preferentially for the production of high-added value components (such as pharmaceutical, biotechnological, food areas). Examples where the authors have most contributed will be illustrated, including the development of BMR for the production and separation of optically pure enantiomers, biophenols, peptides. The perspective of BMR in biorefinery for the production and separation of bioderived chemicals and energy carriers will be discussed.

Biography

Lidietta Giorno is currently Research Director at the Institute on Membrane Technology of the National Research Council of Italy, CNR-ITM. She served as The Director of the Institute from May 2009 till February 2019. She is expert in membrane science and membrane bioengineering. She has served on the European Membrane Society Council as the President of the EMS Council. She is Honorary Member of the European Membrane Society since 2014. Lidietta Giorno is co-author of 13 books, over 220 peer reviewed papers, 2 patents and co-editor of the Encyclopedia of Membranes, Springer, 2016. She is Editor of the Journal of Membrane Science.



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Complimentary set-ups for testing VOC catalytic total oxidation by O₃ at Low temperature in aircrafts and spacecrafts

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In aircrafts and spacecrafts, outside air is not directly fed to passengers, because it contains high ozone concentration at elevated altitudes. In the cabin, inside air contains VOCs, related to treatment products and the food provided to passengers. In this case catalytic converters are necessary to lower the concentration of ozone to the authorized values at the entry of aircrafts, also to treat the air of cabin to eliminate the VOCs; such on-board equipment already exists but have to evolve to be adapted to the future aircraft and spacecraft technologies, and will require to work at much lower temperatures.

Elimination of volatile organic compounds (VOCs) contaminants of indoor air needs the use of new technologies with a low energy cost since VOC concentrations are low and the air flow to be treated is high. Catalytic oxidation with oxygen needs a temperature higher than 200°C to be efficient, leading to an important energy consumption to treat large air flow. This drawback can be circumvented by using oxidative species able to perform total oxidation reactions at room temperature. Amongst the various possibilities we have chosen to use ozone as oxidative species [1-3]. Manganese oxide based catalysts are well-known to be effective for the oxidation of organic compounds by ozone. In order to optimize the role of the catalyst and the gas-solid contact, several catalytic configurations (manganese oxide variously doped by palladium) have been used to both evaluate catalyst in the elimination of VOCs and in the decomposition of residual O₃ and reactor efficiencies.

In the present work the catalytic oxidation of EtOH (chosen as VOC model molecule) is evaluated in a small packed-bed reactor, at high ozone concentrations (13 ppm) at room temperature on our Mn-Pd/TiO₂ catalyst has shown that such system can be used as efficient indoor air treatment.

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Biography

My name is Houcine TOUATI. I am an Assistant professor at the Polytechnic Clermont and researcher at the Institute of Chemistry Clermont Ferrand (ICCF), University Clermont Auvergne France. Researcher attached to the University of Poitiers and visiting researcher at the University of Monastir Tunisia for 2020-2021. I did two postdocs at the Institute of Chemistry of Environments and Materials of Poitiers, University of Poitiers as part of a Project FUI (AirClean- Aerospace valley). I obtained my Ph.D. in 2017 from the National School of Engineering of Poitiers (ENSI) affiliated with the Polytechnic Institute of Bordeaux (INP) France.

I have 10 scientific publications, a book and 3 patents. I have 13 communications (Oral and Poster). I participated in the organization of 3 International Congresses (ISGC - la Rochelle France) and I organized 3 local university seminars and I have 4 prizes



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TiO₂ modifications towards photocatalytic degradation enhancement

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²Nanochemistry group, International Iberian Nanotechnology Laboratory, Braga, Portugal.

Photocatalysis has been studied deeply lately due to its enormous advantages on the degradation of pollutants in a non-selective way. One of the most efficient catalyst is TiO₂. Nonetheless, it has several disadvantages such as the narrow wavelength for its activation and the high recombination of the generated electron and holes (the degradation force of the process). This study is based on the modification of TiO₂ with two approaches: i) the addition of an electronegative element which avoids electron/hole recombination and ii) the addition of a carbon based material which enhances surface area and absorption. Thus, F-TiO₂ and GO-TiO₂ (GO stand for graphene oxide) were successfully synthesized. These catalysts were characterized by different means and compared to raw TiO₂. Indeed, electrochemical measurements were done such as Electrochemical Active Surface Area or Electrochemical Impedance Spectroscopy, in order to understand the electron-transfer behavior. Then, a model pollutant, the dye methylene blue was treated under low consumption UVA-LED lamp. The effect of several parameters such as doping agent dosage, pollutant concentration or aqueous matrix nature were evaluated. Indeed, the future usage of this techniques can be foreseen due to the capacity of these both catalysts to cope with dye concentration fluctuations and real wastewater matrixes. Nevertheless, in some complex cases the addition of small quantities of H₂O₂ to enhance the photocatalysis were required. Under optimal conditions, the catalysts are reused up to three cycles without any detriment. The attained data can compete with previously reported data, opening a path for future research.

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Biography

Aida M. Díez has completed her PhD from University of Vigo, Spain and she is performing postdoctoral research at the same University. She has acquired experience on catalysis thanks to stages on institutions of high expertise on the field (Laboratory of Catalysis and Materials, Associated Laboratory for the Green Chemistry and International Iberian Nanotechnology Laboratory, Portugal). She acts as professor at the University of Vigo since 2016. She is the co-director of several degree projects and participates on numerous journals as reviewer. She has published 12 papers in reputed journals and has participated on more than 30 congresses with oral and poster presentations.



Progress on the removal of contaminants on surface and wastewater: report of case-studies

Laura Scrano¹, Sabino Aurelio Bufo^{1,2} and Lee-Ann Modley²

¹University of Basilicata, Potenza, Italy , ² Department of Geography, Environmental Management & Energy Studies, University of Johannesburg, 2092, South Africa.

Contamination of the water sector represents a global issue known since the 1960s. However, the consequences are still not adequately known as a whole. There is insufficient information on the thousands of molecules released into the environment and, above all, their properties and the quantities produced, capable of determining the global effects of potential toxic actions on living organisms and the environment.

For some time, scholars and researchers from the planet have been directing their activities to identify new integrated technologies and low energy consumption tools aimed at treating and reusing wastewater. For some time, our research group has been experimenting with removing traditional contaminants and emerging contaminants using hybrid techniques (filtration and Advanced Oxidation Processes). In this communication, we report some of our case studies, which have validated the effectiveness of the treatments.

Biography

Associate Professor SSD AGR/13

Visiting professor IUT, University Claude Bernard, Lyon 1, France ANVUR disciplinary expert

Qualified as Full Professor SSD AGR/13

Prof. Scrano has been involved as co-proposer in four national and international research projects, and she coordinated one of them. She is author/co-author of many scientific articles published in international referenced journals (indexed Scopus) and of several scientific papers published in national journals and national and international conference proceedings, in two of which, she has obtained a prize for the scientific activity developed.

Prof. Scrano studies the properties that allow some clay minerals to retain organic molecules present in the soil, including some herbicides of the latest generation, and how the constituents of the soil (organic matter and clay minerals) influence the degradation process).



Preparation and characterization of PVDF-TiO₂ core-shell nanofibers for photocatalytic applications

Carlo Boaretti, Jiayi Yin, Michele Modesti, Alessandra Lorenzetti, Alessandro Martucci and Martina Roso

University of Padova, Italy

A polyvinylidene fluoride (PVDF) - titanium dioxide (TiO₂) core-shell composite nanofibrous membrane (CNM) with photocatalytic activity was obtained from the microwave-assisted hydrothermal treatment of an electrospun PVDF membrane. The effects of the precursor solution acidity, the heating temperature, and the treatment time on the structure and the photocatalytic performance were investigated. The CNM obtained from a 2 M precursor acidic solution showed the presence of nanofibers (NFs) with a proper core-shell structure, wherein a TiO₂ smooth shell was uniformly covering the electrospun PVDF NFs core. The TiO₂ crystallographic phase was found to be temperature-dependent, with the highest anatase content observed at 120°C. The mean PVDF-TiO₂ NFs diameter measured from SEM images and the TiO₂ fraction of CNM calculated from TGA results showed an accumulation of TiO₂ on the PVDF NFs surface as heating temperature and treatment time increased. The photo-oxidation capability of the as-prepared CNMs was evaluated by the photocatalytic decomposition of aqueous methyl orange solution at room temperature under UV-C irradiation. PVDF-TiO₂ CNM exhibited a stable performance after five cycles of the MO degradation due to a strong connection between the TiO₂ layer and the PVDF substrate. The implemented approach has been demonstrated to be a feasible method for the synthesis of core-shell PVDF-TiO₂ fibrous membrane. The influence of hydrothermal process parameters on the structure and final properties of PVDF-TiO₂ CNM was revealed through a detailed mechanism investigation

Biography

Dr. Carlo Boaretti is currently researcher at the Department of Industrial Engineering of the University of Padova. He received his PhD in Industrial Engineering from Padova University in 2016 working on the applications of electrospun nanofibers for energy and environmental applications. His actual research interests are related to the development and characterization of innovative nanostructured membranes and nanocomposites materials, the recycling of polymeric materials and the application of alternative green technologies (ultrasound, UV and microwaves).



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Early Industrial Roots of Green Chemistry: International “Pollution Prevention” Efforts During the 1970’s and 1980’s

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UVLAW Patents LLC, Blowing Rock North Carolina, USA

Many articles in the Academic literature and/or conventional histories of “Green Chemistry” describe its start as being a result of concepts and actions at the US Environmental Protection Agency (“EPA”) and/or in Academia during the 1990’s. But many examples of environmentally friendly Real-World chemical processes were invented, developed and commercialized in the oil refining, commodity chemical, and consumer product industries starting about the time of World War II. Those industrial efforts dramatically accelerated and evolved into explicitly environmentally conscious “Pollution Prevention” efforts during the 1970’s and 1980’s. A UN conference in November 1976 brought together over 150 attendees from industry, academia, and governmental and non-governmental organizations from 30 countries to address environmental issues related to preventing pollution caused by the chemically-related industries. Seventy-nine papers published in 1978 from the conference proceedings (titled “Non-Waste Technology and Production”) addressed a wide variety of technical, economic, environmental, and policy issues and approaches, and documented many examples of already commercialized environmentally friendly chemically based processes. On a parallel track, in 1975 the 3M Corporation initiated a corporate-wide program called “Pollution Prevention Pays (“3P”)” that commercialized thousands of environmentally oriented Real-World processes and/or inventions, in many countries, and simultaneously saved 3M large sums of money. Similar “Pollution Prevention” approaches were emulated by many chemically based corporations in many countries during the 1980s. The “Green Chemistry” terminology and “12 Principals” adopted by the EPA and Academia in the 1990’s evolved from the “Pollution Prevention” approaches, programs, and commercialized inventions that began decades before the 1990s.

Biography

Mark A. Murphy has a Ph.D. in Chemistry from the Univ. of Wisconsin-Madison, worked for 11 years at Hoechst Celanese Corp. as an Industrial Chemist, where he conceived (in 1984) the BHC Ibuprofen Process that was one of the most widely recognized early “Green Chemical” inventions. He later obtained a law degree at the University of Texas -Austin and became a patent attorney and partner in three Intellectual Property law firms. He is currently semi-retired as owner / operator of UVLAW Patents LLC.



Effectiveness of Advanced Oxidation Processes (AOPs) and adsorption on natural materials for the removal of sildenafil from aqueous phases

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Pharmaceuticals represent a large part of the trace organic micropollutants. Most of them reach sewage treatment plants, either metabolised or not. For most of these, occurrence, risk assessment and ecotoxicological data are unavailable. Therefore, it is difficult to predict their health effects on humans and living organisms. In recent years, the widespread use of sildenafil citrate, a drug for erectile dysfunction, has attracted a great deal of attention due to its high use rate, its commercialisation through legal and illegal routes, and its unpredictable use disposal and its potential unknown effects on wildlife and the environment. This study focuses on the removal efficiency of sildenafil by different AOPs and natural adsorption materials. Functionalised bentonite and a local rocky material were tested. Three oxidants were the degradation agents: hydrogen peroxide (H₂O₂), peroxymonosulfate (PMS) and peroxydisulfate (PS). The degradation processes of sildenafil were studied with particular attention to potentially toxic photo transformation products. They were identified by LC-ESI-MS and confirmed by MS/MS. Subsequently, other experiments assessed the toxicity of sildenafil and its phototransformation products on *Daphnia magna* and *Vibrio fisheri*. Results showed that AOPs combined with adsorption on natural materials are essential processes to remove such drugs and their transformation products from aquatic bodies.

Biography

Dr. Filomena Lelario received the Master degree, summa cum laude, in Chemistry in 2000 from the University of Basilicata and the PhD in "Crop Systems, Forestry and Environmental Science" in 2004 from the same university. Since 2004 she has obtained several research grants from the University of Basilicata to determine natural substances and xenobiotics in vegetable, biological and environmental samples by liquid chromatography and low and high-resolution mass spectrometry. Her scientific focus is also on the fate and risk of emerging pollutants such as pharmaceuticals and pesticides in the environment. She is a co-author of several papers published on international peer-review, conference papers and book chapters. She is involved in several research projects supported by national and international grants.



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Novel Insights into Sb-Cu Catalysts for Electrochemical Reduction of CO₂

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Catalysts play a vital role in electrochemical reduction of CO₂ to valuable products. Only based on effective catalysts, CO₂ electrolysis process can be advanced toward industrial application. In this work, we present a Sb-Cu₂O material synthesized via one-pot microwave-assisted solvothermal route. The Sb-Cu₂O derived bimetallic catalyst achieves a highest CO selectivity of 96% and good CO partial current densities of 37.3 and 74.0 mA cm⁻² at -0.8 and -1.2 V vs. reversible hydrogen electrode (RHE), respectively. The Sb-Cu catalyst also displays good stability at current densities ranging from 5.6 to 100 mA cm⁻². Additionally, for the first time, a complete theoretical study reveals the critical roles of Sb in selective CO₂ conversion to CO on this bimetallic material, including stabilizing stepped Cu surfaces selective for the reaction, lowering energy barriers for the formation of key intermediate and favouring CO desorption.

Biography

J. ZENG is a post-doc. researcher in Center for Sustainable Future Technologies @POLITO, Istituto Italiano di Tecnologia, Italy. Her research activities have been mainly focused on carbon-based and metal oxide-based electrocatalysts toward oxygen reduction and carbon dioxide reduction reactions for the applications in Li-O₂ batteries, fuel cells and carbon dioxide valorisation. During her career, J. Zeng has won the award of PHD "Fondazione De Nora" (awarded by the Society of Italian chemistry). She has been involved as First/Corresponding author of 20 articles and co-author of 15 articles in international peer-reviewed journals.

